



A Publication of the U.S. Department of Energy's

National Energy Technology Laboratory

Vol. 01 / Spring 2017

Impact



X_{PV}

5.0e-02
2.0e-02
1.0e-02
5.0e-05
2.0e-05

*Innovation Fast Lane
of the Future:*
**SIMULATION-BASED
ENGINEERING**

NETL Impact

Vol. 01 / Spring 2017

EDITORIAL BOARD

Dr. Grace M. Bochenek
Dr. Randall Gentry
Dr. Linda Kimberling
Dr. Sean Plasynski
James Wilson
Charles Zeh

EDITOR-IN-CHIEF

Paula Turner

DESIGN AND LAYOUT

Alec Grieco

CONTRIBUTING WRITERS

Dr. Paul Battista
Jenny Bowman
Joe Golden
Gerrill Griffith
Shaelyn Patzer

LABORATORY LOCATIONS

Albany, Oregon
Pittsburgh, Pennsylvania
Morgantown, West Virginia

MISSION

Discover, integrate, and mature technology solutions to enhance the nation's energy foundation and protect the environment for future generations.

...

NETL IMPACT is a quarterly publication from the Department of Energy's National Energy Technology Laboratory. The magazine focuses on the exciting, cutting-edge research performed at NETL by our scientists and through our project portfolio to support the DOE Fossil Energy mission.

From the Director

Welcome to the first *Impact*, a new publication that introduces readers to some of the most vital and robust energy research and development focused on improving the lives of Americans through innovation.

NETL, the only national laboratory dedicated to fossil energy research, is a U.S. Department of Energy lab that produces technological solutions to America's energy challenges. For more than 100 years, the Laboratory has developed tools and processes to provide clean, reliable, and affordable energy to the American people.

NETL's current mission is to discover, integrate, and mature technology solutions to enhance the nation's energy foundation and protect the environment for future generations. Our vision is to be renowned as a fossil energy science and engineering resource that delivers world-class technology solutions. We tackle more than 1,500 specific energy research projects with 1,400 employees at 3 research sites strategically located across the nation.

As the only one of the Energy Department's 17 national labs that is both government-owned and -operated, NETL is in a unique position to accelerate the development of technology solutions through strategic partnerships.

Our new publication seeks to inform readers about the latest developments our talented scientists and engineers are advancing. In this inaugural issue, we feature some of the new approaches and computational tools we use every day to increase the efficiency of existing power systems, innovate new ones, and find more efficient ways to harvest the nation's energy resources.

I hope you enjoy learning about these initiatives. We look forward to sharing more about other discoveries in the issues that follow.

Grace M. Bochenek, Ph.D.

Director, National Energy Technology Laboratory



NETL Impact

IN THIS ISSUE

Cover Story

Simulation-Based Engineering **4**

Engineering Applications..... **6**

Seeing the Value of R&D
through Energy Market Modeling **8**

Computational Modeling for
Power Generation Systems **10**

Solving Energy Device Riddles
with Computational Fluid Dynamics **12**

Materials Property Modeling for Tougher Turbines ... **14**

The Umbrella Conundrum:
NETL and Uncertainty Visualization **17**

From Physical to Virtual:
NETL's Multiphase Flow Analysis Laboratory **18**

Merging Computational Modeling and Simulation
Tools with the Power of Progressive Partnerships.... **19**

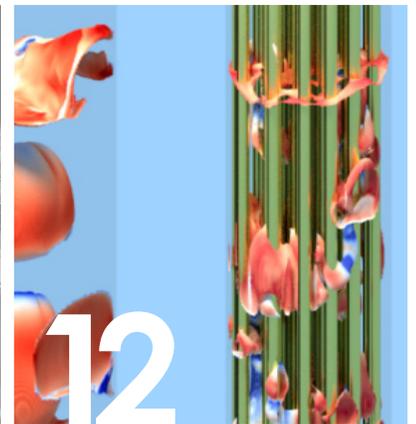
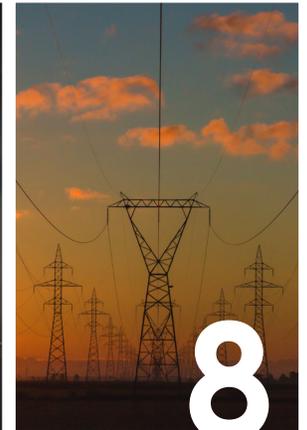
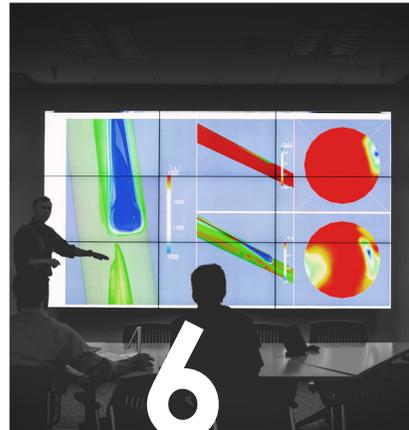
Advanced Manufacturing for Gas Turbines **20**

Low-Cost Carbon Capture Technologies
Investigated in Recent Paper..... **21**

NETL Leadership Transition Builds on
Legacy of Excellence..... **22**

Award Highlights..... **23**

NETL Crowns Regional
Science Bowl Champions **26**



Simulation-Based Engineering

[ENABLING A CLEAN ENERGY FUTURE]

By Dr. Cynthia Powell

Imagine being able to design and optimize an entire fossil-fuel power plant, from fuel processing, through energy conversion, to power distribution, and to include the integration of pollution control devices to assure near-zero emissions, without leaving your desk. At NETL, high-performance computing is bringing once-impossible opportunities and achievements to energy R&D.

Simulation-based engineering has emerged alongside laboratory work and prototype, or pilot scale, testing as a necessary tool in the discovery and development of technologies for sustainable energy systems, enabling scientists and engineers to do their work faster, cheaper, and in a more interconnected manner than physical approaches alone. Simulation-based engineering has become a major part of the way NETL does its job and enables others to do theirs, from the discovery and development of new materials, through the design of ultra-efficient energy

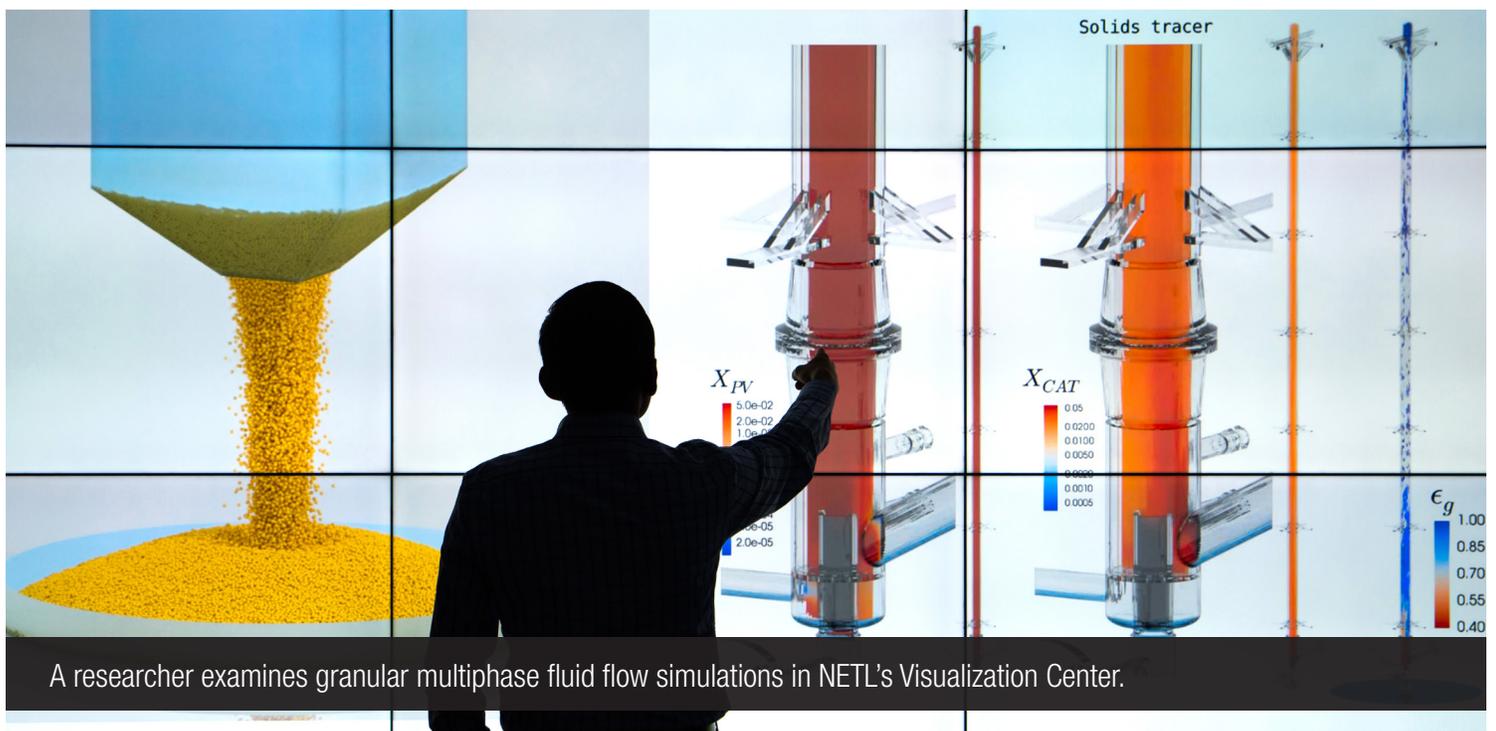
conversion devices, to the integration of processes in the design of new affordable and environmentally sustainable energy systems.

Simulation-based engineering refers to the application of computational models to the study and prediction of the behavior of engineered systems. Leveraging the tremendous power of today's computers, engineers are now able to more efficiently design new materials, devices, and systems, and to better predict and optimize their performance.

NETL has developed an extensive portfolio of simulation-based engineering methods, and in the process, has taken a place at the forefront of energy systems modeling. The advantage of these methods is that the results of months or even years of laboratory experimentation and testing can be obtained at the computer. Simulations can facilitate the engineering of new materials and accurately predict performance under a range of conditions.

Simulations can accurately model complex systems, such as the performance, costs, and environmental impacts of a modern power plant. With recent advances, simulations can be used to study and understand emergent phenomena that may be difficult, or impossible, to observe in the lab.

NETL researchers and analysts model not only the physical-science aspects of materials, devices, systems, and processes, but also the costs, markets, and environmental impacts throughout a technology's life cycle, to understand the real-world prospects for new technology implementation. These models enable simulation of processes and environments for purposes as diverse as research, technology assessment, and forecasting. Many of NETL's models have been packaged as tools, and made available to the public for design, optimization, and planning purposes throughout energy-related industries.



A researcher examines granular multiphase fluid flow simulations in NETL's Visualization Center.

Faster, Better, Cheaper Technology Development

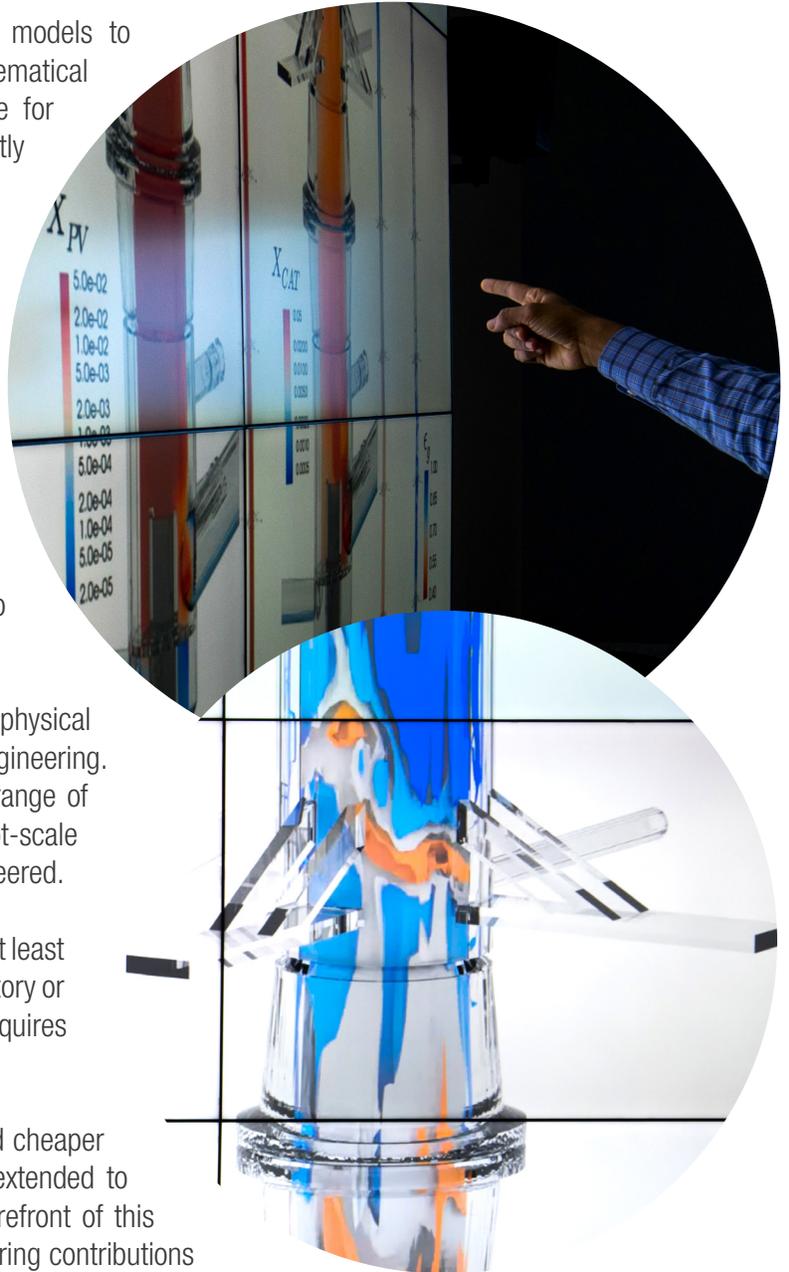
Simulation-based engineering involves the use of computer models to predict the modeled systems' behavior. The models are mathematical representations of systems or processes, sufficiently accurate for the task at hand, but simplified enough to rapidly and efficiently generate the desired results.

NETL uses simulation-based engineering to accelerate development of technologies at reduced cost. The lab has become a lead developer of tools and practices for fossil energy engineering. In 2016, NETL won two R&D 100 awards for products based on computational engineering: Computationally Optimized Heat Treatment of Metal Alloys and the Carbon Capture Simulation Initiative (CCSI) Toolset. This modeling expertise serves as a source of innovation and technology transfer; and simulation-based engineering methods bring further advantages for energy technology development to the lab.

Computer models of energy systems are easier to modify than physical systems, representing another advantage of simulation-based engineering. In other words, simulations can be used to explore a greater range of system's behavior than is typically possible with laboratory and pilot-scale experiments; thus the resulting technologies will be better engineered.

Simulation, however, cannot replace physical experimentation—at least not yet. Models are built from data that are collected in the laboratory or at the power plant. Validation of models and their results also requires “real” data, collected under “real life” conditions.

The ability to design and develop technologies faster, better, and cheaper has wide appeal; and simulation-based engineering is being extended to virtually all corners of the engineered world. NETL is at the forefront of this revolution in the field of fossil energy technology, making pioneering contributions across the fossil energy research agenda, from development of materials able to withstand the high temperatures and pressures needed for highly efficient ultra-supercritical coal power plants and hydrogen-fueled turbines, to the design of hybrid fuel cell/gas turbine power plants. NETL's simulation capabilities for analysis of processes, systems, and markets extend simulation-based engineering out to the domains of technology development and adoption processes. ☰



Dr. Cynthia Powell (*retired*)

Dr. Cynthia Powell is responsible for implementing a research and development portfolio that positions the Laboratory as an international resource for fossil energy technology discovery, development, and deployment. As part of this role, she promotes safe and efficient research operations at NETL and ensures the Laboratory's research personnel are equipped with the technical competencies and knowledge needed to effectively support its research mission. She has more than 15 years of experience in high-temperature phase and microstructural development of structural materials and the effects of these phase changes on the bulk properties of such materials.

ENGINEERING APPLICATIONS

Exploration & Discovery

Physical experimentation must focus on the specifics of implementation, but computer models enable discovery into an extended range of phenomena. NETL's modeling capabilities are crucial to its work in areas like subsurface exploration, in which disparate data types must be integrated to provide insight and reduce uncertainties. NETL develops and uses models for enhanced recovery of resources such as oil and gas in shale formations, and geologic storage of substances including carbon dioxide, natural gas, and waste water.

Life Cycle Analysis

NETL uses life cycle analysis (LCA) as a tool and framework for evaluating energy technology and policy options on a common basis. LCA includes the environmental burdens of converting fuel to useful energy, infrastructure construction, extraction and transport of fuel, and transporting the final energy product to the end user. NETL's LCA method also includes life cycle costing, which applies cost metrics between the same boundaries as these environmental models. NETL has applied LCA to fossil, nuclear, and renewable energy systems that produce electricity and liquid fuels. Products of these modeling efforts include both detailed reports and dynamic software tools.

Risk Assessment & Management

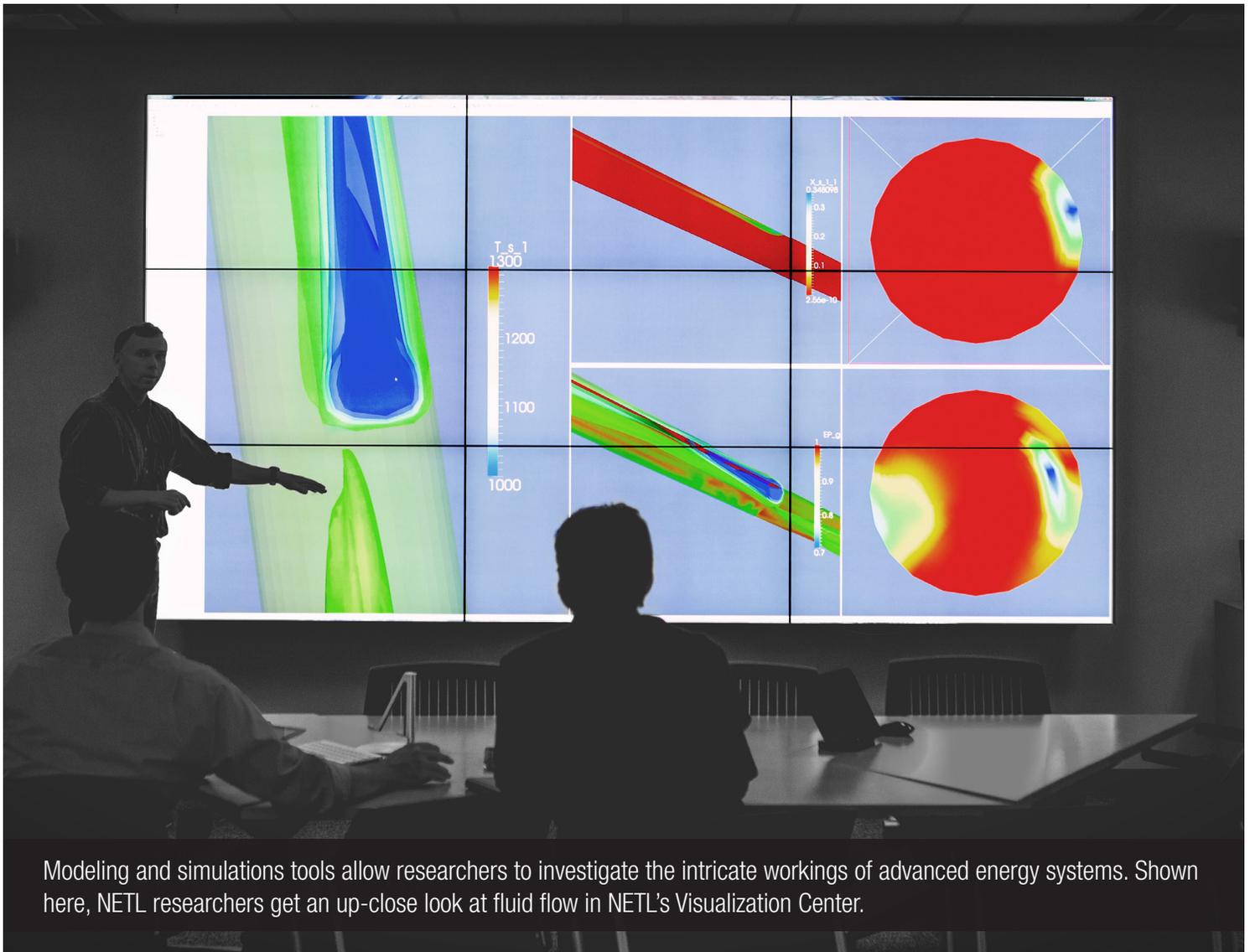
Uncertainties and risks go hand-in-hand with new technology development, and some risks can be severe, as recent experience with the Deepwater Horizon offshore drilling platform illustrates. Accordingly, risk assessment and management have emerged as engineering practices, and NETL is prominently engaged in their development. Two examples are the NETL-led National Risk Assessment Partnership—a multi-national laboratory effort to develop a critical science base and predictive tools that can be applied to risk assessment for long-term storage of carbon dioxide, and Offshore Integrated Assessment Modeling (IAM)—a suite of eight custom tools that model risks involved in oil and gas in the offshore environment.

Operations & Controls

NETL's unique Hybrid Performance (HyPer) facility enables the study of controls and architecture for hybrid fuel cell/gas turbine systems in a simulated environment. Combining fuel cells and turbines in unified systems can generate power with greater fuel efficiency and less environmental impact than either fuel cells or turbines alone. Controlling the flow of power from both the fuel cell and turbine during load changes is more complicated than in conventional power systems. HyPer couples simulations and physical hardware so that researchers can investigate a fully integrated system, designing components and testing and optimizing control strategies to maximize fuel efficiency and performance.

Technology Design & Optimization

NETL's wide-ranging simulation capabilities are used for energy technology design across all areas of fossil energy research, from development of materials able to withstand the high temperatures and pressures needed for highly efficient, ultra-supercritical coal power plants and hydrogen-fueled turbines to design of hybrid fuel cell/gas turbine power plants.



Modeling and simulations tools allow researchers to investigate the intricate workings of advanced energy systems. Shown here, NETL researchers get an up-close look at fluid flow in NETL's Visualization Center.

High-Performance Computing

NETL hosts several high-performance computing facilities, among them the Morgantown, Wv Simulation-Based Engineering User Center with its 503 teraflops supercomputer, Joule; visualization centers at Albany, Or, Morgantown, Wv and Pittsburgh, Pa sites; and GAIA, the Geoscience Analysis, Interpretation & Assessments multiuser facilities. These facilities provide a range of hardware capabilities on which to build and run computationally intensive simulations.

Prediction

Comparisons of alternative pathways—including demand, requirements, use, and costs—and what-if analyses support technology optimization on a range of investigations, from simple components to complex systems. For example, forecasting coal use in coming decades, supports planning for longer-term eventualities. Other comparisons underlie prediction of recovery of rare earth elements from coal byproducts and exploration of diverse means to do so.

Forecasting

Exploration of multiple options and forecasting is important in planning and policymaking for both R&D and technology implementation, where technical concerns such as the efficiency of a prospective process join concerns about systems integration, costs, and environmental consequences. NETL's simulation capabilities for analysis of processes, systems, and markets extend simulation-based engineering to technology development and adoption processes. ☰

SEEING THE VALUE OF R&D THROUGH ENERGY MARKET MODELING

By Joe Golden

Technical Contact: Dr. Charles Zelek

Throughout history, people have yearned to know the future, and the reason is clear. Just as a farmer could greatly benefit from knowing which grains will grow and which will fail, an energy research laboratory like NETL could strategically plan its efforts based on an accurate forecast of which technologies may have the greatest impact on the future energy market.

Shakespeare's characters must consult the fabled Oracle at Delphi to learn their fate, but NETL relies on science-based energy market models that can accurately predict a myriad of scenarios, including how NETL research and development (R&D) will affect the cost of electricity, carbon emissions reduction, job creations, and many other important factors, far into the future.

"We can start with baseline of *no* NETL R&D," NETL's head of market modeling efforts, Chuck Zelek explained, "and then we forecast out to 2040, and see what the energy market looks like. We see things like what the energy mix will be, how much electricity will cost, and how well we're meeting regulations. Then, we run the model *with* NETL R&D. The difference between the two really underscores the importance of our work."

When current NETL R&D is added to the market models, the true value of the laboratory's research becomes apparent. Compared to a baseline of no R&D, cost of electricity is reduced, carbon emissions are mitigated, and environmental targets are met. Even more useful, researchers can see how other scenarios might play



“This modeling work ensures that our work is focused on the best and most efficient path toward enhancing the nation’s energy foundation.”

out. For example, if the Lab increased its carbon capture and storage efforts, the models can project the effects of this change. In this way, NETL can best use its resources to focus on achieving a bright energy future for the nation.

So, what are the models that NETL uses, and how do they work? One of the most widely known models, the National Energy Modeling System (NEMS) was created by the U.S. Department of Energy’s (DOE) Energy Information Administration (EIA). This model is primarily used to develop the *Annual Energy Outlook*—an essential document used by industry and policy makers that focuses on factors expected to shape U.S. energy markets through 2040. NETL not only uses this model, but also contributes to it based on its expertise in fossil energy research. Code developed at the Lab has been integrated into the model and EIA consults NETL on the expanded capabilities of the model.

MARKAL, a name derived from market and allocation, was developed by the Energy Technology Systems Analysis Programme

(ETSAP) of the International Energy Agency. NETL uses this model to find the least expensive combination of technologies to meet a specific goal and calculates resulting environmental emissions, water consumption, and withdrawals.

NEMS, MARKAL, or any of the other various energy market models all work in a similar fashion. Historical data on energy usage patterns, and the current availability and cost of energy sources serve as data for input. NETL R&D directly affects these factors. Assuming that industry will favor the cheapest energy source and economic and regulatory climate persists, the models logically play out possible scenarios with these baseline inputs.

An excellent example of how energy market models can demonstrate the value of NETL R&D can be seen when examining DOE’s Clean Coal Research Program (CCRP) and its potential benefits for consumers. As a fossil energy research laboratory, much of NETL’s work supports the CCRP. Areas like carbon capture, utilization, and storage research

and demonstrations; advanced energy systems, and cross-cutting research all contribute to keeping coal a strategic fuel while enhancing environmental protection. When this R&D data is fed into the energy markets, the projected cumulative benefits through 2040 are remarkable based on the current economic picture:

- \$92 billion in total electricity expenditure savings
- 2.4 million jobs created
- A Gross Domestic Product of \$242 billion
- 2.9 gigatonnes of CO₂ captured
- 4 billion additional barrels of domestic oil from enhanced oil recovery

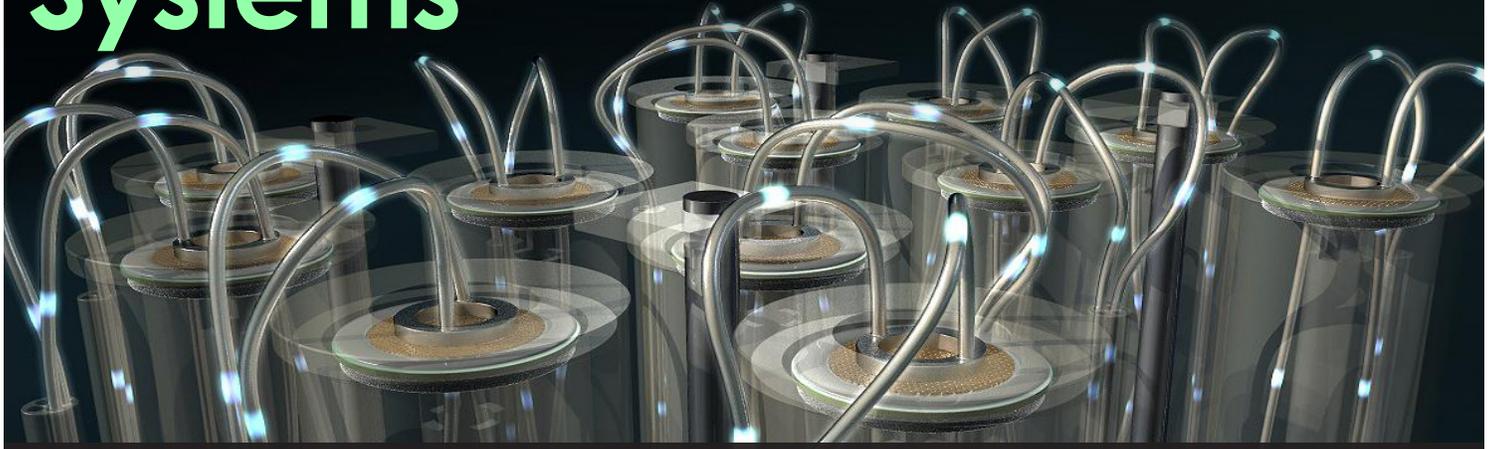
“The models we use at NETL validate the large-scale research efforts we undertake daily,” Zelek said. “Our researchers are solving the nation’s toughest energy challenges, and this modeling work ensures that our work is focused on the best and most efficient path toward enhancing the nation’s energy foundation.” ☰



Dr. Charles Zelek // Charles.Zelek@netl.doe.gov

Dr. Charles Zelek is an economist at NETL in the Systems Engineering and Analysis Directorate within the Research and Innovation Center. In this capacity, he conducts energy market analyses to inform NETL’s fossil energy research, development, and demonstration programs and contribute to related policy and regulatory decision making. Dr. Zelek has worked in the field of climate change and energy for over 15 years across positions in academia and government. He has conducted research on terrestrial carbon sequestration internationally in the Philippines, supported formulation of the Energy Title of the 2008 Farm Bill as a senior economist for the Department of Agriculture in Washington D.C.

Computational Modeling for Power Generation Systems



3D Rendering of NETL's Multi Cell Array (MCA), a unique platform developed to rapidly test multiple fuel cells and determine how they degrade when contaminants exist in the fuel stream, such as might occur when using syngas from a coal gasifier.

By Paul Battista // Technical Contacts: Jason Hissam, Dr. David Miller, Joe Stoffa

The ability to adapt technology design early in the development process is critical to controlling costs and reducing risks. Innovative energy technologies face a lengthy journey from the laboratory bench through commercial deployment that could take up to 15 years for pre-deployment and another 20 to 30 years for widespread industrial-scale deployment. Additionally, it's estimated that 75 percent of the cost of manufacturing occurs at the conceptual design stage. Computational modeling is the key to controlling costs and risks in a timely fashion.

Reducing CO₂ emissions and improving the performance of fossil fuel-based energy systems is a key mission of NETL. Computational tools and models that help identify, design, scale up, and optimize promising technology concepts play a pivotal role. Computational modeling, coupled with high-performance computing, is used to simulate and study the behavior of complex systems and

allows scientists and engineers to conduct thousands of simulated experiments using multiple variables. A multiscale modeling approach allows the evaluation of system components at various scales, ultimately leading to a better understanding and optimization of a complete, integrated system. The results of modeling help researchers make predictions about what will happen in the real system in response to changing conditions.

At NETL, computational tools are used to simulate interacting phenomena associated with fossil fuel-based energy systems, providing vital data about physical properties, thermodynamics, chemical reactivity, heat transfer, hydrodynamics, mass transfer, and other aspects of the device or processes. Two examples of these tools are Modeling of Solid Oxide Fuel Cells and Multiphase Flow with Interphase eXchange.

Jason Hissam

Jason.Hissam@netl.doe.gov

Jason Hissam is a project manager in NETL's Technology Development and Integration Center. He currently serves as the primary contact for the Simulation-Based Engineering and Innovative Energy Concepts programs.

Dr. David Miller

David.Miller@netl.doe.gov

Dr. David Miller is the senior research fellow for NETL's Systems Engineering and Analysis. Additionally, he serves as the Technical Director of the Institute for the Design of Advanced Energy Systems, a virtual organization that includes national laboratories and regional university partners.

Joe Stoffa

Joseph.Stoffa@netl.doe.gov

Joe Stoffa is a project manager in NETL's Advanced Energy Systems Team. His project portfolio focuses on solid oxide fuel cell technology with an emphasis on research activities designed to improve performance.

Modeling Solid Oxide Fuel Cells (SOFCs)

SOFCs are electrochemical devices that convert the chemical energy of a fuel (methane or syngas) and an oxidant (air or oxygen) directly into electrical energy. Because SOFCs produce electricity through an electrochemical reaction instead of a combustion process, they are much more efficient and environmentally benign than conventional electric power generation processes. Their inherent characteristics make them uniquely suitable to address the environmental and water concerns associated with fossil fuel-based electric power generation.

Modeling SOFCs ranges from the nanometer scale to the utility scale. At the nanoscale, electrochemical phenomena and surface reconstruction are modeled to understand electrode performance and material degradation. At intermediate scales, detailed cell and stack performance models yield predictions of performance, degradation, fuel consumption, thermal stresses, and other phenomena. These detailed models are used to create SOFC models that are integrated into chemical process simulators to demonstrate performance and identify costs of utility-scale power generation plants.

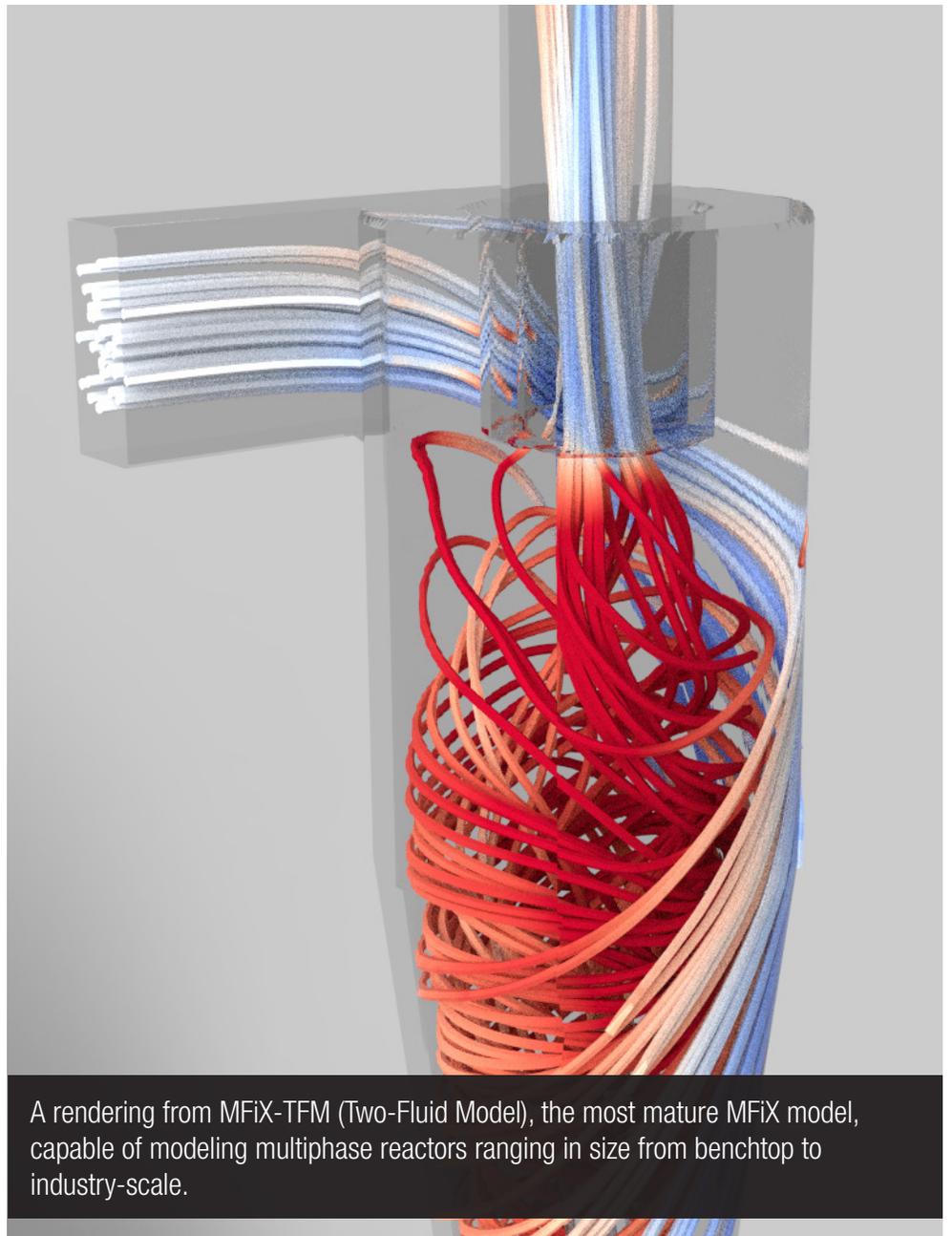
Multiphase Flow with Interphase eXchange (MFiX)

Computational modeling can be used to simulate complex power systems and components like gasifiers and carbon capture reactors allowing for a better understanding of performance prior to finalizing technology design features. Models that quantify uncertainty are important for reducing the cost and time required for developing zero-emission fossil fuel conversion processes and systems.

Multiphase flows—the simultaneous flow of materials of different phases (gas, liquid, or solid)—are encountered in most commercial energy and environmental processes. Understanding the interaction between these phases is critical to understanding and predicting the performance of energy system devices that employ multiphase flows. NETL is a recognized world leader in developing and applying computational fluid dynamic models of multiphase flow reactors.

Information generated using these models is far more extensive than data generated by experiments alone. The models can

integrate experimental and computational results to provide unique insights. MFiX, a suite of the computational fluid dynamics codes developed specifically for modeling reacting multiphase systems, is central to the process at NETL. This open-source software has more than two decades of development history and 4,000 registered users worldwide. MFiX has become the standard for comparing, implementing, and evaluating multiphase flow models. Researchers at NETL use MFiX to perform basic and applied research on advanced fossil energy technologies including gasification, coal combustion, gas cleanup, and CO₂ capture. ☰



A rendering from MFiX-TFM (Two-Fluid Model), the most mature MFiX model, capable of modeling multiphase reactors ranging in size from benchtop to industry-scale.

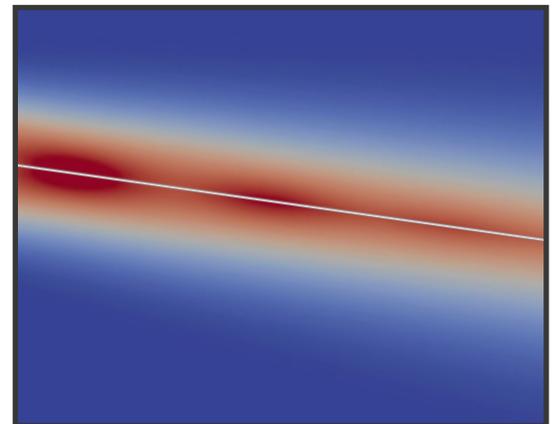
SOLVING ENERGY DEVICE RIDDLES WITH ADVANCED COMPUTATIONAL FLUID DYNAMICS

By Gerrill Griffith // Technical Contact: Dr. Madhava Syamlal

Computational Fluid Dynamics (CFD) is the use of applied mathematics, physics and computational software to describe how a gas or a liquid flows. The CFD simulations require high performance computers such as NETL's Joule. At NETL, it is a critical knowledge tool that is helping to find cleaner, more efficient ways to power the nation. There are many examples at NETL of how CFD has been used to develop devices and processes aimed at energy innovations.

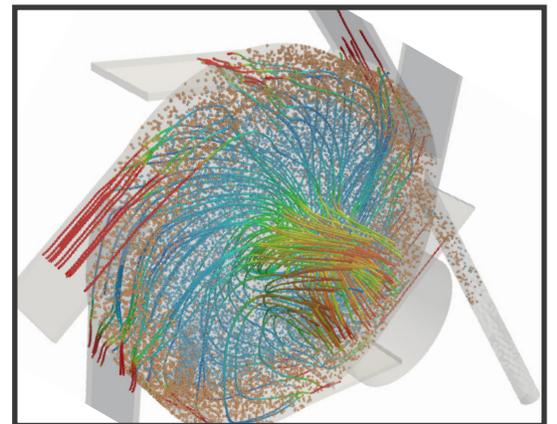
MHD Modeling & Simulation

Magneto-hydrodynamic (MHD) power generation or direct power extraction (DPE) is a process to generate electrical energy directly from the products of fuel combustion without an intermediate mechanical device (dynamo). The electric power is produced from the interaction of the ionized fluid with an applied external magnetic field. MHD power generation systems could be more efficient than traditional fossil power systems, especially when a carbon capture system is integrated. Work will continue to improve accuracy and include the use of laser induced photoionization to increase the conductivity of the gas within a generator channel. The model developed at NETL will help engineers to predict and understand the behavior of such systems.



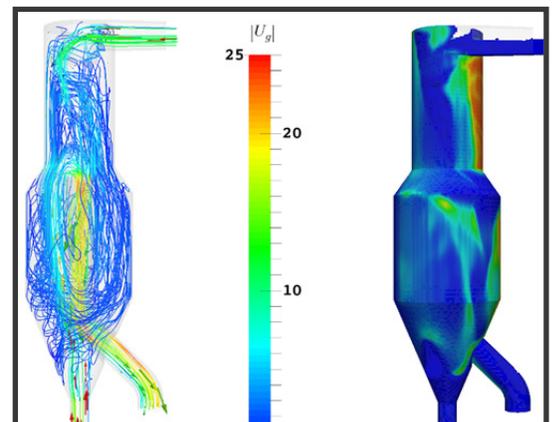
Vortex Chamber Research

Vortex chambers allow for the operation of rotating fluidized beds that can provide a unique fluidization regime where particles experience centrifugal forces much higher than the force of gravity allowing particles to experience intensified gas-solid contact, gas-solids separation, and solids-solids segregation. With a focus on segregation of oxygen carriers and ash in Chemical Looping Combustion, numerical simulations were conducted to understand the flow behavior and particle segregation in a vortex chamber. The information from numerical simulations will be used to guide and help interpret the experimental tests of vortex chambers in the lab.



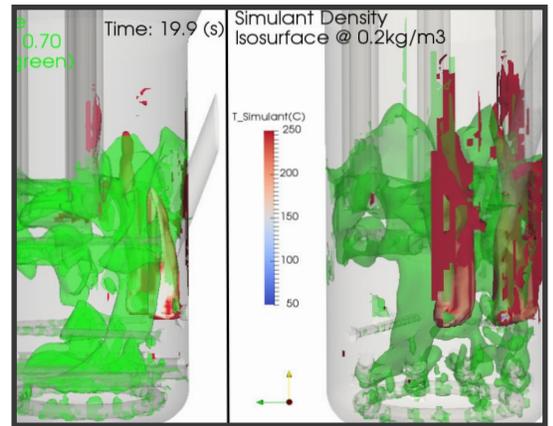
Chemical Looping Modeling & Simulation

Chemical Looping Combustion (CLC) is being investigated by NETL as a way to use fossil fuels at a lower cost and with lower greenhouse gas emissions than more conventional approaches. In chemical looping combustion, the fuel is combusted with a solid oxygen carrier, eliminating the need for separating CO₂ from the flue gas as in the case of combustion in air. NETL researchers used CFD to predict the performance of three CLC designs. Based on the simulations, two separate modifications were identified as possible solutions. The proposed modifications were experimentally tested and proven effective.



CFD for Development of Integrated Waste Treatment Units

NETL used CFD modeling to help develop an Integrated Waste Treatment Unit (IWTU), a first-of-its-kind, 53,000-square-foot facility designed to treat 900,000 gallons of aqueous, radioactive sodium-bearing waste that has been stored in underground storage tanks at a spent nuclear fuel reprocessing facility located at DOE's Idaho Nuclear Technology and Engineering Center (INTEC). IWTU uses a steam-reforming technology to convert the sodium-bearing liquid into a solid, granular material before packaging it in stainless steel canisters for long-term storage. This reforming process uses two fluidized beds to treat the sodium-bearing waste and reform process gases. Fluidized beds suspend solid fuels on upward-blowing jets of air during the combustion process, causing a turbulent mixing of gas and solids and providing more effective chemical reactions and heat transfer.



CFD-Based Optimization

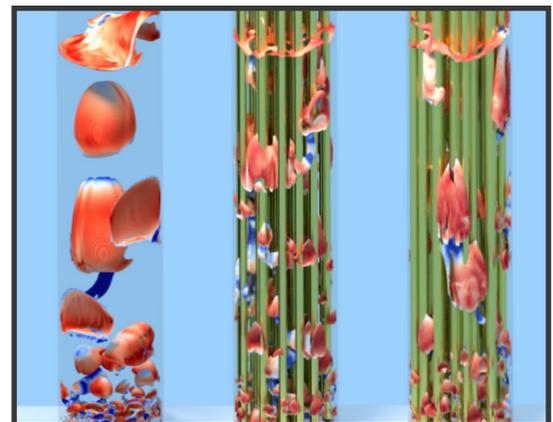
Developing new small-scale systems that convert solid fuel to power and chemicals to suit local conditions and that can be deployed at low financial risk is an important NETL objective. NETL scientists developed an MFIX-based reactor optimization code that enables users to determine optimal reactor design and operating conditions before any physical hardware is constructed. NETL rapidly transforms computational reactor designs into a physical test unit using 3D manufacturing. Researchers use the physical units to validate simulation and design optimization. If discrepancies are found, researchers use this knowledge to refine the simulation optimum, and a new physical system can be created and operated in a day. This method of CFD-based design and rapid prototyping using 3D manufacturing is expected to radically change small-scale system development.



Carbon Capture Simulation

To develop sorbent-based CO₂ capture for conventional coal-fired power plants, NETL conducted CFD simulations for a pilot-plant unit that addressed several challenges including the presence of vertical heat transfer tube banks, patented multi-stage design, and the complex chemical reactions that take place inside the system.

A model built with the help of NETL's multiphase CFD solver, MFIX, was first validated with data from several small-scale experiments. The figure below shows a validation study for a fully resolved flow over an array of vertical tubes. Simulations were performed with square and triangular tube arrangements and results were compared with experimental data found in the literature. Good agreement was found in terms of hydrodynamics and bubble statistics. The validated model was used to predict the performance of a 1 MW carbon capture reactor, well before the unit was operated. ☰



Dr. Madhava Syamlal
Madhava.Syamlal@netl.doe.gov

Dr. Madhava Syamlal is the senior fellow of computational engineering at NETL. He is responsible for the development of science-based simulations to accelerate energy technology development.

MATERIALS PROPERTY MODELING FOR TOUGHER TURBINES

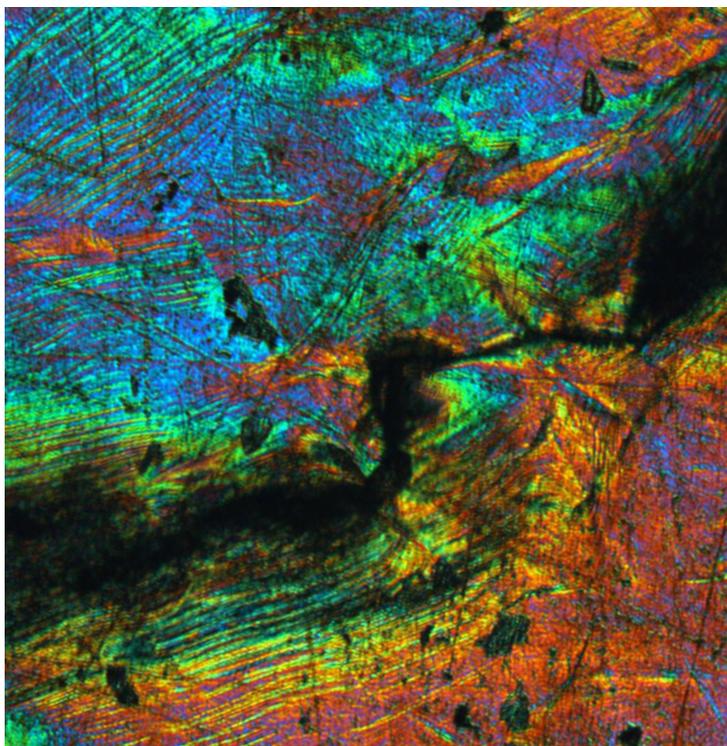
By Jenny Bowman // Technical Contact: Dr. Patrichin "Rin" Burke

Computational materials science enables researchers to predict the behavior of materials, and reduce the difficulty, time and expense of experimentation. Using advanced computing power and software, researchers are able to design, study, test, and optimize materials in a virtual setting. For NETL researchers, computational materials modeling is a powerful tool.

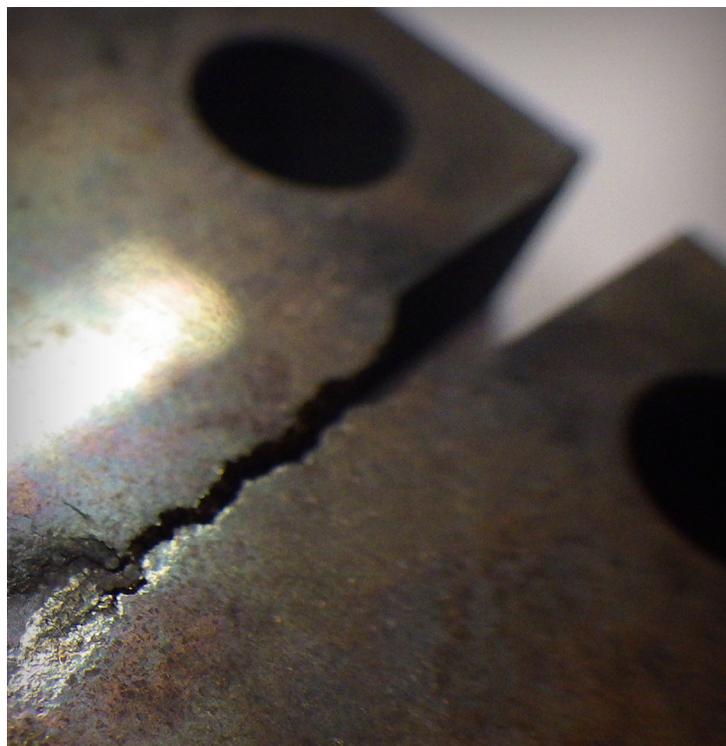
One research area where NETL focuses its materials property modeling is the technology needed for increased turbine temperatures. Ultra-efficient power production requires high-

temperature, high mechanical stress operating conditions. Components of turbines operating at these demanding conditions are subject to damages such as "creep"—the tendency for materials to sag or deform at high-temperatures, and "fatigue"—the propagation of cracks over time. Advanced materials are needed to increase turbine power and efficiency while maintaining low capital costs and protecting components to enable longer service lifetimes. The advanced turbines and turbine-based systems enabled by these materials will operate cleanly and at low cost.

As part of this effort, NETL manages projects under DOE's Office of Fossil Energy Advanced Turbines Program, which supports universities and small businesses to conduct materials R&D. One of the goals of the program is to design and develop new alloys that can be used effectively as large industrial gas turbine (IGT) blade components, withstand harsh operating conditions, and provide superior performance compared to state-of-the-art turbine blades.



A magnified optical contrast image of a turbine sample reveals plasticity as striated, bright-colored regions surrounding the crack. *Photo courtesy of Thomas Siegmund/Purdue University.*



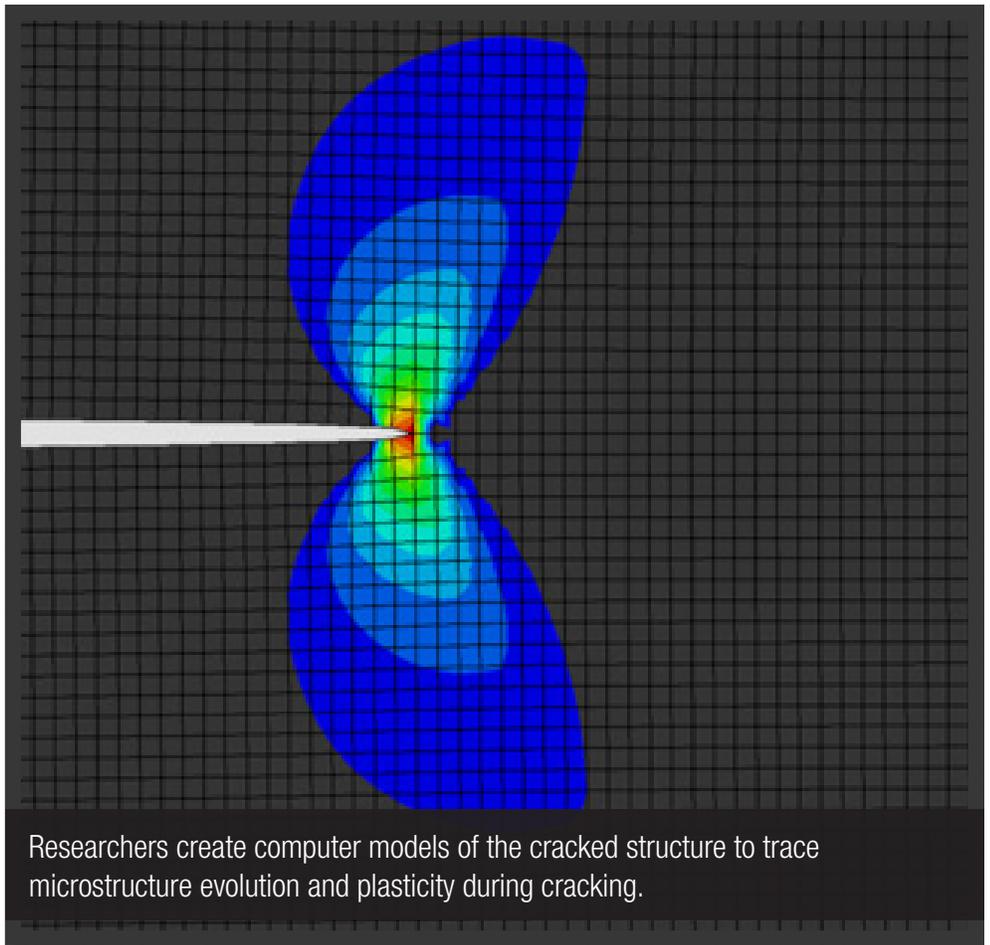
The propagation of cracks has been a long-standing problem in the structural integrity of turbines. This phenomenon is shown here in a test coupon. *Photo courtesy of Thomas Siegmund/Purdue University.*

Developing Stronger, More Durable Alloys through Integrated Computational Materials Engineering

In the world of alloy development, nickel is the material of choice for high-temperature applications because of its outstanding high-temperature strength and corrosion resistance. Alloying nickel with other select materials produces super tough alloys known as “superalloys.” As the need for higher efficiencies grow, superalloys must be made even tougher.

Under an NETL-managed project, QuesTek Innovations LLC is designing and developing an innovative superalloy for industrial gas turbine (IGT) blade components that is more cost-effective and easier to manufacture compared to state-of-the-art superalloys. QuesTek used its proprietary integrated computational materials engineering (ICME) tool and design platform to address the task. ICME tools enable researchers to link materials models at multiple scales to better understand how fabrication methods produce structures on the micro-scale, how those structures affect material properties, and what materials will be most suited for particular applications.

QuesTek designed a new single-crystal nickel-based superalloy called QTSX™ that exhibits superior high-temperature properties—especially creep resistance—and can be cast effectively as large, defect-free components. Major improvements in alloy performance have been associated with optimizing alloying elements, especially reducing rhenium while maintaining creep strength since rhenium significantly drives up costs. Because of its low availability relative to demand, rhenium is among the most expensive of metals. QuesTek’s QTSX superalloy composition achieves the



same superior creep performance of a rhenium-containing alloy, but without the added expense. Another benefit is the QTSX’s castability. Alloys must be easily cast (manufactured) without defects for industry adoption. Traditionally, “freckling” has been an obstacle during casting—a major defect that poses a weakness in the alloy as a crack-initiation site and degrades the mechanical properties. The QTSX single crystal superalloy, developed by use of a novel computational modeling tool, has demonstrated freckle-free casting of full-scale IGT blades. Moreover, preliminary assessments show that QTSX is comparable to alloys containing more than twice the amount of rhenium (1 weight percent versus 3 weight percent) regarding microstructural stability, oxidation resistance, and creep performance. Casting trials at full-scale blade have shown that QTSX is defect free, which would drastically improve manufacturing yields of IGT blades.

[...Continued on page 16]

Single-crystal materials are composed of a continuous, unbroken crystal structure. This single structure means there are no “grain boundaries” or interfaces in the structure, which are weak points along which premature damage can occur. As a result, single-crystal materials have enhanced creep and fatigue properties.

Using Computational Modeling to Improve Component Life-Prediction Methodologies

[...Continued from page 15]

Creep is a permanent deformation that occurs under stress at elevated temperatures. Fatigue is localized, progressive structural damage that occurs under cyclic loading. For designers of high-temperature components, creep and fatigue are serious problems. Materials in high-temperature systems operate at the conditions that will result in both types of damage. Most gas turbine users want increased operating lifetimes and the flexibility to enable various operating cycles or “cyclic loading.” The starts and stops and changes in power generating output imposed on gas turbines during these transient operations can lead to significant materials damage due to thermal and mechanical stress.

*Finite Element Analysis

is a computerized method for predicting how a material will react under operating conditions such as heat, pressure, and fluid flow. Using finite element software enables researchers to determine whether a material will fail or work the way it is designed.

Evaluating the creep-fatigue interactions in IGT materials through computational materials results in increased efficiency and reduced costs by enabling more precise materials design.

Purdue University, as part of an NETL-managed project, is developing tools to predict creep-fatigue interactions in nickel-based superalloys to predict creep-fatigue crack growth, interaction, and life prediction methods for Inconel 718—a nickel-based superalloy that is highly oxidation- and corrosion-resistant. The alloy is also well suited for service in extreme pressure and heat environments.

A team led by Dr. Thomas Siegmund is developing a model to predict creep-fatigue under various loads that will be tested and validated by experiments. Once developed, the Purdue team’s model could be embedded into standard finite element software* as an add-on analysis tool for gas turbine designers. The work will improve the cost-effectiveness of turbine design while ensuring a high level of safety for turbine operation. In addition, the new model can reduce turbine manufacturing costs and maintenance costs through increased blade life, leading to lower plant costs and lower electricity costs.

In another project managed by NETL, Dr. Rick Neu at Georgia Tech is developing a microstructure model for single-crystal nickel-based superalloys to assess long-term creep fatigue interactions and life prediction for turbine components.

Advanced computational techniques enable researchers to predict the structure properties of materials at very small scales. A material’s microstructure—the small-scale structure of a material—can strongly influence physical properties including strength, corrosion resistance, and temperature resistance. The Georgia Tech team will investigate microstructural properties of single-crystal nickel-based superalloys to understand how long-term exposure to the stresses of IGT service environments degrades the microstructure and what this evolution means for performance of IGT components. The model developed under this project will allow improved component life, which will enable decreased maintenance costs and reduced costs for electricity. The model will be validated by long-term experimental studies that systematically ages the alloy under different stress conditions with specific emphasis on the role of microstructure.

Computational materials modeling is enabling the rapid design and simulation of new and novel alloys that are essential for advanced power generation systems to achieve performance, efficiency, and cost goals. ☰



Dr. Patcharin “Rin” Burke // Patcharin.Burke@netl.doe.gov

Dr. Patcharin “Rin” Burke is a materials scientist and federal project manager at NETL. Her projects focus on the technical challenges of developing low-cost solid oxide fuel cell systems for stationary coal-based power applications and advanced materials development for advanced turbines systems and components. Dr. Burke’s main areas of expertise involve fabrication and structure-property-processing relationships of high-temperature materials such as alloys, composites, and perovskite materials and their application to fuel cell systems and advanced turbines.

The Umbrella Conundrum: NETL & Uncertainty Visualization

By Shaelyn Patzer // Technical Contact: Dr. Kelly Rose

We may not always be aware of it, but uncertainty is a constant part of our lives. It figures into decisions as major as where to invest our retirement portfolios and as minor as if we should grab an umbrella on our way out the door.

When the weatherman says there's a chance of rain, when do you decide to bring that umbrella—when there's a 30 percent chance of a drizzle, or when you're 70 percent likely to get soaked?

Understanding likelihoods and the range of potential error in a prediction is important in everyday life, but it's vital in research. Data analysis is an integral part of modern life, providing a foundation of knowledge for decision making in nearly every sector—from economics to energy. However, data is inherently uncertain. No matter how carefully gathered information is or how accurate the testing, no measurement is exact. The credibility of the scientific, technical, management, and policy decisions that are based on the understanding that data needs to include a perception of the accompanying uncertainty and error.

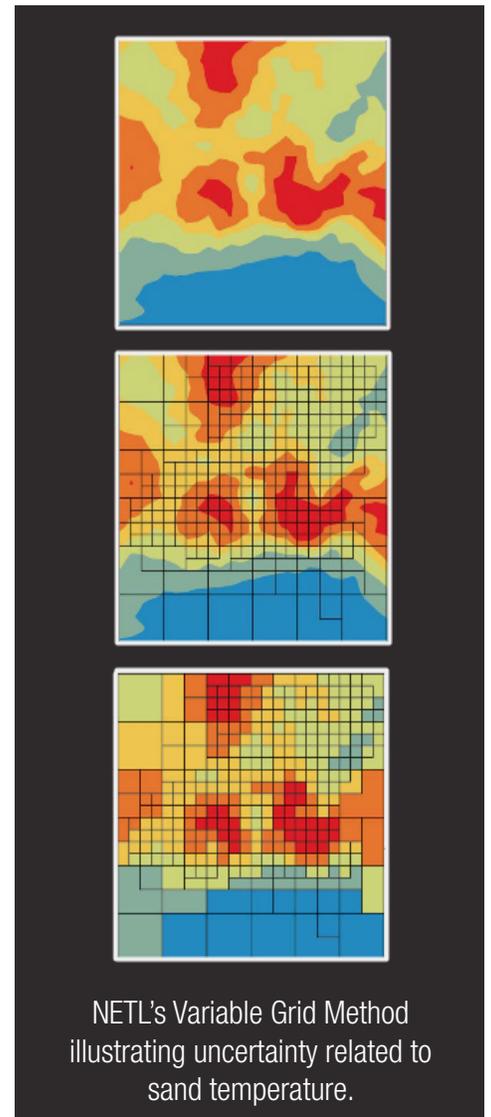
Recognizing this need, researchers at NETL created a technology to help tackle the challenges presented by accurately

representing data uncertainty. The Variable Grid Method (VGM) developed by NETL focuses on the visual quantification and representation of spatial or spatial-temporal data trends—graphics that help illustrate information associated with the data analysis of geography, space, and time, like the constant changing of a weekly weather forecast across a map. Spatial data plays a large role in informing decisions related to today's critical issues, such as energy security, weather forecasting, and human health.

Through the use of computer modeling, VGM allows users to measure the uncertainty associated with their datasets and create a visual representation of both the data itself and its range of error. This technology is not new, but previous tools lacked an important function—the ability to include the role of uncertainty and error, enhancing the accuracy of the data, prediction, or model visualization. By providing information on the unknown, users immediately have a better understanding of the data as a whole, improving the foundation on which to make decisions. After all, when the uncertainty is left out of the equation, it can be pretty difficult to decide if you need to bring an umbrella!

Important decisions can hinge on the provision of uncertainty in data. Spatial data can influence decisions that impact your life every day—decisions that can only be improved by understanding every scrap of information available.

VGM offers an alternative way to visualize knowledge gaps and uncertainty. The modeling tool enables users to represent ranges or categories of uncertainty as variable grid cell sizes. ☰



Dr. Kelly Rose // Kelly.Rose@netl.doe.gov

Dr. Kelly Rose is a geo-data science researcher with NETL's Research and Innovation Center. Her research at NETL is focused on using geologic and geospatial science to reduce uncertainty about, characterize and understand spatial relationships between energy and natural systems at a range of scales. Her work involves development of new data-driven methods and tools for analysis of offshore energy, groundwater, carbon storage, and geothermal systems.

From Virtual to Physical:

NETL's Multiphase Flow Analysis Laboratory

By Shaelyn Patzer // Technical Contact: Dr. William Rogers

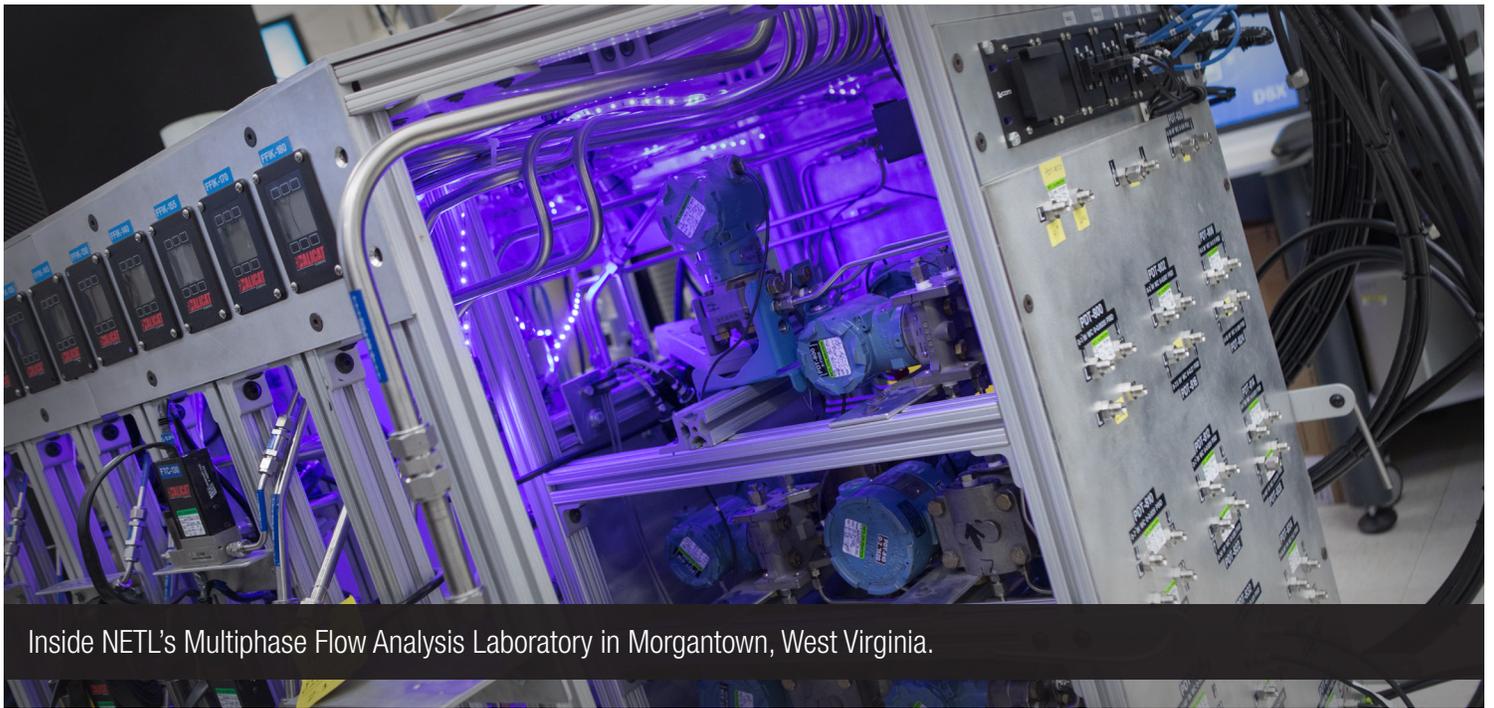
NETL's research teams rely on the advanced capabilities presented by its world-class laboratory facilities. The Multiphase Flow Analysis Laboratory (MFAL) offers researchers unique opportunities for understanding complex multiphase flows encountered in energy applications.

The equipment available in the MFAL allows scientists to validate the multiphase flow computer models through real world experiments in actual conditions. One

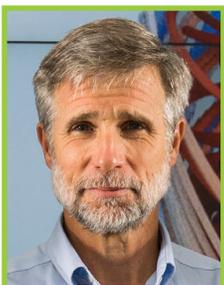
important apparatus is a circulating fluidized bed, a device used to study the hydrodynamics of solids and gases moving through several important flow regimes – from dilute riser to dense standpipe. The laboratory model is representative of commercial systems yet still allows researchers to study the details of the complex gas and particle flows encountered in this system.

It's important to study this phenomenon because many energy systems hinge on

the control of reacting gas-particle flows at high temperatures and pressures. Researchers want to find ways of designing and operating these systems for optimal performance. The MFAL facility also crosscuts many other research areas such as additive manufacturing for the creation of test prototypes. The breakthroughs enabled through this facility are changing the way energy conversion systems are designed, operated, and optimized, leading to a safer, cleaner, and more affordable energy future. ☰



Inside NETL's Multiphase Flow Analysis Laboratory in Morgantown, West Virginia.



Dr. William Rogers // William.Rogers@netl.doe.gov

Dr. William Rogers has worked at NETL for 32 years in various technical and managerial roles associated with energy research and development. He also possesses industrial experience in chemical process and steel industries. Dr. Rogers' research interests include computational fluid dynamics in combustion, gasification, fuel cells, and multiphase experimentation for model validation.

Merging Computational Modeling & Simulation Tools with the Power of Progressive Partnerships

Forging productive new partnerships involving academia, private industry and other federal research facilities that lead to new technologies for improving efficiencies in energy production is a specialty of NETL. The Laboratory's Carbon Capture Simulation Initiative (CCSI) stands as a prime example. Through cooperative partnerships, CCSI and its next generation, CCSI², produced a sophisticated toolset designed to disseminate computer simulation data for more efficient and cleaner fossil energy systems.

The CCSI Toolset provides a way of dramatically speeding up and reducing traditional risks associated with carbon capture technology for use in power plants that use fossil fuels. The CCSI partnership will help develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies through discovery, development, demonstration and, ultimately, widespread deployment to hundreds of power plants.

CCSI comprises a web of collaborators that stretch over eight states and incorporates five laboratories, five universities, and industry partners. It was formed by an organization that is exceptional in structure and scope. CCSI employs computer modeling simulations of complex systems, to advance carbon capture technology development and deployment. The type of modeling done by the initiative relies on expertise from multiple scientific disciplines, from statisticians to chemical engineers to material scientists.

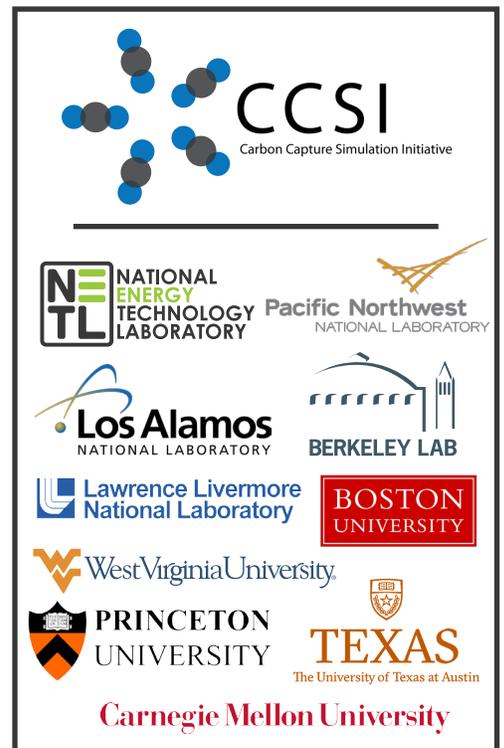
By working closely with industry from the inception of the project to identify industrial problems, CCSI ensures that the simulation tools are developed for the carbon capture technologies of most relevance to industry.

This project was the recipient of an R&D 100 award in 2016 making it an innovation judged by an independent panel to be among the most significant game-changing technologies of the year.

The Toolset is the only suite of computational tools and models specifically tailored to help maximize learning and reduce risk during the scale-up process for carbon-capture technologies. Modules were specifically tailored to guide experimental and pilot-scale testing.

Taking promising new power plant technologies from concept to commercial scale normally would take 20-30 years to manage the overall risk of the scale-up process. Ultimately, the CCSI Toolset will enable promising concepts to be quickly identified through rapid computational screening of devices and processes; reduce the time needed to design and troubleshoot new devices and processes; quantify the technical risks involved with taking technology from laboratory-scale to commercial-scale; and stabilize deployment costs by replacing some of the physical operational tests with virtual power plant simulations. The total cost savings that could be realized by using the CCSI toolset to scale up with wide deployment is estimated to be in the hundreds of millions.

Based on the success of the CCSI team in applying the toolset to industry relevant projects, DOE established CCSI² to create formal partnerships with technology developers that accelerate the development of next-generation carbon-capture technologies. These partnerships will ensure that the full benefits of intermediate-scale projects are reaped by larger-scale projects. ≡



Lynn Brickett

Lynn.Brickett@netl.doe.gov

Ms. Lynn Brickett has worked at NETL for 20 years. Lynn began her career conducting environmental research examining contaminants associated with coal by-products. She moved into Project Management where she managed projects associated with coal by-products, water, NO_x and Hg. She is currently the Technology Manager for DOE's Carbon Capture and Carbon Use/Reuse programs.

ADVANCED MANUFACTURING FOR GAS TURBINES



Ceramic cores are used during investment casting to form the internal cooling passages within the turbine airfoil, ultimately forming an array of pins and standing ribs on the inner wall of the casting, creating an engineered surface to control air turbulence and improve cooling efficiency.

By Richard Dennis

When an advanced manufacturing (AM) process is considered for application to produce a part or subsystem, it typically is evaluated for performance and cost. For example, can the AM process produce the part at a lower cost, with better performance, and be delivered on schedule? Will the new part fit seamlessly into the existing supply chain or assembly process? Cost, performance, schedule and assembly are the criteria that must be considered when a “traditionally” manufactured part is replaced by a new part from an AM process. The magnitude of the criteria, and the trade-offs between them, must be established to evaluate the efficacy of the overall AM process. If the AM process improves all of those factors, then the decision is clear.

For Mikro Systems Inc., this was exactly the case. Using its patented process, TOMO-Lithographic Molding (TOMO), advanced ceramic cores could be fabricated quicker and cheaper allowing revolutionary performance improvements for gas turbine air foils.

Mikro, a high-technology manufacturing company in Charlottesville, VA, has customers that include international high-technology companies, and government and academic institutions. It has applied TOMO and developed a unique ceramic core casting technology that uses precision, three-dimensional, lithographically-derived tooling that permits the intricate design and casting of enhanced heat transfer features for gas turbine blades.

The Mikro approach allows new internal cooling features that are not possible with current casting processes. The replacement core casting technology is intended to seamlessly integrate with established casting processes used by industry, minimizing new capital investment requirements and quickly revolutionizing the ability to enhance existing and future turbines with new blade designs.

Mikro’s technology addresses the need for rapid, cost-effective manufacturing of advanced turbine blades that will

improve the performance and reduce the cost of electricity produced by gas turbine power plants. While facilitating significantly better cooling performance, production lead time can be improved by 70 percent and development costs reduced by as much as 50 percent when compared with conventional core casting manufacturing processes. Tooling costs are also significantly reduced.

Much of the work by Mikro Systems was supported by the DOE Small Business Innovation (SBIR) program. The development and evaluation of advanced cooling features was also supported by NETL, Purdue University and Siemens Energy. Through successful development and validation of TOMO, Siemens signed a commercial license agreement with Mikro, and in 2013 opened a manufacturing facility in Charlottesville, for commercial production of ceramic cores for current products and gas turbines. ☰



Richard Dennis

Richard.Dennis@netl.doe.gov

Mr. Richard Dennis has worked at NETL for 32 years in various technical roles associated with energy research, development and strategic planning. Rich has conducted and managed R&D in gasification, fluidized bed combustion, fuel cells, gas turbines and gas stream cleanup. He is currently the Technology Manager for the DOE’s Advanced Turbines and Supercritical Carbon Dioxide Power Cycle programs.

Low-Cost Carbon Capture Technologies Investigated in Recent Paper

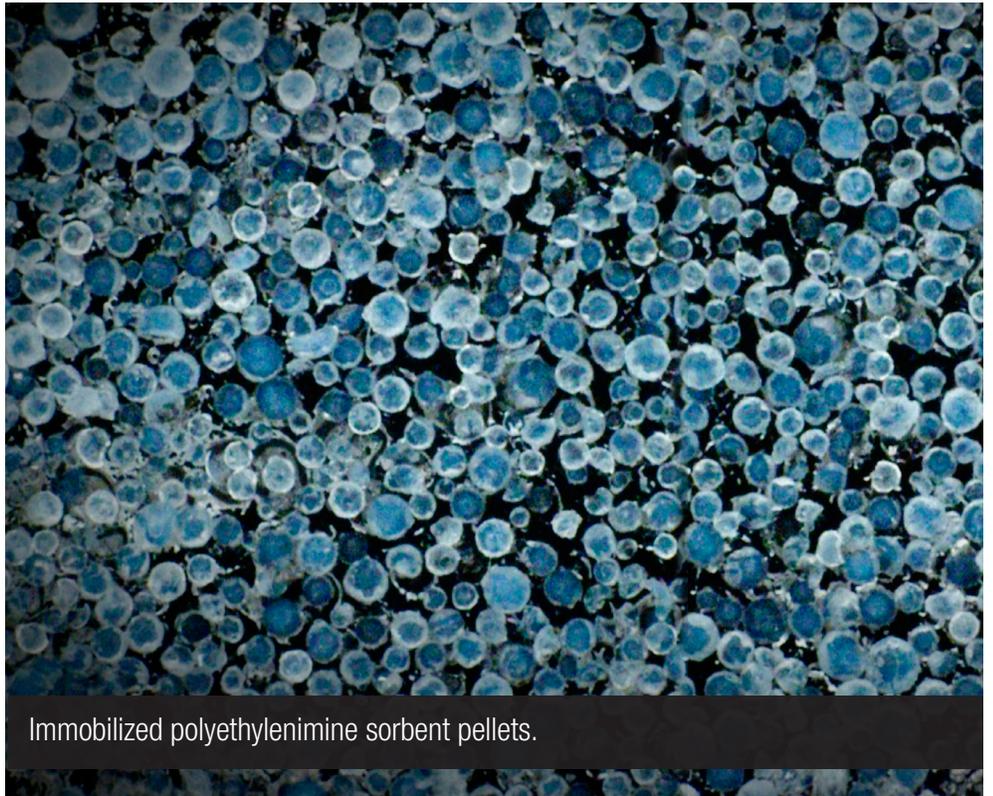
By Joe Golden // Technical Contact: Dr. Ronald W. Breault

More affordable carbon capture technologies may be on the horizon, according to a recently published article in *Chemical Engineering Research and Design*. The article presents NETL's design and development of a test unit that captures carbon dioxide (CO₂) using amine-based solid sorbents rather than traditional liquid solvents.

Solid sorbents have the major benefit of reduced cost over liquid solvent counterparts—a feature that could help put more of these CO₂ scrubbing systems into more coal-fired power plants.

As described in the paper, a test unit was built that employed fluidized bed technology, in which a solid and fluid mixture can be made to behave like a fluid that facilitates an effective flow. NETL researchers aimed to use this technology, along with specially engineered reactor components, to enable the solid sorbent to efficiently adsorb CO₂ from simulated flue gas and then be successfully transported to the regenerator.

Maintaining constant circulation of the solid sorbent was a major obstacle during experimentation, but a series of modifications to the system design



Immobilized polyethylenimine sorbent pellets.

solved this challenge. As a result, NETL researchers succeeded in increasing CO₂ adsorption while maintaining sorbent regeneration. This study provided an in-depth characterization of the amine-based solid sorbents and defined the critical parameters necessary to demonstrate their increased performance, opening the door to more research on this promising low-cost alternative to liquid solvents.

The article, “Carbon capture test unit design and development using amine-based solid sorbent,” was written by NETL researchers Ron Breault, James Spenic, Larry Shadle, James Hoffman, McMahan Gray, Rupen Panday, and ORISE intern, Richard Stehle. ☰



Dr. Ronald W. Breault // Ronald.Breault@netl.doe.gov

Dr. Ronald W. Breault is the thermal science team supervisor and a senior researcher in the Energy Conversion Engineering Directorate of NETL's Research and Innovation Center. In this capacity, he leads a team focused on reactor development for advanced energy production and emissions reduction processes. Dr. Breault has more than 35 years of industrial and government research experience in energy conversion technologies.

NETL Leadership Transition Builds on Legacy of Excellence

By Jenny Bowman

NETL wished a fond farewell to Dr. Cynthia Powell, long time director of the Lab's research and development work. Dr. Powell retired as Executive Director of NETL's Research & Innovation Center, with nearly 25 years of federal service, to take a leadership position with Pacific Northwest National Laboratory. During her tenure at NETL, Dr. Powell served as the Lab's first Deputy Director and Chief Technology Officer and created a robust environment for scientific and technical achievement benefitting the nation. Dr. Powell received a Secretary's Appreciation Award for her efforts and is well regarded

for imbuing the laboratory with her passion for collaborative technology discovery, development, and delivery. Dr. Powell received a B.S. and M.S. in ceramic sciences and engineering from Clemson University and earned her Ph.D. from Case Western University.

Continuing the tradition of excellence in leadership is Dr. Randall Gentry, who succeeds Dr. Powell as NETL's Deputy Director for Strategic Plans and Programs and acting Executive Director of the Research & Innovation Center. Dr. Gentry brings a wealth of experience in technology

and research leadership to NETL, with more than 20 years of experience working at the interface of science and engineering and a well-honed leadership approach that embraces open communication, change management, and decision making with transparency in large multi-disciplinary research organizations like NETL. He came to NETL from Argonne National Laboratory. Dr. Gentry received a B.S. in civil engineering from Memphis State University and earned his M.S. and Ph.D. in civil engineering from the University of Memphis.



Dr. Randall W. Gentry—Deputy Director, Science and Technology Strategic Plans and Programs



AWARD HIGHLIGHTS



R&D 100 Awards Honor NETL Technology

By Shaelyn Patzer

The R&D 100 Awards are often referred to as the “Oscars of innovation.” For over 50 years, R&D Magazine, a publication dedicated to research and development efforts across the globe, has been recognizing excellence in technological innovations—honoring the efforts put forth by scientists and engineers and bolstering the success of new, ground-breaking technology. In 2016, NETL was the recipient of three individual R&D 100

Awards for innovations it discovered and developed that were judged by an independent panel to be among the most significant game-changing technologies of the year. These three award-winning innovations are just a few of the Laboratory’s initiatives, which seek to discover, integrate, and mature technologies that enhance the nation’s energy security and protect the environment for future generations.

Computationally Optimized Heat Treatment of Metal Alloys

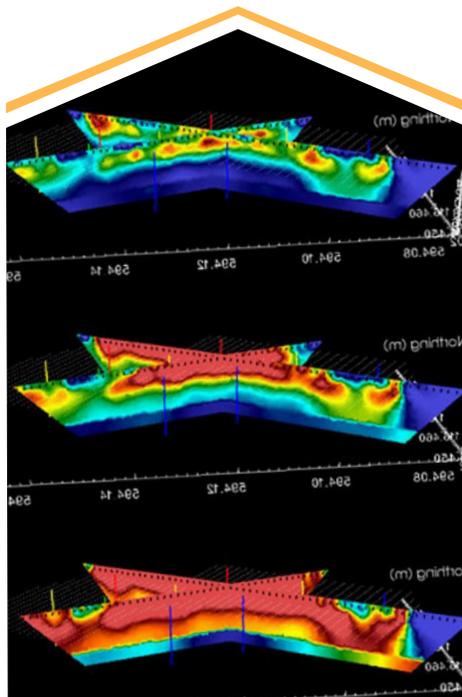
Conventional processes for homogenizing metal alloys are trial-and-error in their approach, resulting in increased process cost and limits to the possible paths that may be explored. NETL’s Computationally Optimized Homogenization Heat Treatment Process provides an easy method to optimize heat treatment to achieve the desired degree of homogenization with a minimum of furnace time.

The primary application for this technology is for alloys that are exposed to extreme environments, including heat-resistant alloys or those needing corrosion/oxidation resistance. A properly homogenized alloy will not only perform better but will also have an extended lifecycle.



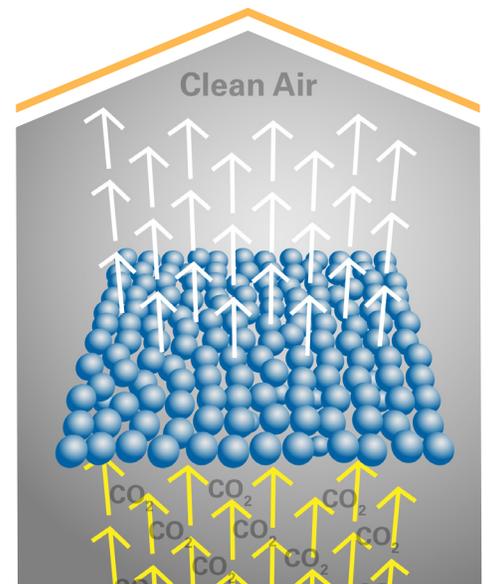
Carbon Capture Simulation Initiative (CCSI) Toolset

The CCSI Toolset is the only suite of computational tools and models specifically tailored to help maximize learning and reduce risk during the scale-up process for carbon-capture technologies. This is critically important because carbon-capture pilot projects represent an expensive, limited opportunity to collect the data necessary to move to commercial scale. Each module in the toolset is specifically tailored to properly guide experimental and pilot-scale testing to acquire important data.



HVAC Load Reduction Technology for Commercial Buildings

Leveraging the laboratory’s proven expertise in sorbent technology development, NETL partnered with enVerid Systems to create unique multi-functional sorbents that can capture carbon dioxide (CO₂) and volatile organic compounds at ambient temperatures and which regenerate below 60 degrees Celsius. With these new sorbents, enVerid was able to develop an HVAC load reduction (HLR) technology, which uses a module integrated into existing HVAC systems to scrub the air of dangerous indoor air contaminants. This technology helps to reduce energy use and lower costs by recirculating already-cooled inside air. ≡





AWARD HIGHLIGHTS



NETL Researcher Alexandra Hakala Received U.S. Government's Highest Honor for Early Career Research Scientists

By Gerrill Griffith

Dr. Alexandra Hakala, (a geochemist at NETL), has been named as a recipient of the Presidential Early Career Award for Scientists and Engineers (PECASE)—the highest honor the U.S. government can bestow on scientists or engineers in the early stages of their research careers.

The awards were announced by the White House on January 9, 2017. Awardees are selected for their pursuit of innovative research at the frontiers of science and technology and their commitment to community service as demonstrated through scientific leadership, public education, or community outreach. The awards are conferred annually by the president and are based on recommendations from participating government agencies.

Dr. Hakala was selected for her impressive accomplishments, innovation, and technical leadership. Her work has focused on increasing the efficiency of domestic energy production while minimizing the environmental impacts associated with the use of fossil fuel.

Dr. Cynthia Powell, executive director of NETL's Research and Innovation Center said, "Ale is an excellent geochemist, and her research is making a tremendous impact on our understanding of how fossil energy development can impact the environment. She is a tireless advocate for sustainable energy systems, and an inspiration to her colleagues at



the laboratory and her friends in the community. It is easy to see why she was selected to receive the PECASE award." Dr. Hakala joined NETL in 2008 and has made contributions to research on groundwater chemistry, carbon capture and storage, and shale gas development. Her environmental geochemistry skills have greatly improved understanding of toxic and nontoxic metal mobility in ground water systems, long-term geologic storage of CO₂, and safe natural gas development—important to long-term energy resource development.

Dr. Hakala serves as one of the Energy Department's representatives on the Technical Subcommittee for the Interagency Oil and Gas Task Force. She also serves as a Science Ambassador for the National Academies of Science and Engineering, sharing her enthusiasm and dedication to her profession and

encouraging others to pursue careers in the science and technological fields. In addition, Dr. Hakala mentors students and postgraduate researchers through the ORISE research associate program at NETL, and serves as an external committee member for PhD dissertation and MS thesis committees.

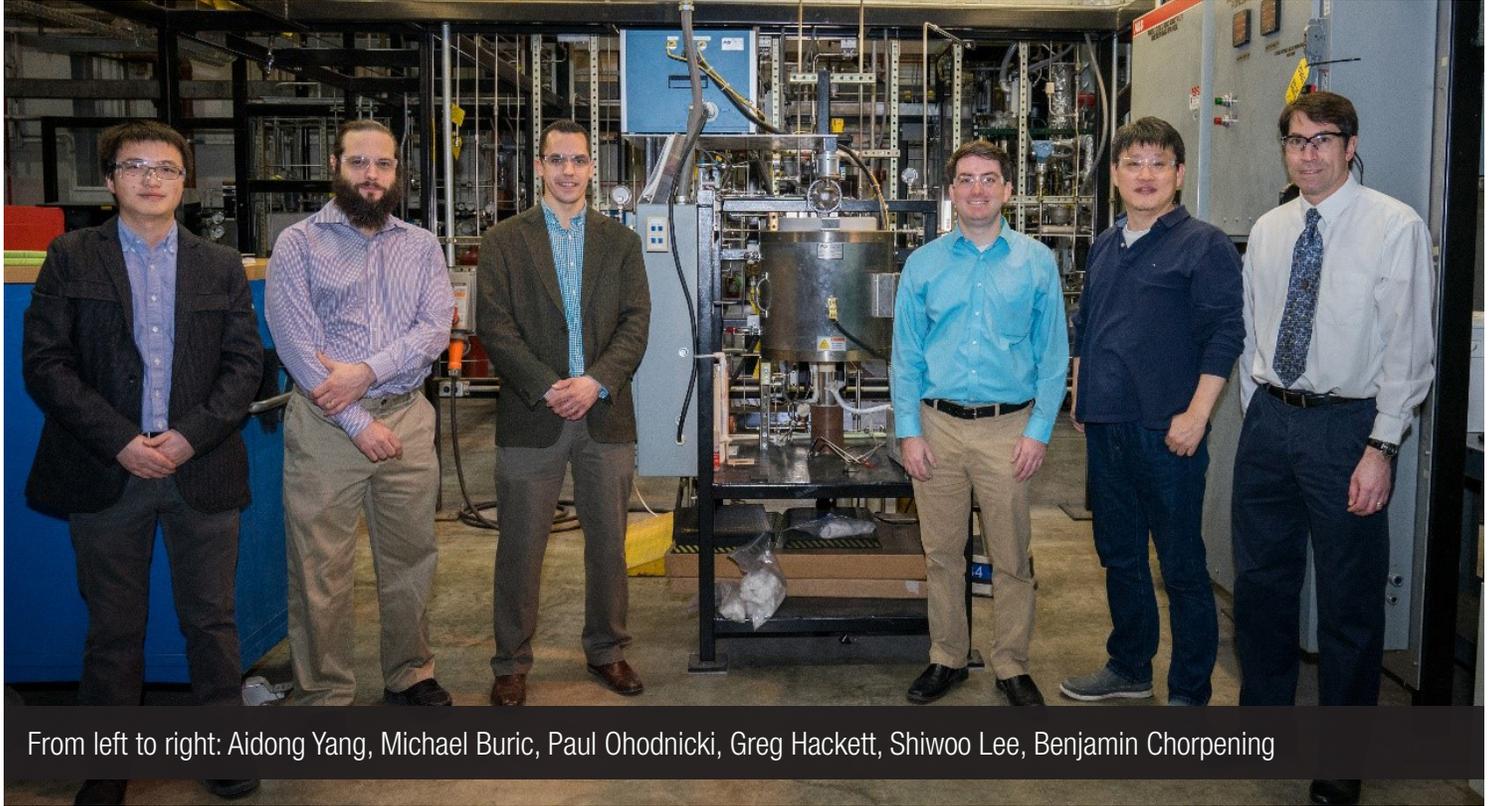
PECASE Awards have encouraged and accelerated American innovation to grow the economy and tackle scientific challenges. In addition to Dr. Hakala, this year's award recipients are from the U.S. Departments of Agriculture, Commerce, Defense, Education, Energy, Health and Human Services, Interior, and Veterans Affairs; the Environmental Protection Agency; the National Aeronautics and Space Administration; the National Science Foundation; Smithsonian Institution; and the intelligence community. ≡



AWARD HIGHLIGHTS



NETL Research Team Wins Carnegie Science Award



From left to right: Aidong Yang, Michael Buric, Paul Ohodnicki, Greg Hackett, Shiwoo Lee, Benjamin Chorpeneing

By Shaelyn Patzer

An NETL research team has been honored with a Carnegie Science Award in recognition of work supporting manufacturing and materials science.

In a collaboration with the University of Pittsburgh, NETL assembled a multi-disciplinary team tasked with developing high-performance optical sensors capable of operating in harsh environments, such as those found in fossil-fuel power generations systems including solid oxide fuel cells (SOFCs).

Western Pennsylvania relies on the coal and natural gas industry, which provides jobs and stimulates the local economy while also serving as primary energy sources for the region. However, the environments in fossil fuel-based power generation and

advanced manufacturing processes can be extreme, with temperatures ranging from 800 °C to 1,600 °C and highly oxidizing, reducing, erosive, or corrosive conditions. Sensor technology is meant to monitor and maximize the efficiency of industrial and power generation processes, but it often fails under these conditions—limiting the ability of operators to optimize efficiency, minimize environmental impacts, and transition to next-generation processes.

The research team set out to develop high-performance sensors capable of withstanding the environmental factors to which previous sensor technology would succumb. Particular attention was paid to the development of sensors compatible with SOFC systems—a promising, emerging technology for electricity

generation, which can be fueled by coal-derived syngas. The team demonstrated a new optical sensor technology capable of measuring temperatures and gas compositions inside an operating SOFC. This cutting-edge technology holds promise for future commercialization and industrial adoption, resulting in regional economic growth and job creation.

The Carnegie Science Awards were created by the Carnegie Science Center two decades ago to recognize and promote outstanding science and technology achievements in western Pennsylvania. The achievements of the multi-disciplinary team assembled between NETL and the University of Pittsburgh are remarkable and will benefit the region for decades to come. ☰

NETL Crowns Regional Science Bowl Champions

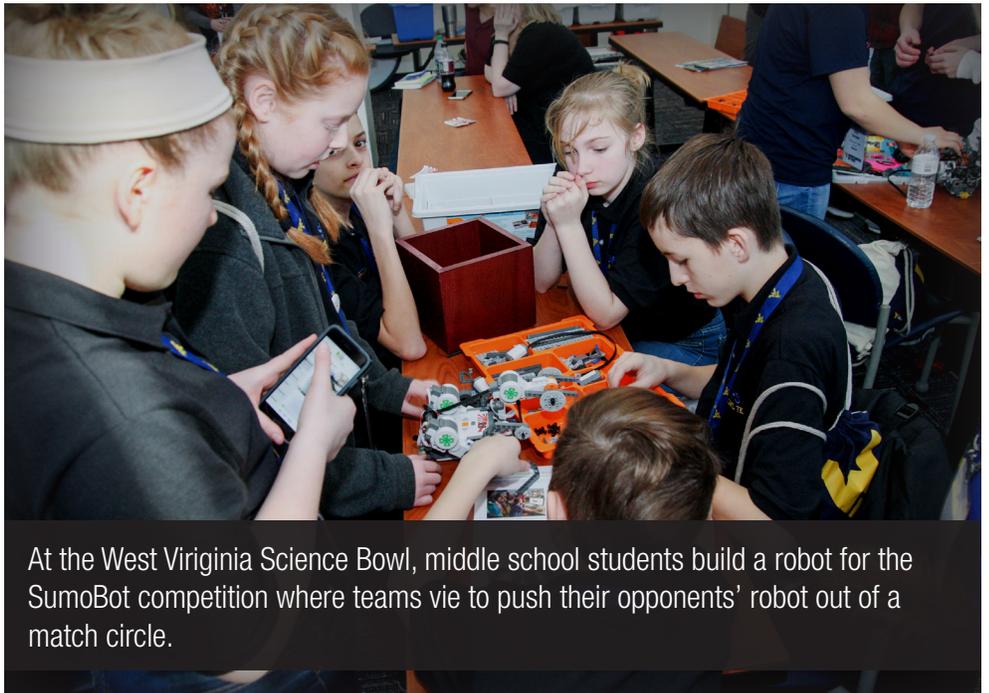
By Jenny Bowman

Each year, NETL hosts regional science bowl competitions in West Virginia and Southwestern Pennsylvania to determine each state's champion teams. Science Bowl is just one of many NETL educational outreach activities, but it draws numerous enthusiastic volunteers from across the sites. For 2017, competitions were held in conjunction with West Virginia University and the Community College of Allegheny County. Four teams were crowned victorious: **Suncrest Middle School** and **Morgantown High School** from West Virginia, and **Winchester Thurston School** and **North Allegheny Intermediate High School** from Pennsylvania. The teams earned an all-expenses paid trip to represent their states at the National Science Bowl in Washington D.C.

The Science Bowl is academically vigorous and conducted in a round-robin question and answer format. Students must be both quick witted and quick handed, buzzing in to answer questions before the opposing team. This tournament style offers participants a fast-paced and energetic experience, different from traditional academic competitions that revolve around completing and presenting projects. Science Bowl also encourages the students to learn how to strategize as a team, and encourages adults (from parents to teachers) to take a more active role in STEM education. In addition to the actual competition, NETL's events feature special guests and engineering activities and have been an effective way to encourage student engagement in science, technology, engineering, and math.



Students face off against sponsors and NETL leadership in a practice round to kick off the SWPA Final Competition.



At the West Virginia Science Bowl, middle school students build a robot for the SumoBot competition where teams vie to push their opponents' robot out of a match circle.



U.S. DEPARTMENT OF
ENERGY



1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochran's Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

Program staff are also located in **Houston, TX**
and **Anchorage, AK**.

Visit us: www.NETL.DOE.gov



@NationalEnergyTechnologyLaboratory

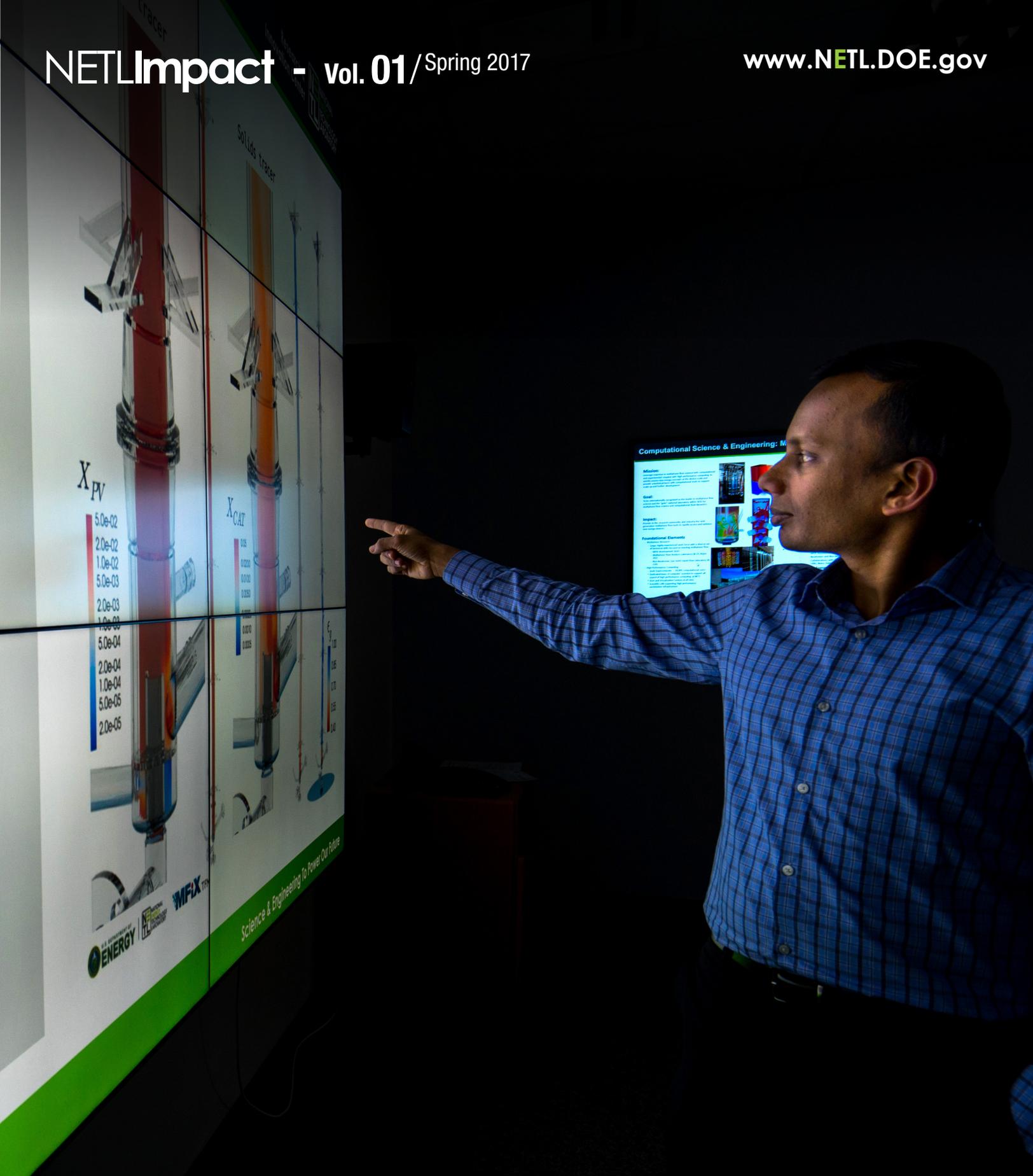


@NETL_DOE



@NETL_DOE

Customer Service: **1-800-553-7681**



Computational Science & Engineering: M
Mission
Goal
Impact
Fundamental Elements



U.S. DEPARTMENT OF
ENERGY

