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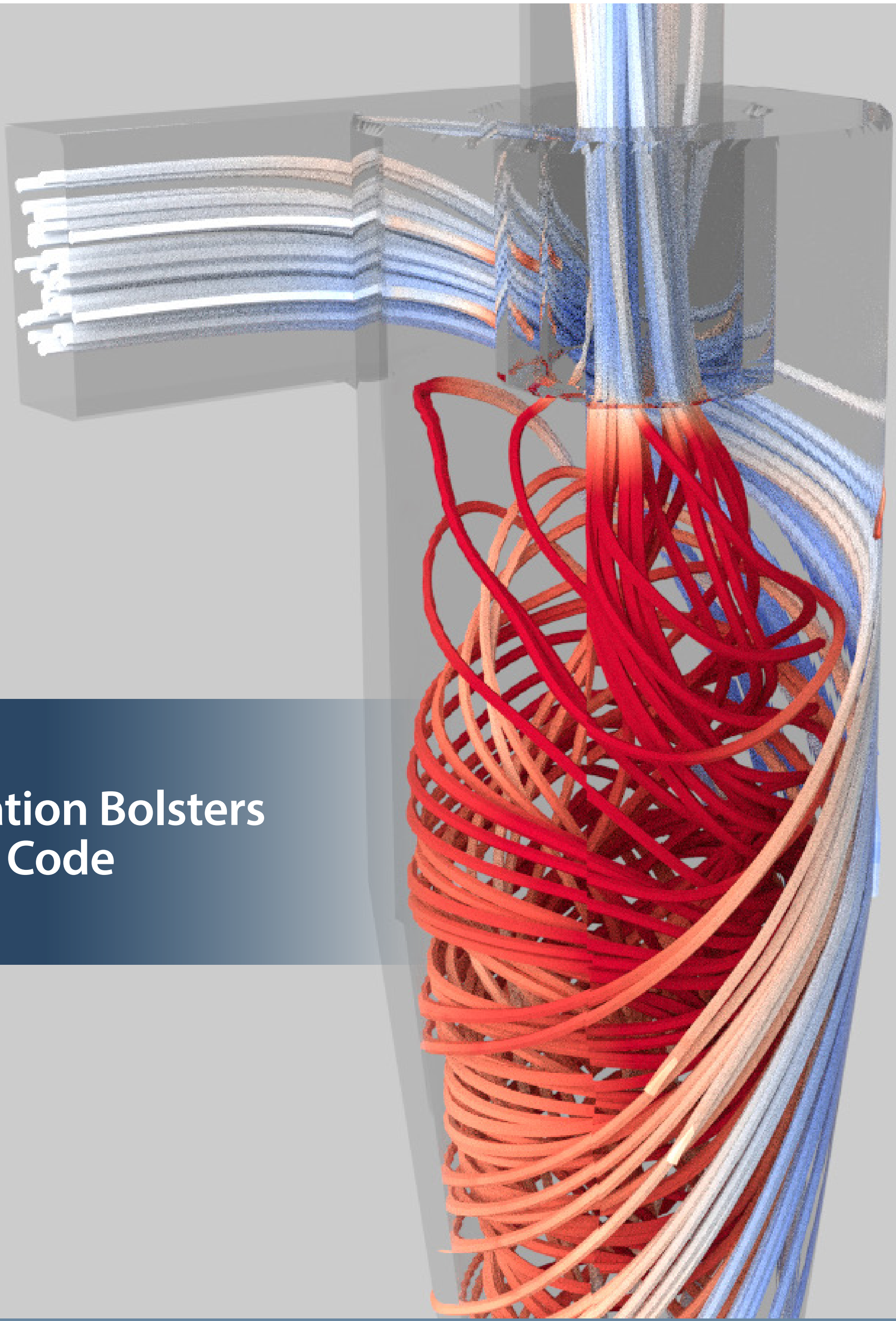
Research news

September 2015, Issue 12



FOCUS STORY:

New Equation Bolsters Modeling Code

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the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DEPARTMENT OF ENERGY

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MULTIPHASE FLOW Science Solves a Nuclear Site Cleanup Challenge

Until the late 1980s, nuclear reactors at the Hanford site in Washington State processed uranium metal fuel, producing plutonium for America's defense program. The process of extracting plutonium from uranium fuel rods yielded millions of gallons of radioactive waste. After decades of sitting in large underground tanks, the waste was to be treated using mixing vessels outfitted with pulsating jets, converted into a glass-like material, and stored. However, the design and performance of the 38 pulse jet mixing vessels needed to be confirmed, ensuring that they could mix and treat various combinations of liquid and solid radioactive waste safely and reliably for more than 40 years without human intervention. NETL is providing its considerable expertise in multiphase flow to the U.S. Department of Energy's Office of Environmental Management to make sure the vessels will perform as needed.

How do you begin to address the largest nuclear waste cleanup project in the United States? "You have to use all the tools available," **Chris Guenther**, director of the Computational Science & Engineering Division, said. "NETL is starting with small-scale testing and computer modeling—along with existing large-scale testing at the Hanford site—to aid in verifying the design and performance of the pulse jet mixing vessels."

Researchers are combining modeling and small-scale experiments to determine when a pulse jet mixing vessel lightly loaded with solids can be represented by a single liquid. This liquid may or may not have properties

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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.

Cover image

A simulation of a cyclone is seen here with stream lines depicting the motion of the gas. The stream lines are colored to indicate gas velocity, with red indicating the fastest moving gas.

Construction of the original storage tanks at the Hanford Site. These 530,000-gallon capacity underground storage tanks were built between 1943 and 1944, and put into service in 1945 to store radioactive sludge. NETL is modeling part of the process to clean up this radioactive waste for permanent storage.

that mimic the effect solids have on the mixing and velocity within the vessel. A computational fluid dynamic model based on this work will then be used to confirm the design and performance for most of the 38 pulse jet mixing vessels.

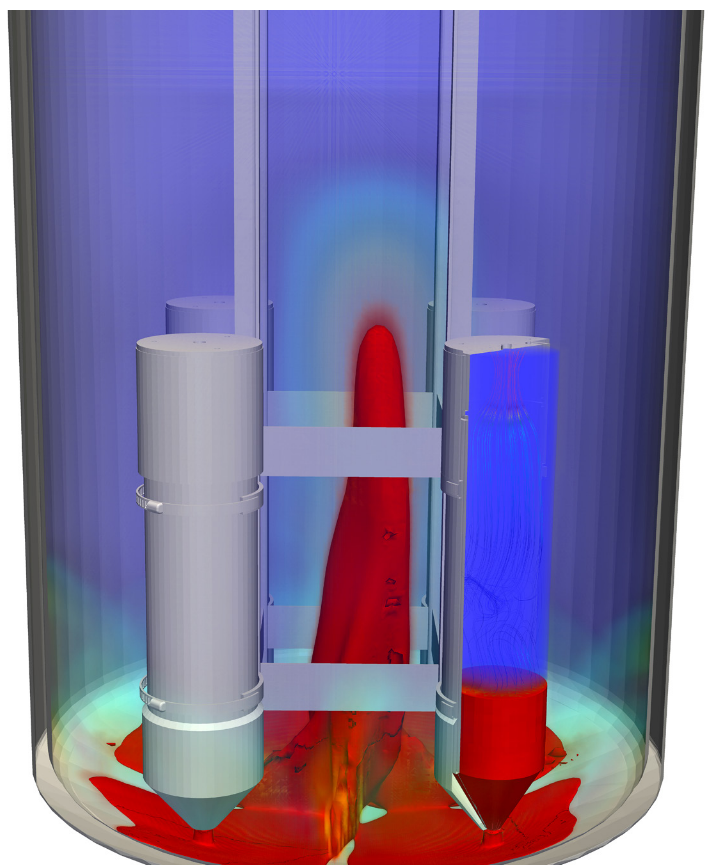
To date, NETL testing has demonstrated the feasibility of the intended work and the ability of a computational fluid dynamic model to capture the pulse jet mixing vessels' complex behavior. Using a computational fluid dynamic model to confirm the design and performance of these vessels will significantly reduce the need for large-scale testing at Hanford, saving hundreds of millions in tax-payer dollars and expediting the start of waste treatment at the Hanford site.

After the waste moves from the underground storage tanks and through the pulse jet mixing vessels, it will undergo vitrification, which involves mixing with glass forming-materials and fusing at high temperature. While liquid, the material will be poured into cylinders to cool and solidify as a glass-like material. Eventually, it will be buried for permanent storage.

NETL's involvement in this waste cleanup effort exemplifies the Laboratory's world-class multiphase flow expertise and its commitment to addressing national problems. Now, NETL is uniquely positioned as the go-to laboratory for future projects involving multiphase flow science, and its capabilities may be called on again for similar cleanup efforts. The Department of Energy is cleaning up multiple U.S. sites where government-sponsored nuclear weapons development and nuclear energy research took place, helping transport and dispose of low-level wastes, decommission and decontaminate old facilities, remediate contaminated soil and groundwater, and secure and store nuclear material.

Contact: Chris Guenther

NETL's experimental vessel was designed based on this full-sized vessel at Hanford.



This computer model shows the inside of the experimental pulse jet mixed vessel at NETL.

Going Airborne to Find Old Well Sites and Detect Greenhouse Gas Leaks

Like F-22 pilots establishing air superiority over a battlefield by conducting reconnaissance, NETL researchers are dispatching helicopters through rural skies that are armed with sophisticated sensors to detect forgotten and abandoned oil and gas wells. They identify potential sources of greenhouse gases that could be seeping from those lost wells from long ago and then share the data with appropriate individual state agencies for remediation.

The next step in the evolution of the approach is to reduce the costs of the sorties by using small unmanned helicopters and then begin monitoring additional locations where carbon dioxide (CO_2) is being permanently stored underground. It's all part of NETL's mission to fuel the economy, strengthen security, and improve the nation's environment.

Abandoned wells that do not have identifiable owners are called "orphan wells." States began aggressively searching for and plugging orphan wells after passage of the federal Safe Drinking Water Act to protect groundwater. But before orphan wells can be capped, they have to be found. For several years, NETL has helped locate abandoned oil and gas wells with manned helicopters equipped with magnetometers and other equipment that can detect the magnetic signatures of old oil and gas well casings. The flyovers are augmented and verified with ground-based detection follow-ups.

Rick Hammack of the Engineered Natural Systems Division said the flights are important because undetected orphan wells may pose safety and environmental concerns. He said that the NETL efforts are focused on state-owned lands. Results of the flyovers are conveyed to individual state governments with remediation responsibilities.

"Improperly sealed wellbores sometimes seep methane gas that can trigger explosions, contaminate water supplies or impact modern drilling operations," he said. "Estimates are that there are 1.2 million orphan wells nationwide."

The results of the NETL aerial monitoring campaigns are positive. In one 2014 survey conducted by a manned helicopter over Hillman State Park in Washington County, PA, NETL detected 194 potential well sites with the helicopter's magnetometers. Once pinpointed, ground teams examined 75 of those sites and confirmed that 47 were indeed former well sites. Using ground-based monitoring equipment, they determined that 19 of them had detectible methane leakage.

Once the effectiveness of the manned helicopter flights became obvious, NETL began looking for ways to improve the economics of the airborne monitoring approach. After considering the successes that the Department of Defense and the Department of Homeland Security attained with smaller unmanned craft for security work, NETL researchers believe the solution is to develop a fleet of small unmanned helicopters that can provide a low-cost option for surveillance of oil and gas fields. The mission could then be expanded to monitor underground CO_2 storage sites and locations where CO_2 is used to force previously unrecoverable oil to the surface in a process known as enhanced oil recovery (EOR).

"These are small helicopters that can be equipped with light-weight sensors and used to perform accurate, repeatable airborne surveys with costs that are one or two orders of magnitude below what it costs to use a full-size manned helicopter," Hammack explained. "The lower cost would allow us to use these smaller aircraft to conduct routine surveillance of large CO_2 storage sites of up to 4 square miles. That way, the sites can be monitored on daily, weekly, or monthly intervals."

Reduced cost of aerial monitoring using the little autonomous helicopters could also permit multiple repeat surveys to be conducted of oil and gas fields under different weather conditions. That is an important capability as researchers investigate phenomena like mid-winter ozone exceedances that are sometimes observed in oil and gas fields in the Rocky Mountains.

According to Hammack, the little helicopters are inexpensive to both buy and operate and can fly 2-hour surveys without refueling.

NETL's aerial monitoring projects are an important part of the Laboratory's overall mission to enhance the nation's energy security and improve the environmental acceptability of fossil energy production and use.

Contact: Richard Hammack, Garret Veloski

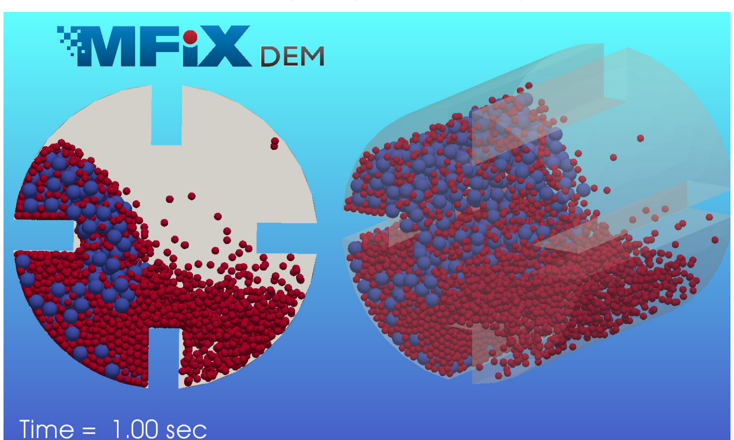
NEW EQUATION BOLSTERS MODELING CODE

While designing models for the Multiphase Flow with Interphase Exchanges (MFiX) code, one of NETL's most robust computational tools, Physical Research Scientist **Jordan Musser** realized that an important component of energy system behavior was not accurately accounted for in the existing code. In energy systems, it is common for more than one phase of matter to interact with another, a phenomenon known as multiphase flow. For instance, during combustion and gasification, coal particles interact with gases, creating a gas-solid flow (See examples of other types of multiphase flow in the Fundamental Facts section).

Within these flows, the constituents may change phases during reactions, releasing heat energy that researchers must carefully account for as they build models to predict how energy systems will behave. More accuracy provides greater confidence in these tools which may be used to reduce scale-up time and decrease capital investments, leading to cheaper, more efficient systems that will be deployed more rapidly.

Musser explained that it is important to accurately quantify the heat energy released during a phase transition. "Reaction rates are strongly based upon the temperature of the reacting fields," he said. "So if a reaction occurs and the heat transfer is not allocated correctly among these two phases, the reaction in the model may proceed more slowly or more quickly than researchers anticipated."

Either way, the characteristics of a real-world product—syngas quality in the case of gasification—could be different than what the model predicted. If the temperature is too high, for instance, gasification reactions may be hampered, resulting in a different than expected mix of carbon monoxide and hydrogen. These results could mislead design engineers working to optimize the operation of a gasifier, reducing the usefulness and effectiveness of computational tools.

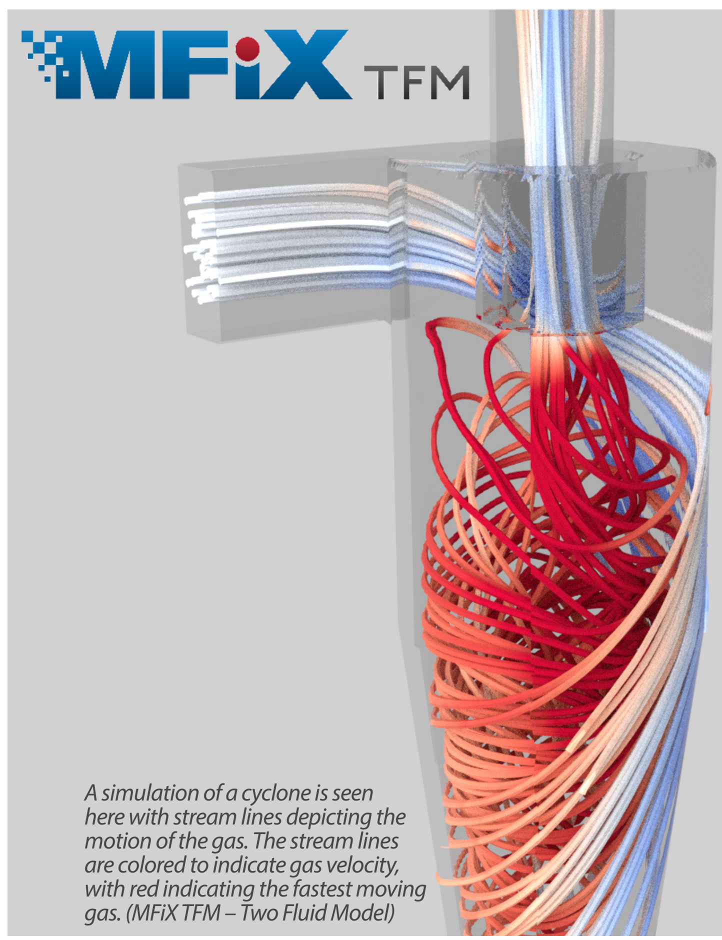


This simulation demonstrates how a rotary drum is used to mix different types of solid particles. (MFiX DEM – Discrete Element Model)

Musser set out to improve heat transfer accounting in reactive flow modeling. He designed an equation to account for the energy released during mass transfer between phases. This code was then incorporated into the MFiX code and verified by physically capturing data that are measured experimentally on the evaporation and condensation of a liquid droplet. When the physical data aligned with the model's prediction, the researchers verified that the new model was much more physically accurate than the old model.

Musser published his research in Chemical Engineering Science in an article titled "Constitutive Equation for Heat Transfer Caused by Mass Transfer." News of Musser's improved model quickly spread, and soon a commercial software code, Barracuda, had implemented the NETL mathematical model to increase its ability to accurately account for heat transfer.

Contact: Jordan Musser



A simulation of a cyclone is seen here with stream lines depicting the motion of the gas. The stream lines are colored to indicate gas velocity, with red indicating the fastest moving gas. (MFiX TFM – Two Fluid Model)

Research Sheds Light on Sensor Material Behavior in Harsh Environments

John Baltrus uses X-ray photoelectron spectroscopy to analyze a material's surface chemistry.

Surface characterization is important for determining how materials interact with their environment. Researchers rely on their understanding of how surfaces behave in order to improve the performance of materials being incorporated in sensors. NETL is developing optical gas sensors, capable of operating in harsh environments, which can be used to monitor and control critical processes in a variety of energy systems including coal gasification, solid oxide fuel cells, gas turbines, and oxy-fuel combustion. For example, using optical gas sensors to monitor and adjust the gas environment during coal combustion or gasification can enable more efficient coal utilization and improved power plant efficiency. Using X-ray photoelectron spectroscopy (XPS)—a technique used to examine the surface chemistry of a solid material—NETL researchers have begun to understand the operating principles and sensing mechanisms behind promising nanocomposite thin film materials.

Samples placed in the ultra-high vacuum chamber of the X-ray photoelectron spectrometer are exposed to an X-ray beam.

XPS provides information about surface elemental composition as well as the chemical and electronic states of the elements. Elements within the top 3-5 nanometers of the surface of a material emit characteristic electrons when excited by an X-ray beam. The number of electrons having specific energies can be plotted to yield spectra that permit determination of the relationship between electronic properties and surface composition of thin films. Understanding this allows researchers to adjust composition to improve the electronic properties and thus the performance of the sensing films.

Using this technique, NETL researchers gained insight into the sensing mechanism associated with yttria-stabilized zirconia (YSZ) nanocomposite films containing noble metal nanoparticles. Gold-containing YSZ thin films demonstrated a sensing mechanism involving the transfer of electrons back and forth between the gold nanoparticles and YSZ in response to experimental variables, including high temperatures and exposure to oxidizing and reducing gases.

The effects of changes in electron density of gold can be measured as part of the gas sensing process. By understanding what is responsible for such changes, different noble metals and configurations can be exploited to engineer new and better surface materials for use in optical gas sensors.

According to NETL Research Chemist **John Baltrus**, "Understanding how materials behave under harsh operating conditions is essential to developing materials with better performance characteristics. The results of our work can be used to engineer new surface chemistries leading to more durable, corrosion-resistant, and sensitive optical gas sensors."

NETL has developed a broad portfolio of advanced optical sensor materials that address process monitoring in harsh environments. These technologies are available for licensing and/or further cooperative development.

Contact: John Baltrus

WEST VIRGINIA NATIVE BRINGS HIS LOVE OF CODE TO NETL

Research Scientist **Jordan Musser** was recently recognized by the Council for Chemical Research (CCR) as a "Rising Star." The CCR Rising Star award recognizes emerging talent in the United States in chemistry and chemical engineering. One of seven recipients of this award in 2015, Jordan was recognized for his outstanding development efforts to enhance the code capabilities of MFiX. We asked Jordan, who contributed the story about MFiX in this month's Research News (RN), to tell us more about his work and his experience at NETL in his own words.

RN: Can you tell us about your education and what brought you to NETL?

Musser: Sure! I have a bachelors and master's degree in mechanical engineering as well as a master's and Ph.D. in applied mathematics from West Virginia University. I've been a part of NETL for a little while now and I've worked here in several capacities. I first became acquainted with the Laboratory as a post-graduate researcher with the Oak Ridge Institute for Science and Education program in 2009. After completing my Ph.D., I accepted a post-doc position at NETL before transitioning to a contractor through the West Virginia University Research Corporation for almost two years before beginning federal service in late 2013.

RN: It sounds like you've really experienced the whole range of support roles for a researcher here at the Lab. What are your responsibilities in your current capacity?

Musser: Since 2009, I have been working as a developer on NETL's open-source multiphase flow code called MFiX. We use this computational tool to study the interactions between different phases of matter in energy systems. We focus on modeling gasification systems here, where you have coal reacting with air and steam, but multiphase flows are found outside of industrial applications as well. For instance, outside researchers use MFiX to model volcanos, where volcanic debris and atmospheric gas form a gas-solids flow. That is what we

mean when we talk about multiphase flow— the simultaneous flow of materials of different phases (gas, liquid, or solid) or different chemical properties.

RN: MFiX sounds like an incredibly versatile computational tool. How do you see the code evolving in the future to contribute to the field of multiphase flow modeling?

Musser: We're always working to improve our modeling capabilities. Recently, we developed an equation to account for the transfer of heat energy during phase transitions and that has aided in our ability to accurately predict reaction rates (read more about this work in this month's Focus Story). The more accurately we can model these systems, the faster the advanced technology can be deployed with less capital investment. I would like to see the capabilities of MFiX continue to increase in the future and gain a wider user base.

Contact: Jordan Musser

NETL's In-House Research Program:
Innovative Process Technologies

Reducing costs and speeding product development will help position carbon capture and storage for widespread use and hasten the adoption of clean, energy-efficient power systems that could help conserve our nation's resources and protect our environment. Through the Innovative Process Technologies Program, researchers at NETL are searching for ways to reduce these costs and shorten development timelines. The research program comprises the following tasks:

- Developing innovative sensors and controls that improve the performance of power generation and enhance carbon capture, utilization, and storage. An example of an innovative sensor is NETL's world-class Raman Gas Composition Analyzer, a novel high-temperature fiber-optic gas sensor that uses spectroscopy to reveal a material's chemical properties by exposing the material to a laser beam and observing how its molecules respond, shifting the wavelength of the laser light.
- Developing heat-resistant, energy-efficient, advanced structural materials to lower the cost of ultrasupercritical and advanced ultrasupercritical power plants (by using computational methodologies and tools to predict how materials will perform and explain when and why selected components might fail).
- Generating engineering data sets, simulation tools, and new materials to advance direct power extraction (DPE) (converting thermal or kinetic energy in a fluid directly to electrical power) using a device called a magnetohydrodynamic (MHD) generator. MHD refers to the forces and properties of electrically conductive fluids in a magnetic field. Using electrically conductive gases instead of the turning mechanical blades in a turbine allows operation at very high temperatures, and results in very high system efficiency. The high efficiency of DPE and MHD compensates for the energy inefficiency that carbon capture introduces to a power plant.
- Advancing the use of simulation-based engineering and design in fossil energy by developing methods and software for characterizing dense granular flows (the movement of dry granular particles in a fluid); constructing simplified mathematical representations of systems or processes (known as reduced order models) for multiphase applications; and analyzing data.

To learn more about NETL's development of sensors and controls, contact Benjamin Chorpening. For more information on NETL's new ultrasupercritical and advanced ultrasupercritical materials, contact Jeffrey Hawk. Contact Rigel Woodside to discuss NETL's work in support of MHD energy conversion, or Mehrdad Shahnam to discuss simulation-based engineering and design.

FUNDAMENTAL FACTS

What is Multiphase Flow?

Multiphase flow refers to the simultaneous flow of materials of different phases (gas, liquid, or solid). NETL researchers frequently encounter multiphase flow as they investigate energy systems, and understanding the interaction between these phases is critical to their research. In reacting multiphase flow, the gases and solids react chemically with one another (as opposed to simply interacting) as they move around. Some examples of reacting multiphase flow that NETL researchers study include the following areas:

- During combustion and gasification when coal particles interact with gases
- In a CO_2 capture system where CO_2 in a gas phase reacts with solid phase sorbents or liquid phase solvents
- The chemical-looping combustion of gaseous and solid fuels (in which fuels are indirectly oxidized with air, converting their chemical energy to thermal energy)

Equations used to describe these reactions and interactions are complex, and NETL researchers use a suite of specialized code called Multiphase Flow with Interphase eXchanges (MFiX) to create computer models of reacting multiphase systems. These models eliminate the need to conduct time-intensive real-life experiments during the preliminary stages of energy system planning. Thousands of different variables can be calculated with the code so only the most efficient systems are scaled up for

A researcher records a multiphase flow with a high-speed camera.

industrial use, saving time, money, and other resources.

NETL has performed fluidized systems research for more than 50 years and currently maintains a Multiphase Flow Science Laboratory facility with experimental units that can run tests of various sizes and fluidization conditions.

Researchers studying multiphase flow also use the NETL Supercomputer, capable of performing 503 trillion operations per second—a million times faster than most high-end desktop computers, to speed through intricate computer models with ease.

Contact: Bill Rogers

APPLAUSE

Recognizing the Achievements of Hispanic STEM Role Models

Great Minds in STEM recently announced the 2015 Hispanic Engineer National Achievement Awards Corporation (HENAAC) Luminary Honorees. This year's class of 19 STEM role models comprises leaders who represent professionals from industry, government, military and academic institutions. This recognition honors their efforts leading, collaborating and initiating key programs and research within their respective organizations. NETL physical scientist **Nicolas Huerta** is a Luminary Honoree this year. Luminary awards will be presented during the 27th HENAAC STEM Career Conference, "Ignite, Inspire," taking place October 14-18, 2015 in Pasadena, CA. Full story here.

License Issued for NETL Intellectual Property

A license was issued on August 10, 2015, to Cognitek Management Systems, Inc. This license was for two patents: U.S. Patent No. 8,470,276, issued 6/25/2013, titled "Process for CO_2 capture using a regenerable magnesium hydroxide sorbent," and U.S. Patent No. 8,617,499, issued 12/31/2013, titled "Minimization of steam requirements and enhancement of water-gas shift reaction with warm gas temperature CO_2 removal."

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