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Research news

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FEATURE STORY:

Science is the Key to Sustainable Shale Gas Production

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the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DEPARTMENT OF ENERGY

Research news
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Contents

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.

Science is the Key to Sustainable Shale Gas Production

Natural gas and crude oil provide two-thirds of the nation's primary energy supply. Gas produced from shale gas plays has become an important part of the nation's energy mix. It has grown rapidly from almost nothing at the beginning of the century to near 30 percent of natural gas production. Shale gas production is expected to expand to as many as 100,000 wells over the next several decades.

Through its Unconventional Fossil Energy Resource Program, NETL is performing assessments and providing data that are important to understanding the impacts of gas and oil recovery from shale. Using field monitoring, laboratory experiments and characterization, data mining, and modeling, NETL-led

Cover image
Drill site in the Marcellus shale play. "Horizontal Drilling Rig" by Meredithw, licensed under COM:CC-BY-SA

Marcellus Shale containment pond, Pennsylvania. Photo credit: Dwight Nadig via iStock photo.

multidisciplinary teams of scientists and engineers are uncovering—with the help of sophisticated facilities (see Shale Gas Field Samples Analyzed With Cutting-Edge Tools, this issue)—information that will help predict and address potential environmental impacts to the air and water associated with recovery of these resources. Ultimately, this research will help to ensure sustainable, reliable, affordable, and environmentally sound oil and gas production for a secure energy future.

Air

Using a mobile air monitoring lab that conveys findings via satellite, NETL conducts onsite measurements of emissions from oil and gas activities and then uses the data to develop atmospheric chemistry and transport models for understanding local and regional air quality impacts. Researchers look for gas emissions like methane, particulate matter, oxides of nitrogen, volatile organic compounds, and other species that could cause changes to air quality.

Drill sites have become common throughout Marcellus Shale areas. NETL helps monitor air, water, and underground conditions associated with hydraulic fracturing gas recovery operations.

In the mobile station, a temperature-controlled laboratory space, multiple instruments measure atmospheric concentrations of pollutants associated with natural gas development. **Dr. Natalie Pekney**, a principal investigator in NETL's Engineered Natural Systems Division, leads NETL's air quality monitoring research. She said, "It is just one of the tools we are using at natural gas development sites to measure fugitive atmospheric emissions that could escape during drilling, hydraulic fracturing, production, and transmission."

NETL is working closely with University of Pittsburgh researchers to track nitrogen emissions from well pads using isotope

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tracers. Excess nitrates can contribute to forest degradation, soil and stream acidification and, in coastal systems, contribute to algal blooms and hypoxia. The joint research measures gaseous reactive nitrogen concentrations, samples particulate matter, and collects nitrogen gases for analysis.

Pekney said the research informs decision makers about the air quality impacts of large-scale natural gas production from shale and helps reduce environmental impacts.

NETL's Mobile Air Monitoring Laboratory

NETL's Karl Schroeder, far right, collects natural gas samples to test for the presence of tracers detecting upward migration of gas from the hydraulically fractured Marcellus Shale. No tracers were detected in the process. Assisting were Shikha Sharma, a researcher with West Virginia University, and an unidentified well tender.

Water

Methane in drinking water and the safe storage, transport, and disposal or reuse of water co-produced with oil and gas are key concerns in many communities. NETL continues to examine water issues associated with hydraulic fracturing to understand the processes, identify problems, create innovations to ensure safety, and guide regulatory decision makers. The work incorporates chemistry and data-mining as well as an examination of the chemical make-up of the water recovered during unconventional oil and gas development and production.

"Decision makers will face well placement and water management issues on a case-by-case basis," NETL's **Dr. Alexandra Hakala**, an environmental geochemist, explained. "The information that NETL provides will help planners consider critical environmental parameters instead of just cost alone."

Surface water concerns surround what is known as produced water— naturally occurring water that flows to the surface throughout the entire lifespan of a well. The water typically has high levels of total dissolved solids. NETL teams evaluated produced water from active shale gas sites and performed laboratory experiments to identify biogeochemical processes that affect water quality. With that knowledge, NETL researchers created modeling tools to be used in developing methods for processing produced waters so they can be recycled for other traditional uses.

NETL's work also examines potential groundwater issues. **Dr. Dustin Crandall**, research engineer in the Predictive Geosciences Division, noted that research indicates, "A fracture reaching into underground sources of drinking water from hydraulically fractured deep shale reservoirs is highly unlikely because of geological properties of targeted shale formations, stress conditions in the subsurface, and overburden thickness."

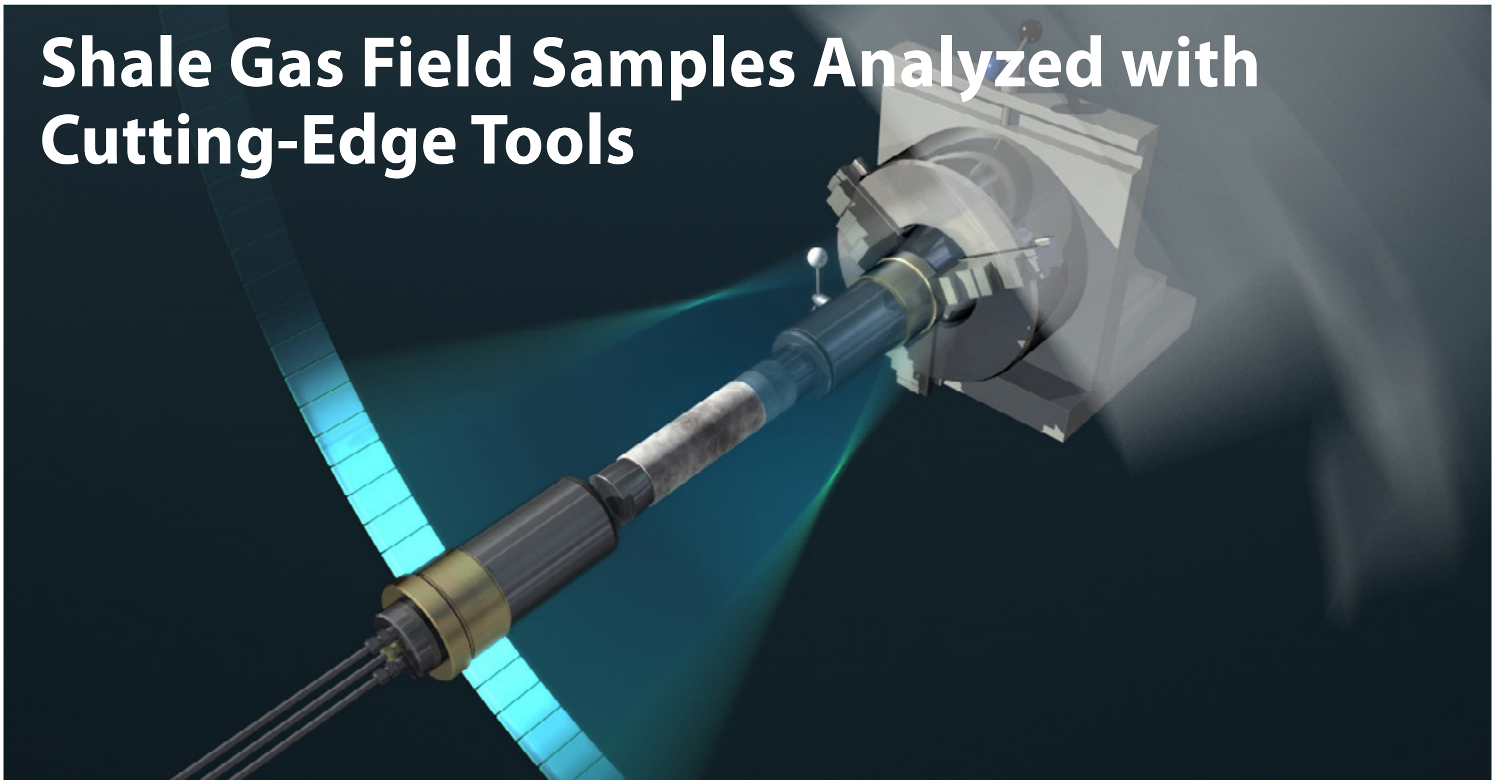
The laboratory developed optical sensor-based tools to monitor fluids in shale gas reservoirs, tools that will serve as analytical tracers in the field. The influence of shale gas development on shallow groundwater was also evaluated by examining wellbore cements, and the potential for gas migration in groundwater aquifers.

NETL experts have also used microseismic monitoring and specific tracer tools to evaluate how hydraulic fracturing could influence the upward migration of fluids from hydraulically fractured formations. **Richard Hammack**, physical scientist with NETL's Engineered Natural Systems Division, explained that NETL monitored a gas-producing zone that is 3,800 feet above the Marcellus Shale in Greene County, PA, to detect tracers that would indicate whether gases and fluids had migrated. Analysis showed that fractures created by hydraulic fracturing did not reach the monitored zone, and tracer analysis identified no detectable migration of gas or fluids.

NETL shale research addresses issues facing shale gas production. The data, technologies, and tools developed through NETL's research will help industry and regulators make decisions and optimize operations so that development of the nation's unconventional fossil energy resources is environmentally sustainable.

Contacts: Alexandra Hakala, Natalie Pekney, Dustin Crandall, Richard Hammack

Shale Gas Field Samples Analyzed with Cutting-Edge Tools



X-ray beam of an adapted medical computed tomography scanner scanning a geologic core sample under pressure .

Shale gas researchers collect a lot of field samples (air, water, rock) to be analyzed in NETL's labs. The timing of sample collection and analysis, coordination of samples between the field and lab, and effective analysis techniques are critical to making the best use of NETL's facilities to generate valid data. Air and water samples are particularly sensitive, changing over time, so field researchers must collect them according to strict protocols, then get them into the lab as quickly as possible. There, lab researchers use a dynamic collection of special tools to analyze them:

- Computed tomography scanners are used to peer into geologic core samples to determine how liquids, solids and gases flow through them.
- Software and visualization hardware provide static and time-dependent data to study how
- A multi-collector inductively coupled plasma mass spectrometer analyzes a broad range of elements to give insight into the complex chemical interactions that occur beneath Earth's surface.
- Geochemical tracer tools help verify the sources of fluids in complex geologic systems.
- Mobile air monitoring facilities assess impacts to air quality from oil and gas exploration and production activities onsite.

Most facilities are located onsite at NETL, with additional resources accessed through collaborative arrangements with the University of Pittsburgh and West Virginia University. (Watch videos of NETL's labs here and here.)

See an animation of how the geologic CT scanner works.

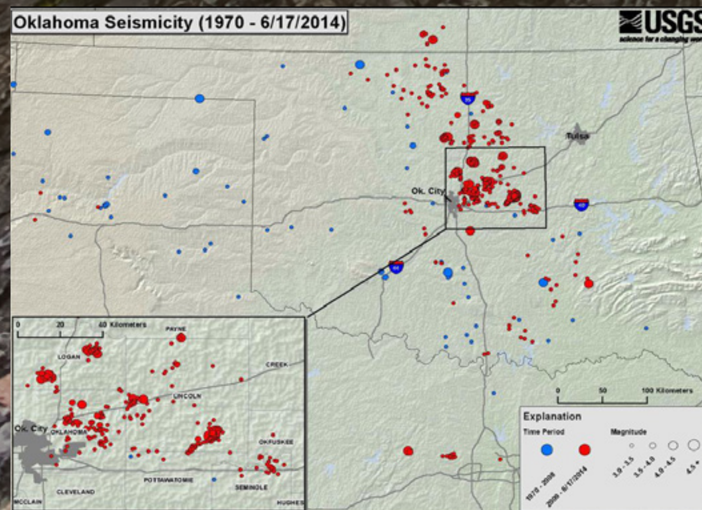
Dr. Dustin Crandall with an adapted medical computed tomography scanner used to study geologic core samples.

Under Pressure:

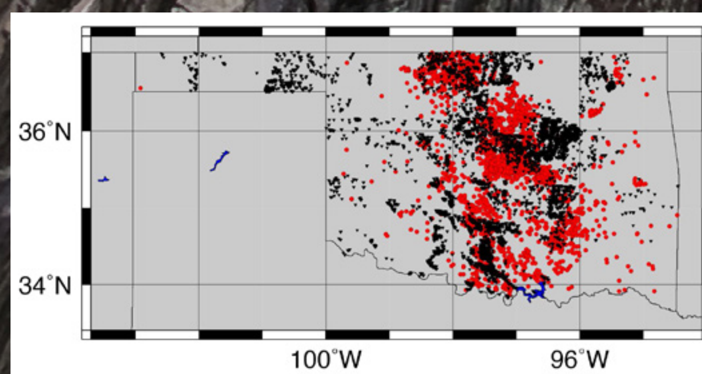
What's Causing the Shake-up?

Until recently, Oklahoma was not known as a hotbed for earthquake activity. Historically, California has been more famous for tremors, but last year Oklahoma surpassed California in seismic activity. What is causing this increase in seismicity? NETL is combining its expertise in geology, computer modeling, and predictive sciences to find answers.

NETL and Virginia Tech gathered information on seismic activity dating from 1882 to 2014 (website of data compiled available here). Researchers compared this information to data on the locations of hydraulic fracturing sites and waste water injection wells. Their findings disagree with the popular perception that hydraulic fracturing cause earthquakes. The majority of well operations, like fracking, cause no increase in seismic activity, although a relationship does exist between some waste water injection wells and earthquake activity. This correlation indicates the possibility of induced seismicity—or earthquake activity that corresponds to human activity.



This seismicity map of earthquakes in Oklahoma since 1970 shows activity of at least 3.0 magnitude on the moment magnitude scale with pre-2008 events in blue and post-2008 events in red. (Courtesy of the U.S. Geological Survey)



This map of Oklahoma shows earthquakes in red and waste water injection wells in black. (Courtesy of the Virginia Tech Seismological Observatory)

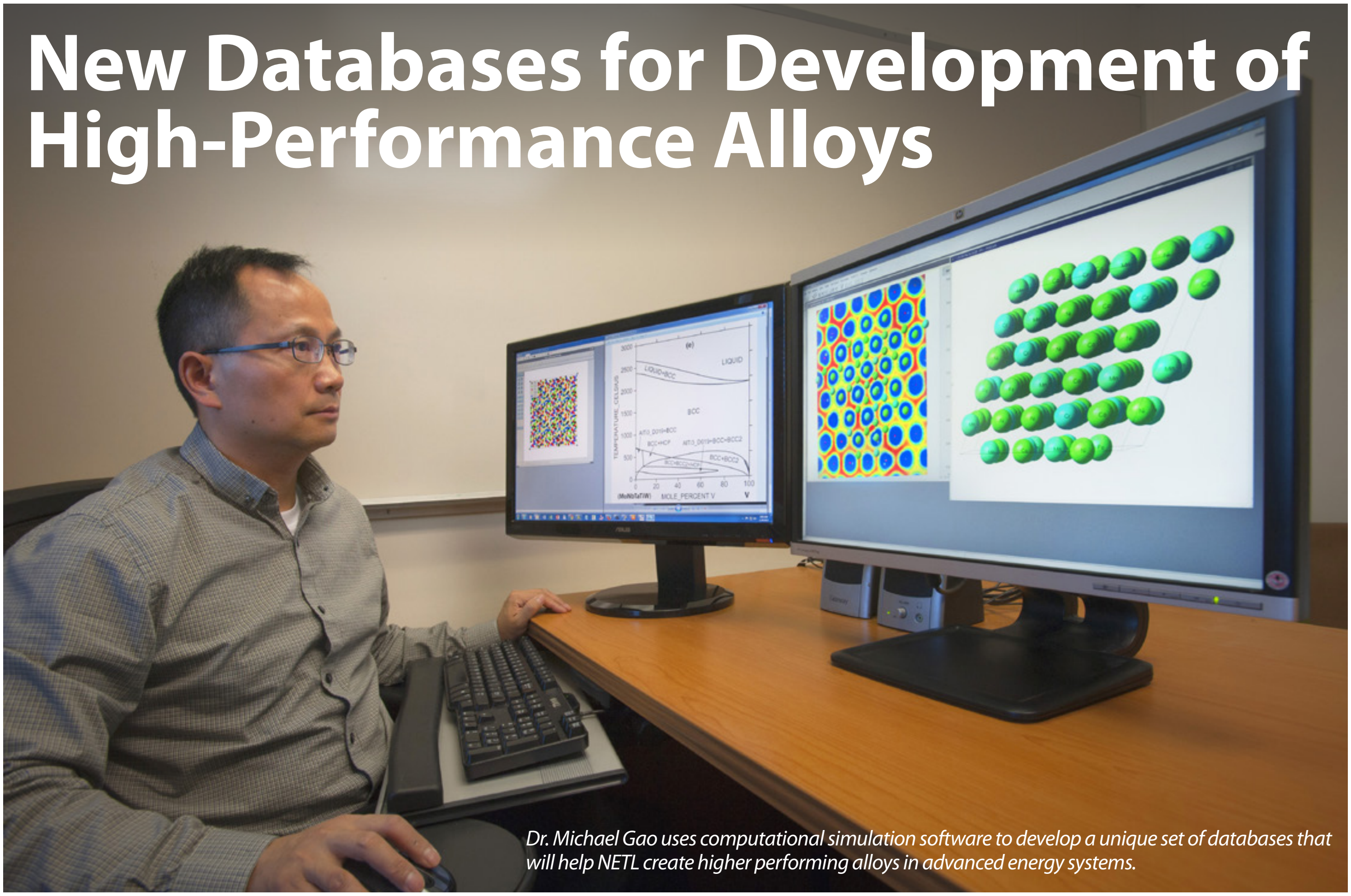
The rock beneath the Earth's surface contains fractures and pores. Fluid injection into these spaces increases pressure within the rock. Changes in the existing pressure can cause rock to move, shearing along the fractures and causing earthquakes. Most of these earthquakes cannot be felt at the surface, but several larger earthquakes have been recorded that researchers believed to be associated with high-volume waste-water injection.

Dr. Dustin Crandall, Research Engineer, emphasized that it's not hydraulic fracturing causing the vast majority of induced seismic events, but "the injection of large volumes of waste water that are pulled back up from the subsurface after hydraulic fracturing is over."

NETL is working to provide a clearer picture of the possible causes of induced seismicity by creating a detailed picture of the subsurface and performing modeling to link injection rates and locations to changes in the subsurface pressure. This research will help inform industry about when and where larger seismic events could occur from hydraulic fracturing and waste water injection—information that can point to optimum injection sites for minimizing the effects of induced seismicity.

Contact: Dustin Crandall

New Databases for Development of High-Performance Alloys



Dr. Michael Gao uses computational simulation software to develop a unique set of databases that will help NETL create higher performing alloys in advanced energy systems.

Advanced technologies for fossil energy power generation, such as ultra-supercritical steam plants and oxyfuel combustion boilers, will increase efficiency and facilitate the capture of carbon dioxide. Such advanced systems will operate at higher temperatures, pressures, and under potentially harsher and more corrosive conditions compared to traditional power plants. They require alloy-based materials that are both cost-effective and able to withstand severe environments.

Computational models capable of predicting how alloys will perform in complex environments are important tools in successful development of new alloys, but predictive models and simulations for designing complex alloys are often limited by the availability and integrity of the data they are constructed from. Researchers at NETL, recognizing a need for more complete input data for alloy design, worked in collaboration with their partners at Pennsylvania State University to develop new databases incorporating specific design parameters to better predict how environmental factors will affect alloy oxidation.

The research team used a combination of multi-scale computational simulation tools to develop a unique set of thermodynamic and kinetic databases for an alloy system consisting of five components: nickel, iron, aluminum, oxygen, and hydrogen. The databases help simulate the oxidation of metal alloys based on alloy composition and environmental factors, such as presence and quantity of oxygen and steam. These simulations are used to identify the best alloys to test in experiments.

According to **Dr. David Alman**, Director of the Structural Materials Development Division, "the power of this integrated approach is that experiments are limited to those alloy compositions with the highest likelihood of success." The result is that high-performing alloys are developed more quickly and cheaply.

This work was part of NETL's Innovative Process Technologies project portfolio, which is focused on developing innovative cost-effective technologies that promote efficiency, environmental performance, and availability of advanced energy systems. NETL is leveraging unique capabilities in computational simulation and metallurgy to develop tools that will shorten development times for the implementation of new alloy systems.

Alloy materials formed from NETL's five-component alloy system are complex structures containing multiple phases that offer distinct advantages over single-component or single-phase materials. The properties of complex structures can be tailored for specific uses by the appropriate combination and distribution of elements, constituents, or phases. The development of these first-of-their-kind databases will allow for more efficient and cost-effective development of complex oxidation-resistant alloys.

Contact: David Alman

Modeling Predicts Gasifier Performance

NETL has earned a reputation for successfully developing and applying innovative computational fluid dynamics (CFD) models for evaluating multiphase flow in energy systems. The core of this expertise lies in computer scientists and their use of the NETL-developed software platforms Multiphase Flow with Interphase Exchanges (MFiX) and Carbonaceous Chemistry for Computational Modeling (C3M). MFiX is a general purpose computer code developed for describing the hydrodynamics, heat transfer, and chemical reactions in fluid-solid systems. C3M is a coal chemistry tool that works with MFiX to analyze the complex chemical kinetic reactions associated with coal gasification.

Gasification is an energy-efficient way to convert fossil fuels to power and/or chemicals while reducing carbon emissions. Researchers are using computational modeling and simulation tools like MFiX and C3M to help gasification become more marketable as a coal conversion technology. Understanding the complex multiphase flow within the gasifier will enable researchers to optimize system performance, improve conversion efficiency of fossil fuels, and reduce capital and operating costs—critical parameters for positioning gasification for the commercial market.

Using the NETL supercomputer, NETL researchers in collaboration with partners at Southern Company Services recently completed a comprehensive set of detailed multiphase CFD simulations using MFiX and C3M software for gasification of Mississippi lignite coal.

The team used data obtained from the DOE-sponsored National Carbon Capture Center which is managed by Southern Company and houses a pilot-scale transport integrated gasifier (TRIG™) reactor. Researchers were able to develop and validate CFD models and chemical kinetic tools to more accurately predict TRIG performance. "We were really pleased with the results of this work," said NETL researcher **Bill Rogers**, leader of the multiphase flow team. "It clearly demonstrated the capability of NETL's computational tools to successfully model gasifier performance over a wide range of operating conditions." Applying these will assist designers and operators of industrial gasifiers to optimize the gasification process and reduce the risk and time required to scale-up and demonstrate the technology for commercial application.

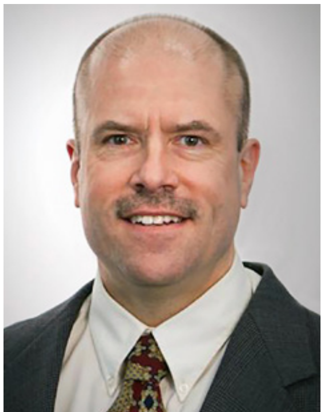
Leveraging unique capabilities in computational modeling and simulation, supercomputing, and demonstration facilities, NETL and its strategic partners are making significant advances in the modeling of multiphase flow—efforts that will be key in meeting U.S. Department of Energy program goals for the design and operation requirements of advanced, coal-based power systems with 90 percent carbon capture capabilities.

Contact: William Rogers

NETL's Multiphase Flow Team—Bill Rogers, team lead, front and center.

Optimal Sensor Networks

Unlock Greater Efficiency from Power Plants



Dr. Stephen E. Zitney leads the dynamics and control research area at NETL.

Modern power generation systems—like integrated gasification combined cycles (IGCC) with carbon capture—rely heavily on sensor networks to provide feedback for use in plant operation, control, and monitoring. Sensors are physical devices that measure process variables like temperature, flow rate, pressure, and chemical composition. Years of experience help plant designers and operators to select the number, location, and type of sensors, but the myriad of possible configurations makes it nearly impossible to manually design an optimal plant-wide sensor network.

Powerful computational tools are required for systematically determining where best to locate sensors. Sensor network design (SND) involves multiple complex objectives including maximizing the accuracy of process measurements, minimizing the sensor network cost, and improving process monitoring and fault diagnosis capabilities. This daunting large-scale SND problem can be solved effectively and efficiently only by using sophisticated optimization algorithms.

The IGCC dynamic simulator at NETL allows researchers to predict how sensor placements would affect plant efficiency.

Anyone who has attempted to solve a puzzle like a Rubik's Cube probably used algorithms. For example, there is an algorithm to move a colored piece from the bottom to the top of the cube. Once a person learns the sequence of moves, or the algorithm, they can solve this problem in the most efficient way possible. Developing an algorithm to solve the SND problem gives a similar result; the algorithm will inform the researcher of the most efficient placement of sensors in the plant.

NETL researcher **Dr. Stephen E. Zitney** and researchers at West Virginia University (WVU) have developed a powerful optimization-based SND algorithm for large-scale power plant applications. Dr. Zitney leads research projects in dynamics and control at NETL, and he describes his team's cooperation with WVU as "allowing NETL to both broaden and deepen our research capabilities."

"Historically, sensor placement has been done for large plants on an *ad hoc* basis, using expert knowledge and rules of thumb," Dr. Zitney explained. This research aims to automate the sensor network design process for plant-wide applications. The comprehensive objective is to maximize overall plant efficiency while simultaneously satisfying sensor network accuracy and budget requirements, which has never before been accomplished through SND algorithms.

To date, the NETL and WVU researchers have applied the new SND algorithm to the CO_2 capture process for an IGCC power plant. Results show that an optimal sensor network design can lead to a reduction in CO_2 emissions of more than 12,500 tons per year for a 735 megawatt IGCC power plant with 90 percent CO_2 capture—that's the equivalent of taking over 2,600 cars off the road.[1]

Future work will include the application of the optimal SND algorithm to the high-fidelity, real-time, IGCC dynamic simulators deployed at NETL and WVU. These virtual IGCC power plants will facilitate the testing of new sensor network designs under real operating constraints, such as limits on CO_2 release. When deployed, the optimal sensor placement strategies developed by this multidisciplinary research will provide more efficient power generation with less CO_2 released into the atmosphere.

Contact: Stephen E. Zitney

[1] EPA, "Greenhouse Gas Emissions from a Typical Passenger Vehicle, " May 2014, http://www.epa.gov/otaq/climate/documents/420f14040.pdf

ORISE Internships:
An Opportunity and Inspiration

Dr. Alexandra Hakala leads NETL's Analytical Bio-Geochemistry Team.

For young scientists, graduating and leaving academia to take the first steps into research or industry can be an exhilarating but turbulent time. Internships provide a valuable opportunity to gain skills and hands-on experience and to help shape the aspirations, passions, and career paths of promising young researchers as they make that transition.

The Oak Ridge Institute for Science and Education (ORISE) offers a range of internships, scholarships, fellowships, and research experiences. Many researchers at NETL, including Alexandra Hakala and Evan Granite, first came to the laboratory as interns in the ORISE program.

Alexandra came to the lab in 2008 to work on oil shale development and on the groundwater impacts team for the National Risk Assessment Partnership. She remembers the program as a formative experience that helped to mold her career aspirations. "It helped me to understand areas within fossil energy research that needed environmental and risk assessment considerations in order to ensure safe and reliable development of U.S. energy resources."

Evan came to NETL on his ORISE internship in 1996 to study sorbents for the removal of mercury from coal-derived flue gas. Now he's been at NETL for over 18 years— 3 years as an ORISE post-doctoral appointment, and 15 years as an NETL researcher. He, too, remembers the internship as foundational. "My mentor was Henry Pennline—one-in-a-million—a terrific researcher and role model, and the subject was very interesting, and the experience helped me settle on a career in research."

The ORISE program continues to enable early career scientists to gain experience and make contributions at NETL. Often, these contributions are rooted in the fresh perspectives the interns bring, as well as their vital role in keeping NETL on the forefront of scientific trends and thoughts. Sometimes the early career scientists choose to stay and make a home at NETL. Consequentially, researchers who were once ORISE interns themselves have the opportunity to watch new interns flourish. Evan views it as one of the most rewarding aspects of his job. "I have mentored many ORISE interns (postdocs and undergraduates) over the past 13 years, and consider it the most enjoyable part of my job. I try to impart the excitement of research. I am very proud of my ORISE students, and many have gone on to great success."

Dr. Evan Granite works as a researcher on NETL's Separations Materials Team.

NETL's In-House Research Program:
Unconventional Fossil Resources

Some energy resources can't be extracted in conventional drilling or mining. Economical recovery of these resources requires the use of more novel (or unconventional) methods, such as hydraulic fracturing and horizontal drilling. Researchers supporting ORD's Unconventional Fossil Resources Portfolio investigate the sources and magnitude of fugitive emissions that these innovative extraction processes cause. They also explore ways to use field-monitoring tools to find abandoned oil and natural gas wells, and they evaluate ground movement and fluid and gas migration associated with hydraulic fracturing. ORD researchers also assess the integrity of wellbores, shale reservoirs, and groundwater aquifers.

The results of this broad research will protect air quality and groundwater, and increase public information about shale gas operations. ORD researchers and their collaborators from academia and other national labs work on numerous tasks, which include:

- Continuing to develop facilities and equipment used to maintain the Energy Data eXchange.
- Developing models that optimize water use during hydraulic fracturing and predict the effects of hydraulic fracturing activities.
- Applying NETL-developed FRACGEN and NFFLOW software to calculate the potential flow of fluids from rock fractures.
- Collecting field data to identify the locations of existing wells, monitor fracture growth during hydraulic fracturing, and measure fugitive methane and air pollutants.
- Conducting laboratory work and geochemical modeling to predict the impact of microorganisms, acids, and oxidation-reduction processes on well integrity or the environment.
- Conducting laboratory testing to develop sensors (e.g., pH and isotopic sensors) able to detect the migration of fluids and gases underground.
- Performing laboratory tests to reveal the leakage pathways in geologic formations.
- Evaluating the impact that shale gas development has on shallow groundwater, including studying ways to naturally remediate groundwater aquifers and monitoring fluctuations in groundwater chemical constituents.
- Working with Sandia National Laboratories and the Energy & Environmental Research Center to provide an understanding of how chemical and physical properties of crude oil affect its safe development and transportation.

To learn more about the Unconventional Fossil Resources Portfolio, contact Alexandra Hakala, Dustin Crandall, Richard Hammack, or Natalie Pekney

FUNDAMENTAL FUN

Marcellus Shale Essentials

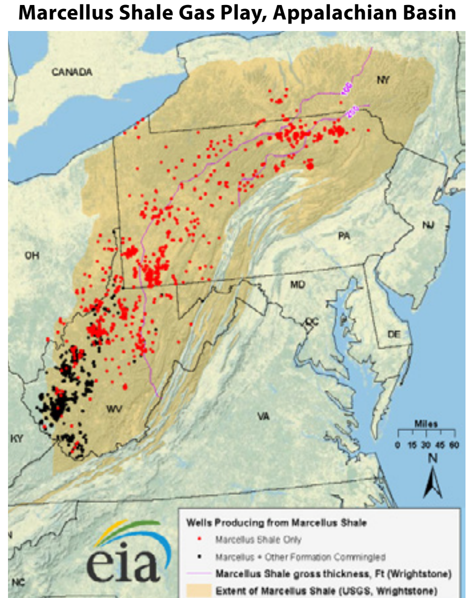
Stretching over six states from Virginia to upstate New York, the Marcellus shale is a storehouse of natural gas. Named for an outcropping in the town of Marcellus, NY, the Marcellus formation runs as deep as 9,000 feet under the surface and is millions of years old. Here are a few quick facts:

- The formation ranges from 50 feet thick to more than 200 feet thick.
- The Marcellus is estimated to contain from 1,925 billion cubic feet of gas to over 500 trillion cubic feet, potentially enough natural gas to meet the needs of 500 million households for 15 years.[1]
- According to the U.S. Energy Information Administration, the Marcellus shale accounts for almost 40 percent of U.S. shale gas production. Production in the Marcellus region increased from 2 billion cubic feet per day in 2010 to over 15 billion cubic feet per day in 2014.[2]

Shale is a fine-grained sedimentary rock. Within the Marcellus shale, natural gas and oil occur mostly in the pore spaces. However, the pores are tiny, and the network of pore spaces is not well connected. This makes it difficult for gas to flow through. Gas also accumulates in vertical seams, called joints, that occur throughout the formation.

So how is the gas extracted? Special recovery techniques, such as horizontal drilling and hydraulic fracturing, have made it possible to tap into as many of these joints as possible to economically release the gas and oil. NETL funded the original research for horizontal drilling that has made it possible to economically produce this gas and other shale gas plays in the United States.

Marcellus Shale Gas Play, Appalachian Basin



Source: US Energy Information Administration based on data from WVGES, PA DCNR, OH DGS, NY DEC, VA DMME, USGS, Wrightstone (2009). Only wells completed after 1-1-2003 are shown. Updated June 1, 2011.

[1] Speight, James. 2007. Natural Gas: A Basic Handbook. Houston: Gulf Publishing. Page 73.

[2] EIA, "Marcellus Region production continues growth," August 2014, http://www.eia.gov/todayinenergy/detail.cfm?id=17411

APPLAUSE

Patents Issued

Method of Purifying a Gas Stream Using 1,2,3-Triazolium Ionic Liquids, **Chau Tang** (ORISE); **David Luebke** (DOE/NETL); **Hunaid Nulwala** (ORISE); 8,906,135, issued December 9, 2014.

1,2,3-Triazolium Ionic Liquids, **David Luebke** (DOE/NETL); **Hunaid Nulwala** (ORISE); **Chau Tang** (ORISE), 8,907,105, issued December 9, 2014.

Poly(Hydroxyl Urethane) Compositions and Methods of Making and Using the Same, **David Luebke** (DOE/NETL); **Hunaid Nulwala** (ORISE); **Chau Tang** (ORISE), 8,912,303, issued December 16, 2014.

Production of Methane-Rich Syngas From Hydrocarbon Fuels Using Multifunctional Catalyst/Capture Agent, **David A. Berry**; **Dushyant Shekhawat**; **Wayne Surdoval**; **Nicholas Siefert** (DOE/NETL), 8,920,526, issued December 30, 2014.

Laser Interlock System, **Steven D. Woodruff**; **Dustin McIntyre** (DOE/NETL), 8,934,511, issued January 15, 2015.

EXTRA! EXTRA!

Natural Gas & Oil Program Research Portfolio Accomplishment Reports

The Office of Fossil Energy and the National Energy Technology Laboratory are releasing a series of nine Research Portfolio Accomplishment Reports to provide a snapshot of accomplishments completed to-date for active and completed projects.

The first report titled, "Unconventional Oil & Gas Resources: Subsurface Geology and Engineering," was recently released. This report details a decade of subsurface geological and engineering research carried out by NETL and the laboratory's partners, which has enhanced our ability to produce natural gas and oil from reservoirs once considered "unconventional."

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