NETL EDGE

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NEW USES FOR THE SAME OLD COAL

NATIONAL ENERGY TECHNOLOGY LABORATORY

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NETL Research Embodies the 21st Century Meaning of Innovation

Time, circumstance and societal and scientific progress can change the meaning of common words over generations.

For example, in the 1600s, the word "innovation" was a pejorative term that symbolized rebellion, revolt and heresy.

By the time the Industrial Revolution occurred, the concept of innovation became associated with science and the invention of new products, machines, industries and jobs.

Today, innovation is now also associated with creative thoughts, new ideas and new methods.

Now, innovation is a process and an outcome.

At NETL, innovation in its modern meaning is at the heart of sophisticated energy research and development that spans a wide array of technology areas related to energy and the effort to enhance the nation's energy security and ensure continued economic growth.

NETL has compiled stories for the summer 2019 edition of Edge magazine that stand as examples of the innovation that drives our progress and outcomes. Research and development stories explain how NETL:

- Developed technologies to convert coal, one of the nation's most abundant natural resources, into valuable products that can create more jobs and industries.
- Advanced carbon capture technologies that use new mixed matrix membranes at reduced costs compared to conventional carbon capture approaches.
- Used computer modeling capabilities to help the U.S. Department of Energy solve a problem that threatened the start-up of a sophisticated integrated waste treatment unit designed to treat radioactive liquid waste.
- Improved enhanced oil recovery processes in Alaska that can help strengthen the viability of the Trans-Alaska Pipeline System.

We hope you will be entertained and enlightened with this edition of our magazine and continue to follow our Laboratory's progress.

ON THE COVER

NETL has a long affinity with coal, beginning with the Lab's foundation in 1910 and its focus on mine safety. Today, NETL continues its research in coal. Despite a downward trend in using this abundant domestic resource for electricity production, there is vast potential to use coal as a feedstock for manufacturing high-valued carbon products and materials. NETL is a leading innovator in research to develop new technologies for these applications. **Read more on page 6.**

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NEW USES FOR THE SAME OLD COAL

By Jenny Bowman

NETL Innovation Is Creating New Applications for America's Most Abundant Domestic Energy Resource

Researchers at NETL are making big strides in the form of tiny dots — coal-based graphene quantum dots that are useful in a range of energy applications such as catalysis, electronics, light emitting diodes (LEDs), sensors, solar cells and more.

The work is part of NETL's research to manufacture common products and materials from domestic coal, which is breathing new life into one of our nation's most abundant, affordable natural resource industries. Most importantly, NETL innovation is finding new applications for coal that do not generate greenhouse gases.

Coal is an abundant natural resource in the United States, and although it's typically associated with energy production, its utility is far more wide ranging. Coal, or additives from coal, can be used to manufacture or improve the performance of a wide range of in-demand consumer products, from carbon fiber to textiles to cements, plastics, water filtration devices, battery materials, 3D printing materials — to name just a few examples.

> "We're focusing on using coal to make carbon nanomaterials, such as graphene, which can be used directly, or which can be used as an additive in composites and coatings to improve performance."

Christopher Matranga, Ph.D., a researcher in NETL's Functional Materials Team, who leads the Manufacturing High-Value Carbon Products from Domestic Coal Initiative, said the Lab is a leading innovator in research aimed at developing new coal-based technologies for applications not previously considered by industry.

"We're focusing on using coal to make carbon nanomaterials, such as graphene, which can be used directly, or which can be used as an additive in composites and coatings to improve performance," Matranga said.

At the foundation of the research are carbon nanomaterials, which made a grand entrance in the 1980s with the discovery of C_{60} fullerene (a molecule of carbon in the form of a hollow, soccer-ball-shaped sphere). But, carbon nanomaterials are not widely commercialized, in part, because they are very expensive and in limited supply.

"These commercialization barriers partially arise from the cost of the petroleum, natural gas, and graphite feedstocks used, as well as

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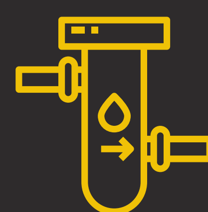
JUST A FEW SURPRISING USES FOR COAL

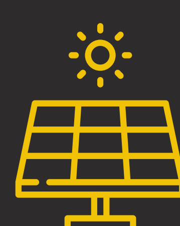
LEDs

3D Printing Materials



Water Filtration

Battery Materials



Solar Cells

> “We started with a coal feedstock costing about one penny. With just a few hours of processing we converted this penny’s worth of coal into 1 liter of graphene quantum dots in water, which has a current market value of approximately $50,000."

processing approaches commonly used to make carbon nanomaterials,” Matranga explained. “Coal offers unique opportunities to bring down the feedstock and processing costs of carbon nanomaterials, which would increase their use in innovative products.”

Coal is cheaper per ton of carbon than the petroleum, natural gas, or graphite feedstocks used to make carbon nanomaterials. The processes for turning coal into graphene-type nanomaterials are simple, inexpensive and scalable. From this foundation, coal-based manufacturing has the potential to drive new economic opportunities for jobs, products and markets.

Coal feedstocks at $30 to $60 per ton could be converted, through NETL’s innovative manufacturing processes, into carbon products selling for much more. For example: carbon fiber and structural composites can cost $140,000 per ton, specialty 3-D printing materials can cost $700,000 per ton, and graphene nanomaterials can cost over $100,000,000 per ton, based on current nanomaterial prices.

To realize these economic benefits, NETL is working to address cost and supply issues that prevent commercialization. The tiny graphene quantum dots are making a big impact in that effort. Graphene quantum dots are small nanoparticles with sheet-like structures that are one carbon atom thick and a few hundred atoms in diameter. The unique size of these materials imparts amazing optical and electronic properties to these coal-based derivatives. Their chemical composition and small size impart unique properties that make graphene quantum dots useful for LEDs, photocatalysis, solar cells and more.

NETL researchers have successfully processed anthracite, bituminous and sub-bituminous coal samples from regional partners in Wyoming, Kentucky, Virginia, and Pennsylvania to manufacture small graphene quantum dots suspended in water, which the research team is now evaluating for use as additives for cements and plastics.

In one application, researchers found that coal-based graphene improved the corrosion resistance and mechanical properties of cements for everyday construction and paving applications.

With additional processing methods that were developed by NETL, researchers can produce large, micron-sized graphene materials as dry, solid powders. These forms of graphene are being investigated for use as electrode materials for batteries, water filtration materials and for chemical sensing applications.

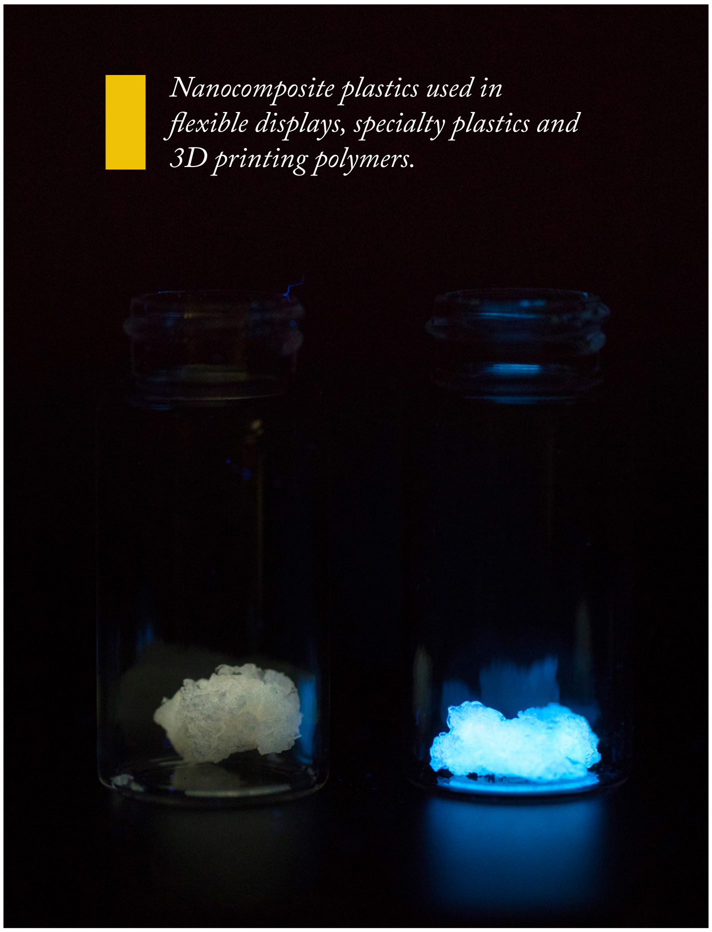
Although graphene nanomaterials are currently too expensive to use in most commercial applications, NETL research is illustrating that the manufacturing costs can be brought down to levels comparable with other commercially used additives. Research at NETL is already illustrating how coal can make a difference in the price of nanomaterials.

“We started with a coal feedstock costing about one penny,” Matranga explained. “With just a few hours of processing we converted this penny’s worth of coal into 1 liter of graphene quantum dots in water, which has a current market value of approximately $50,000. This work shows that coal-based feedstocks will reduce manufacturing costs and are easy to process into extremely high value materials.”

Looking forward, NETL is working closely with private industry to build upon its innovations. For example, in June 2018, NETL launched a partnership with Ramaco Carbon to collaborate on innovative projects that use coal as a manufacturing feedstock for high-value products. A cooperative research and development agreement signed June 7, 2018, enhances NETL’s materials engineering and manufacturing capabilities by allowing Lab researchers access to the coal-based manufacturing and research facilities being developed by Ramaco Carbon near Sheridan, Wyoming.

Once completed, Ramaco Carbon will operate the world’s only fully integrated coal-based research, development

Carbon quantum dots used in LEDs, paints/pigments and 3D printing.



Nanocomposite plastics used in flexible displays, specialty plastics and 3D printing polymers.

and production facility. Ramaco's areas of interest include the use of coal to create carbon-based product precursors and resins, rare earth elements from coal and coal byproducts, feedstock production for carbon-based products, and production of advanced carbon materials — all areas in which NETL has extensive expertise. The Lab is working to establish programmatic research activities in coal-based manufacturing, which will be aided by the agreement.

As research and innovation continues to drive opportunities, coal-based industries could provide a more affordable alternative to the ubiquitous petroleum-based materials that are used to make consumer products and specialty materials that are critical for the United States' energy independence and security. The research is another example of how NETL is developing technological solutions to America's energy challenges. ≡

ARCTIC RECOVERY

First-of-Its-Kind Enhanced Oil Recovery Project to Tap into Vast Arctic Resources

By Joe Golden

> "The ANS and the Arctic region in general are **brimming with potential fossil energy resources**, and the groundbreaking research by NETL and its partners is helping to capitalize on this important opportunity."

Beginning on the coast of the Arctic Ocean and stretching to the mountains of the Brooks Range, the Alaska North Slope (ANS) holds enormous petroleum reserves. Some estimates put Alaska's total store of high-viscosity crude oil, known as heavy oil, at upward of 30 billion barrels, and most of this (20-25 billion barrels) lies undeveloped within the ANS. This immense fossil energy resource could play a vital role in meeting the nation's energy needs, so NETL is committed to enabling the development of this key energy asset.

The Lab began managing a $9 million project in June 2018 that is investigating the first-ever polymer flood for heavy oil on the ANS in the Milne Point Field 30 miles northwest of Prudhoe Bay. Polymer flooding refers to the technique of adding a polymer to the flood water to increase the fluid's viscosity. A thicker fluid will help to better push out the oil during production. This technique is a form of enhanced oil recovery, which increases the amount of oil that can be recovered from a reservoir. Success in this project could pave the way for commercialization of the ANS' vast resources and strengthen the viability of the Trans-Alaska Pipeline System (TAPS).

The primary goal of the project is to acquire scientific knowledge and gain polymer flood performance data, via the first-ever advanced technology-based field pilot to optimize the polymer flood design. This research will address critical gaps in the understanding of enhanced oil recovery for not just the ASN, but across the nation, ultimately enhancing the nation's energy foundation and security.

In addition to the research value, this project also has significant positive implications for TAPS, which transports crude oil from the ANS to the port at Valdez. TAPS can transport up to 2 million barrels of oil per day, but output has significantly diminished since its peak in the early 1980s. When less oil flows through the pipeline, its efficiency decreases because the oil is colder and flows more slowly. Ultimately, the pipeline would have to cease operations if the daily flow fell below an economically sustainable level, so the development of technology to increase production in ANS could help boost flow back to this important pipeline.

Furthermore, work like this will help to position the nation as a global leader in unconventional oil and natural gas resource development technologies and ensure that the nation benefits from the maximum value of all its natural resources. With increased oil production in the Arctic region, Alaska will benefit from more jobs and more residual income from petroleum sales.

"This project is a notable example of how NETL is working toward assuring American energy dominance," NETL Technology Manager for Oil and Gas Jared Ciferno said. "The ANS and the Arctic region in general are brimming with potential fossil energy resources, and the groundbreaking research by NETL and its partners is helping to capitalize on this important opportunity."

MEET NETL DIRECTOR

Brian Anderson

By Gerrill Griffith

“I am a firm believer that the director works for the people of NETL and that means making sure that the hundreds of focused and productive energy researchers and program managers have the tools they need to move the mission of the Laboratory forward.”

Shortly after Brian Anderson, Ph.D., was named the new Director of NETL by DOE Undersecretary for Fossil Energy Steven Winberg in November 2018, a Pittsburgh Post-Gazette reporter interviewed him about his ascension to the leadership chair of the nation's only national laboratory dedicated to fossil energy research. The headline that appeared on the resulting article summed up Anderson's past and present succinctly: “New NETL Director Brian Anderson has coal in his blood, and now in his job description.”

To accurately carry the headline's analogy further, you would have to add geothermal energy, methane hydrates, deepwater oil and gas exploration and a host of other energy topics to that busy bloodstream of his.

The grandson of a West Virginia coal miner, Anderson grew up in Ripley, West Virginia, where he was the third generation in his family to work at the aluminum manufacturing facility in Jackson County. In the middle of last century, the then Kaiser Aluminum smelter was built in West Virginia because of the economics of mining coal from the earth to power the residential and industrial needs of the nation.

Blessed with a rich tenor voice, the future scientist once trifled with the idea of becoming an opera singer before the mysteries and challenges of science beckoned him down another path.

At West Virginia University, where he earned a bachelor's degree in chemical engineering and graduated in 2000, his appetite for research was only whetted. He went on to earn a master's degree and doctorate in chemical engineering from the Massachusetts Institute of Technology (MIT) in 2004 and 2005 respectively and grew his energy research expertise beyond traditional fossil energy topics from gas hydrates and geothermal energy possibilities to carbon capture.

He returned to West Virginia University in 2006 as a faculty member to teach and conduct research. He brought a deepening curiosity about the state and nation's energy future and how new technologies and economic development opportunities could breathe new life into the once burgeoning coal fields where he spent his formative years. He was fascinated by the prospects of unlocking the energy potential in new technologies like geothermal energy and the promise of new sources deep under the earth's oceans.

At the same time, he maintained close contact and pursued research with MIT colleagues. For example, he was a co-author of an important MIT report called “The Future of Geothermal Energy: Impact of enhance Geothermal Systems on the United States in the 21st Century.” The report is considered the seminal report on enhanced geothermal systems and the future of geothermal energy.

With a growing body of work attracting the attention of key national organizations, Anderson was selected to the National Academy of Science's 2010 Frontiers of Engineering Education Workshop, named the College of Engineering and Mineral Resources Teacher of the Year, and served as the opening keynote speaker at the inaugural 2010 Gordon Research Conference on Gas Hydrates.

He collaborated with NETL on a range of energy issues

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and, at the same time, received additional recognitions. For example:

- He served as NETL's coordinator for the International Methane Hydrate Reservoir Simulator Code Comparison Study that helped researchers understand the potential of the crystalline structures of ice that contain methane gas and are found on ocean floor sediments.
- In 2011, Anderson was awarded a Secretary Honor Achievement Award from the Secretary of Energy for his role on the Flow Rate Technical Group — a team of national laboratory researchers who worked to respond to the Deepwater Horizon oil spill.
- In 2011, working with colleagues from Stanford University, MIT, Cornell, the University of Utah, Southern Methodist University and the University of Nevada, he co-founded the National Geothermal Academy.
- In 2014, he was selected as a National Academy of Science's Kavli Fellow as part of their Frontiers of Science Program.

Recently, Anderson answered Edge magazine questions about his work and vision for NETL. Here are the questions and his answers:

Edge: What is a typical day at the facility like?

Anderson: With a talented and experienced executive staff, I manage the complete NETL complex including delivery and execution of our mission and national programs in fossil energy. I am a firm believer that the director works for the people of NETL and that means making sure that the hundreds of focused and productive energy researchers, and program managers have the tools they need to move the mission of the Laboratory forward.

The mission of NETL — to discover, integrate, and mature technology solutions to enhance the nation's energy foundation and protect the environment for future generations — is complex, so no two days are precisely alike. Every day, our team implements a broad spectrum of energy and environmental research and development programs that enable domestic coal, natural gas and oil to economically power our nation's homes, industries, businesses and transportation while protecting our environment and enhancing our energy independence.

My job, by interacting with our research teams, the Department of Energy leadership, and partners in the field, is to make sure the mission is advanced by coordinating resources, securing needed equipment and expertise and managing the overall needs of the researchers. That remains challenging because of the wide-reaching nature of our work in coal, natural gas and oil technologies; contract and project management; analysis of energy systems; and international energy issues. In addition to applications in fossil energy, the NETL team applies their talents in research and project management and execution to other programs across the Department of Energy portfolio, such as in Energy Efficiency and Renewable Energy, the Office of Electricity, and the Office of Cybersecurity, Energy Security, and Emergency Response. It is my role to work across the Department as well as coordinate our efforts across the full complex of the Department's 17 national laboratories.

Our NETL project portfolio also includes R&D conducted through partnerships, cooperative research and development agreements, financial assistance, and contractual arrangements with universities and the private sector. Together, these efforts focus a wealth of scientific and engineering talent on creating commercially viable solutions to national energy and environmental problems. It is my honor and challenge to work with our team to help keep those obligations running on time, on budget and vital for the nation.

Edge: What are the key research projects currently underway at NETL and what is their potential impact?

Anderson: Let's look at just five with long-range implications that have found their way into the public discussion over the past few months:

- In January 2019, we announced that an ambitious computational modeling project led by NETL identified membrane materials that will make carbon capture more affordable for coal-fired power plants, reducing the cost to less than $50 per metric ton of carbon dioxide (CO_2) removed. That's within reach of the U.S. Department of Energy's goal of $40 or less for pulverized coal plants. NETL will

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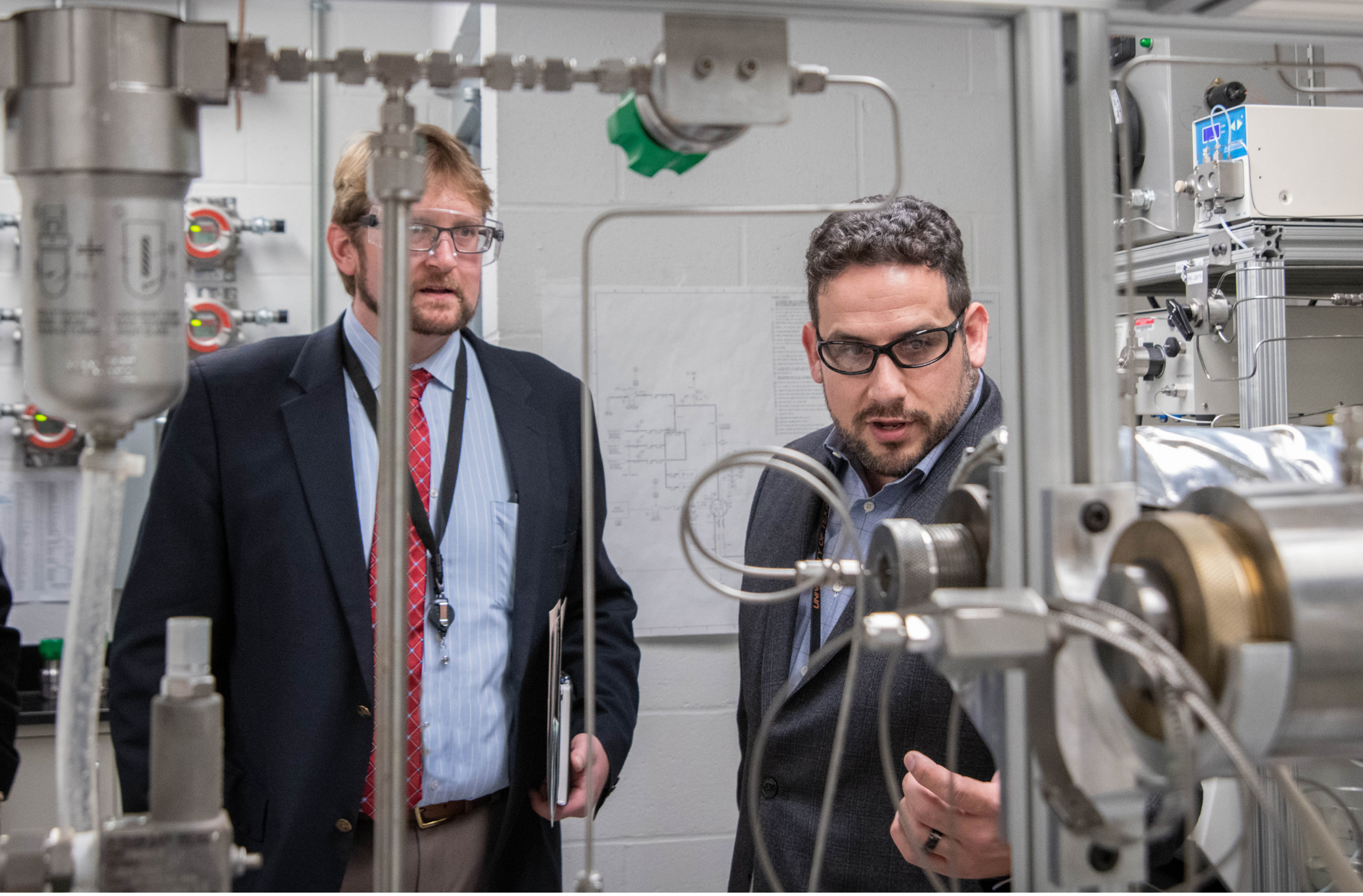


rely on the project's results to focus and refine ongoing efforts to develop innovative membranes that effectively capture CO_2 at an affordable cost as the Lab continues its work to ensure clean, reliable use of the nation's abundant fossil energy resources.

- In December 2018, we announced that Data gleaned from three years' worth of research from the Marcellus Shale Engineering and Environmental Laboratory (MSEEL) — a research partnership funded by NETL — will guide more extensive new testing at a second well site. The work will advance hydraulic fracture stimulation techniques that were pioneered by NETL researchers years ago. A key objective of the field test is to develop advanced completion capabilities that can be applied to other areas of the Marcellus Shale play to improve resource recovery efficiency. The project will yield a tool set and analytical techniques that can be used on individual wells or pads to improve future resource recovery efficiency throughout the region.

- Also, in December 2018, we announced work being done by NETL research to measure and analyze geochemical signals — information that lies buried in the liquids, gases and mineral deposits of the earth — to keep tabs on groundwaters and produced waters at Texas oil fields where CO_2 was injected as part of enhanced oil recovery operations. Across the U.S., when efforts to extract oil with conventional means have diminished, one commonly employed strategy involves enhancing oil recovery with CO_2 injection. NETL researchers study the effects of CO_2 enhanced oil recovery thousands of feet below ground by examining the chemistry of oilfield produced waters, in this case within the Permian Basin in Texas. The work is helping to describe and predict how injecting CO_2 affects the producing formation and to ensure that changing field practices are not causing unwanted migration into groundwaters and that changes in the baseline geochemistry from normal operations are not confused as signals of leakage.

- In November 2018, NETL researchers made progress creating more efficient and environmentally benign electrochemistry technologies that turn CO_2 and excess energy back into valuable chemicals and fuels. One of the challenges associated with power plant economics is excess energy generation. Fossil fuel power plants can't simply be turned off and on as demand increases or decreases. This picture becomes more complicated when renewables are added to the grid because wind and solar don't generate a steady supply of power; it's intermittent as weather conditions vary throughout the day. As a result, over-supply of energy becomes an issue. Storing electricity is not practical because of high costs, low-efficiency and poor reliability of methods for retaining energy that is generated during off peak hours. Electrochemistry can be used to convert CO_2 from fossil fuel power generation into chemicals like carbon monoxide, hydrocarbons, and alcohols. NETL is designing the catalysts needed to create those products.
- In October 2018, we talked about rare earth elements (REEs) — an integral component of high-technology products from smart phones and lasers to computer hard drives, medical devices and national defense systems — and how our researchers have developed a way to effectively filter water from oil and natural gas well flowbacks, industrial waste streams, acid mine drainage and even municipal drinking water to recover valuable REEs.

Edge: How does working with academic, industry and other partners help accelerate research at NETL?

Anderson: Working with industry helps identify immediate research needs that we can then help address through focused research. Working with experts in academia not only allows us to harvest new ideas for conversion into solid research results, it also allows us to help prepare the next generation of energy researchers to carry our progress forward. Then, there is the technology transfer piece to partnerships with the private sector. Fostering connections and forming collaborations through research partnerships and licensing agreements is the route to realizing the true value of technology and encouraging entrepreneurship in the United States. Without technology transfer, innovation would flounder in the gap between the laboratory and the market. Our technology transfer activity is focused on fostering innovation in any way possible, matching the most promising new inventions and technologies to the right people for commercialization. NETL's technology portfolio contains a broad range of innovations that have resulted from research in areas such as carbon capture and storage, mercury capture, fuel cells, sensors and controls, computational modeling, and materials science, among many others.

Edge: What does the future of energy research look like?

Anderson: My 2019 vision for the immediate future of NETL calls for us to:

- Expand existing and build new external partnerships as a vehicle for innovation, commercialization and dissemination of the knowledge and technology we build together. I believe effective partnerships are the most efficient and effective way to conduct informed research and then make sure the results are put to work in support of a bright energy future.
- Use the Laboratory's well-known and expanding competencies and facilities to image, characterize, model, engineer and manage the development and use of geologic systems that help the U.S. master the subsurface — the origins of more than 80% of the nation's energy needs. This frontier of science is ripe for the application of artificial intelligence and machine learning to make a tremendous impact for future generations.
- Create an enhanced energy infrastructure that accommodates new demands, emergent markets and changing energy consumption patterns with carbon capture, utilization and storage innovation and modified pipeline networks to reduce environmental impacts, enhance reliability and assure robust energy delivery.
- Increase the efficiency of technologies that convert the stored energy in fossil resources into heat, power, fuels and chemicals through research that focuses on greater system flexibility and resiliency, rapid technology deployment, and reduced pollutants, waste and freshwater use.
- Develop and promote evolving NETL technologies for recovery of REEs from coal, coal byproducts and water resources for use by U.S. industries for consumer products and defense technologies. ≡

NETL Modeling Effort Helps Solve Start-Up Challenges at Nuclear Waste Treatment Facility

By Joe Golden

In a cost-saving computer modeling effort, NETL assisted in solving a critical technical issue at the DOE Office of Environmental Management (EM) Integrated Waste Treatment Unit (IWTU), preventing a long-term delay of start-up operations.

IWTU is an Energy Department facility designed to treat 900,000 gallons of radioactive liquid waste by heating and essentially drying it into a solid granular material for long-term storage. The heat required in this process is created by a piece of equipment called a denitration mineralization reformer (DMR), in which coal, steam, air and oxygen interact. Because this mixture contains multiple phases of matter (i.e., solids and gases), an understanding of multiphase flow is critical for design and troubleshooting.

"NETL is a globally recognized leader in multiphase flow," said NETL researcher Chris Guenther, Ph.D., who worked on the project. "So, when IWTU encountered an issue with their DMR, they called on the Lab's expertise."

Using the Lab's Multiphase Flow with Interphase eXchanges (MFiX) software suite, NETL researchers demonstrated that the problem — solids accumulating or agglomerating in the lower regions of the DMR — was inherent to the DMR's design and could not be overcome under normal operating conditions.

"Once we figured out the reason for the problem, we realized that the reactor would need to be redesigned," said Guenther.

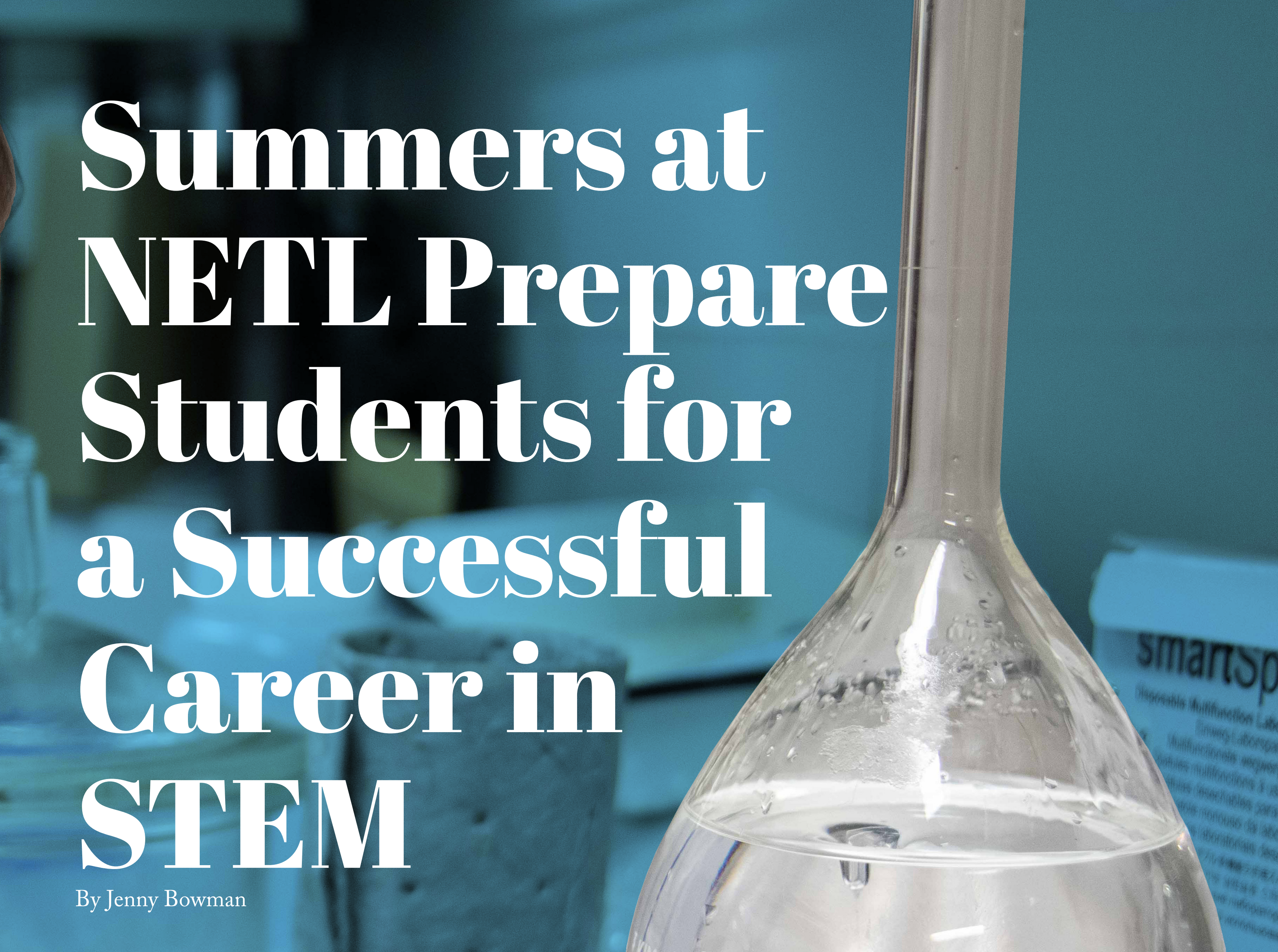
NETL researchers then began a highly successful collaboration with EM support contractor Flour Idaho and the Idaho National Laboratory to create MFiX simulations that screened three alternative reactor designs under a range of conditions. This partnership was an exceptional example of teamwork in which a DOE contractor leveraged a variety of powerful resources, including cutting-edge modeling tools, the expertise of two national labs and thousands of computational cores on NETL's supercomputer Joule, to efficiently solve a difficult technical issue. The team created exceptional value, as the task was accomplished with only two full-time employees working for eight months on the modeling effort.

The simulations were pivotal in the design selection and guided both sub-scale and full-scale experiments. This computational approach eliminated the need to test each design under a range of operating conditions at full scale, saving tens of millions of dollars in the design phase alone. IWTU made the selected design change to the DMR, which was successfully tested with no evidence of further accumulation of solids.

"This was the first nuclear application of MFiX software using a reacting two-fluid model," said Guenther. "This project's success has really demonstrated the versatility of the modeling tool."

This is just one example of how NETL's computational modeling efforts are working to not only better predict and optimize the performance of fossil fuel power generating systems but are also finding new applications throughout DOE.

NETL researchers Yong Liu and Chris Guenther study MFiX-generated simulations in the Lab's Visualization Center.



Summers at NETL Prepare Students for a Successful Career in STEM

By Jenny Bowman

What's special about joining NETL for the summer? Hands-on experience in the lab and life-long connections with mentors and fellow innovators.

Each year, NETL hosts research associates from the Mickey Leland Energy Fellowship (MLEF) and Consortium for Integrated Energy Systems in Engineering and Science Education (CIESESE) programs. The Lab's summer internships also include opportunities within NETL's Professional Internship Program and Postgraduate Research Program.

For students, an internship with NETL is an opportunity to collaborate with world-class scientists and engineers on leading-edge research projects in state-of-the-art facilities. For the Lab, it's an opportunity to educate the next generation of energy researchers and ensure NETL's mission — to discover, integrate and mature technology solutions to enhance the nation's energy foundation and protect the environment for future generations — continues on a productive course to serve the American people.

June 3, 2019, NETL welcomed 35 students from the MLEF program and eight participants from the CIESESE program for 10-week internships. The students joined NETL from universities all across the country, from Maryland to California, Puerto Rico to Colorado and many locations in between. They came with a common goal: to get time in the lab, make life-long connections, and develop the skills they will need to make an impact in the world of energy.

Named after the late Congressman Mickey Leland of Texas, the MLEF program was created in 1995 to improve opportunities for under-represented students in STEM fields and strengthen a diverse pipeline of future STEM professionals. The program has mentored several hundred talented students from across the nation and provided participants the unique opportunity to gain hands-on research experience with fossil energy. Students

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gain insight into how DOE is developing solutions to meet the energy challenges of the future, including policy and regulation, project finance, and strategic performance measures at the Office of Fossil Energy headquarters. The program will wrap up in August with a technical forum in which the participants present their research findings.

CIESESE interns' research focuses on the infrastructure, technologies, and procedures to generate, store and distribute energy for use by individual consumers and by the public and private/industrial sectors. The program directly supports DOE's goal to build a sustainable professional and academic pipeline, particularly professionals from the Hispanic community, ready to take on the challenges of current and future energy systems.

Brianna O'Neil-Hankle is a participant in the MLEF program. She is an environmental science student from Allegheny College and is building on her experience performing water chemical tests. She is applying those skills to meaningful research with NETL mentor Christina Lopano, who works with the Lab's Geochemistry Team. O'Neil-Hankle said she hopes to improve her laboratory skills and get outside her comfort zone in the lab.

"Lopano's research is a perfect next step for me to grow and learn in the STEM field," O'Neil-Hankle said. "I hope this experience will help me decide my future career path. I have always loved nature and wish to pursue a career protecting the environment. Specifically, I plan to focus on reducing the impacts of natural gas drilling on groundwater."

MLEF research associate Marina McCue, a mechanical engineering student at Northern Arizona University, came to NETL with a deep passion for energy.

"I want to learn and gain first-hand experience working with energy, and I hope to pursue a career working with renewable, sustainable or clean energy technologies," she said. "This summer internship with NETL will give me the experience I need."

McCue's passion for energy stems from her desire to contribute toward mitigating climate change.

"I believe one of the greatest and most important challenges society currently faces is climate change and it is my plan to contribute to finding a viable solution…by making traditional energy technologies cleaner, increasing system efficiencies, reducing energy consumption or conducting research with carbon dioxide recapture capabilities," she explained.

McCue's summer research is in collaboration with mentor Larry Kincell of NETL's R&D Engineering and Facility Operations Team.

CIESESE research associate Bernardo Restrepo-Torres joins NETL from the Universidad Ana G. Mendez (Puerto Rico), where he studies mechanical engineering. At NETL, he is collaborating with mentor David Tucker in the Hybrid Performance (Hyper) facility. Here, Restrepo-Torres applies his engineering knowledge toward the development of new power generation technologies.

"It is very exciting to be part of the solution of the state-of-the-art and future generation systems that are developing in NETL facilities," he said. "As a former researcher in the Hyper lab, I consider this system very exciting because of the number of phenomena involved. It represents a challenging opportunity for anyone who loves research in energy systems."

Restrepo-Torres, who interned at NETL in 2017, hopes to run experiments related to system identification, obtain data, and develop methodologies that help in the operation of the hybrid system.

"I hope that my skills in developing algorithms and my knowledge in energy system integration go further after this experience," he said.

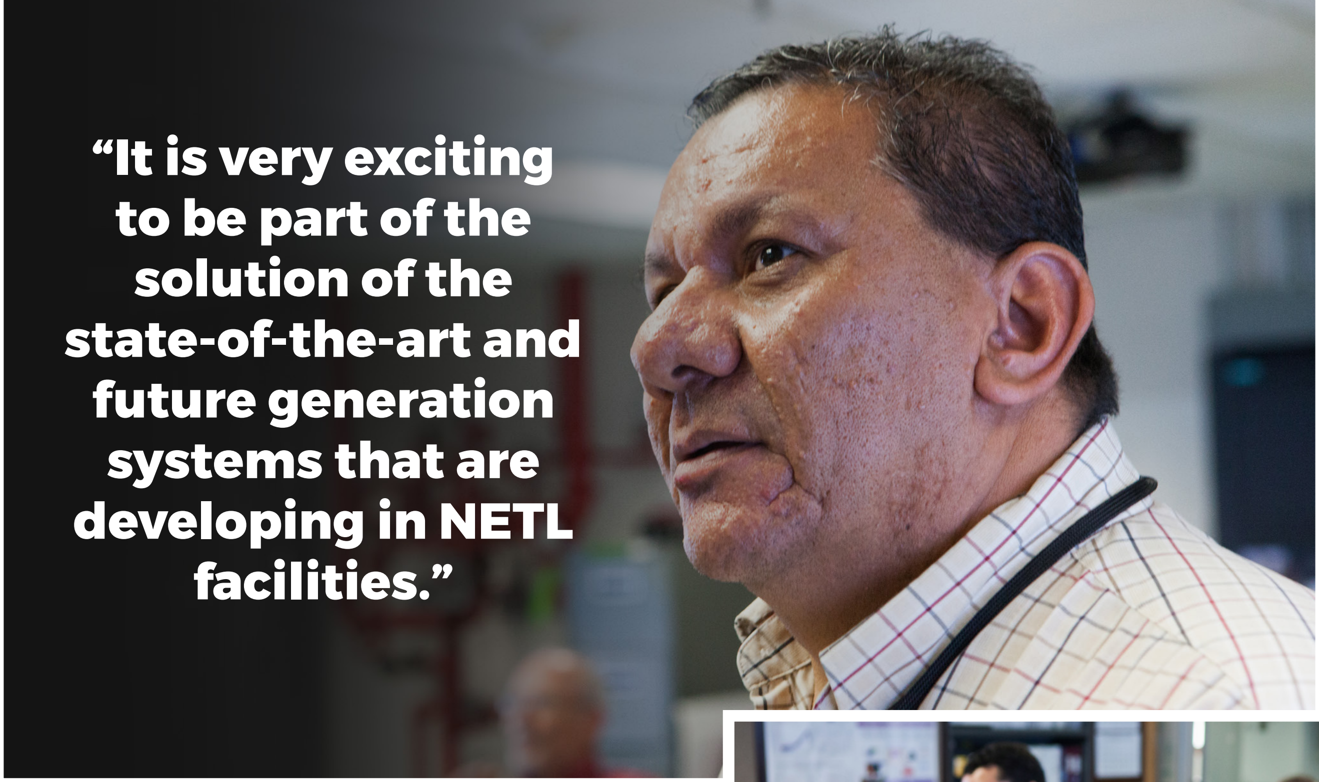
NETL's Hyper facility is a cyber-physical system that couples a simulated fuel cell with an actual turbine to study a range of phenomena, from improving power infrastructure to developing control strategies for the reliable operation of these highly efficient systems.

At NETL's Albany lab, MLEF research associate Emily Davis is interning with Rigel Woodside, who works with NETL's Innovative Energy and Water Processes Team. A student at Rutgers University in New Brunswick, Davis sought a summer research opportunity at NETL because she wanted to conduct research in the lab environment and make meaningful contributions toward finding technology solutions to today's energy challenges.

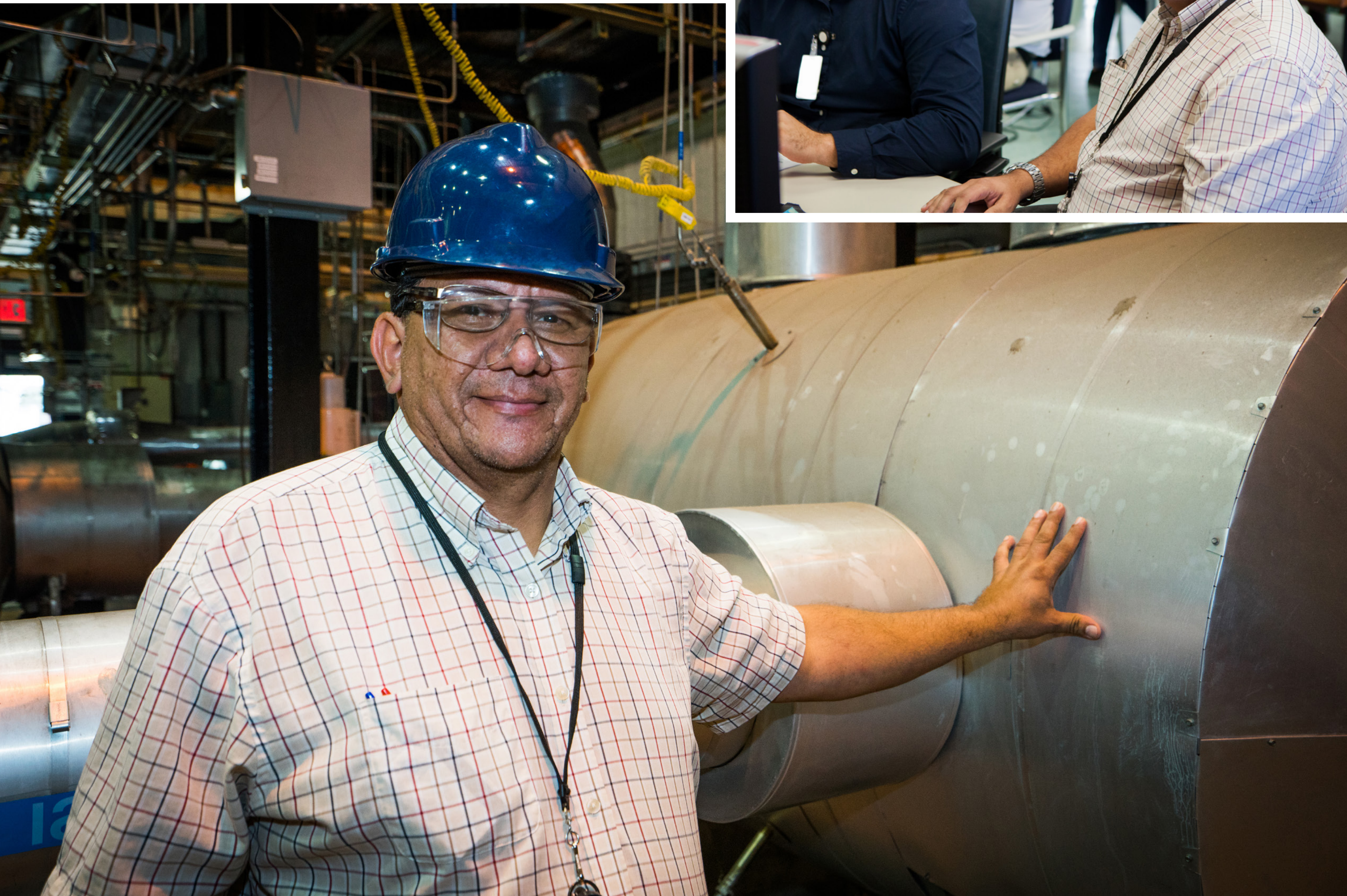
"I hope to become more skilled in running simulations and better understand the goals of the Department of Energy as a whole," Davis said. "I love mechanical engineering because it forces me to draw new conclusions every day, and those conclusions are eventually going to contribute to a positive impact on the world and its development."

Davis said she hopes to make improvements on sustainable energy solutions for people around the world.

These research associates are only a few of the talented students who are conducting important research with NETL's innovation experts. The contributions of these up-and-coming scientists and engineers are making positive impacts in NETL's research to provide breakthroughs and discoveries that support home-grown energy initiatives, stimulate a growing economy, and improve the health, safety and security of all Americans. ☰



CIESESE student Bernardo Restrepo-Torres, a professor from the University of Turabo is working in the HYPER Lab at NETL in Morgantown, W.Va. The purpose of the project is to develop a supervisory control scheme for load following in a hybrid system.



Computational Tools Accelerate Development of Innovative Membranes to Cut Cost of Carbon Capture

By Cassie Shaner

As the U.S. energy landscape evolves, the nation's abundant coal resources continue to provide valuable energy that helps meet growing demand at an affordable cost. Coal accounted for more than 27% of U.S. power produced in 2018, supplying more than 1.1 trillion kilowatt hours of electricity. Yet, as energy demand continues to rise around the world, cost-effective carbon capture technologies are needed to boost the viability of the nation's coal-fired power fleet and ensure responsible stewardship of the environment.

Carbon capture technologies reduce harmful greenhouse gas emissions by capturing carbon dioxide (CO_2) from coal-fired power plants; however, existing options are often costly for industry and consumers. Polymer-based membranes used to separate CO_2 from post-combustion flue gas offer simplicity for conventional pulverized-coal plants, with reduced up-front and long-term costs. However, capturing significant amounts of CO_2 using current technology remains cost-prohibitive, with costs estimated at about $60 or more per metric ton of CO_2 captured.

NETL is working to cut that cost by exploring the use of mixed matrix membranes (MMMs), which combine sturdy polymers with inorganic crystalline particles that enhance selectivity and permeability. An ongoing project is using powerful computational tools to screen more than 1 million potential MMMs, evaluate their properties and estimate the associated cost of carbon capture (CCC) — ultimately indicating that costs could be reduced to less than $50 per metric ton of CO_2 removed using MMMs.

Bridging atomic-level models to real-world challenges is what first attracted Jan Steckel, Ph.D., to NETL about 16 years ago. She appreciated that NETL, as an applied lab, offered an opportunity to use her education in theoretical chemistry to solve timely problems. Now, Steckel is collaborating with the University of Pittsburgh's Chris Wilmer, Ph.D., and NETL colleagues Olukayode Ajayi, Ph.D., and Samir Budhathoki, Ph.D., to accelerate development of innovative carbon-capture membranes that boost performance and affordability using the Lab's advanced computational tools. Their work was highlighted on the cover of the April 2019 print edition of the prestigious journal *Energy and Environmental Science*, featuring artwork by Steckel's 13-year-old daughter.

The cover art for the April 2019 edition of the high-impact Energy & Environmental Science journal was created by Anastasia Piacentini, daughter of NETL's Jan Steckel. Each petal features the chemical structure of a metal-organic framework.

"We just keep trying to make materials that are better," Steckel said. "We're trying to discover crystalline materials that can make mixed matrix membranes that are more permeable and selective than existing polymers."

DEFINING MMM RELATIONSHIPS

An ideal carbon-capture membrane is both highly selective and highly permeable, meaning that it captures CO_2 while allowing other gases to pass through. Though membranes fabricated from pure polymers are cheap and possess good mechanical properties, their ability to be both highly selective and highly permeable is limited.

Metal-organic frameworks (MOFs) are crystalline materials made from metal or metal oxide subunits joined with organic linking molecules. MOF particles incorporated with polymers in MMMs can either enhance or worsen membrane performance, depending on the structure of the MOF. A polymer must be paired with a complementary MOF to create a membrane that achieves optimal results, but millions of possible MOF structures exist. To add an additional challenge, it is not feasible to measure the gas permeation properties of an MOF in the lab. NETL's computational effort addresses these challenges by enabling researchers to predict the properties of a large number of MOFs as well as determine which MOF-polymer pairings will create the best MMMs.

NETL's world-class supercomputing tools offer the capability to screen a vast number of MOFs for use in MMMs, understand the relationship between MOF and MMM properties and connect atomistic calculations with process simulations to predict carbon-capture costs. Steckel's team used databases of real and hypothetical MOFs and experimental properties for nine pure polymers to predict properties for more than 1 million MMMs.

The computations allowed researchers to draw useful conclusions about the performance of MMMs, separate from cost considerations. For instance, many MOFs can be used to create MMMs that improve upon the performance of pure polymers for carbon capture. MOFs offer the most significant gains when paired with highly permeable polymers. To achieve an MMM with the highest possible CO_2 permeability, a polymer with the highest possible

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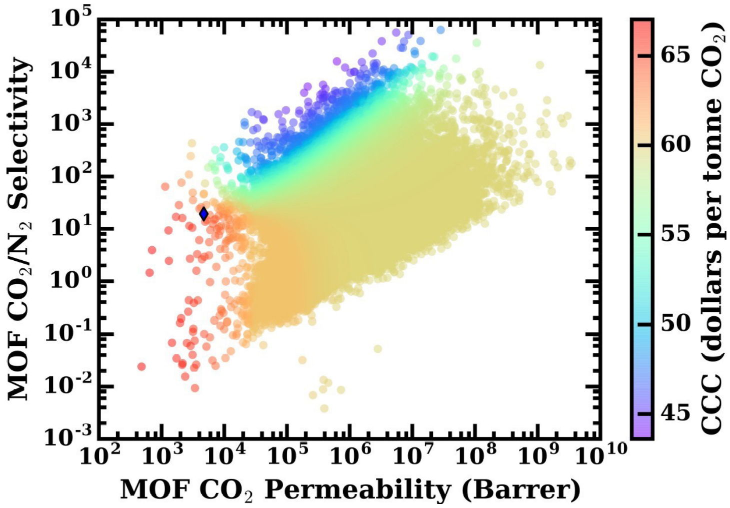

This chart depicts selectivity as a function of CO_2 permeability for the hypothetical MOF database. Color denotes the predicted CCC for a MMM generated with the MOF and PIM-1 polymer. The performance of a membrane composed of PIM-1 alone ($64 per metric ton of CO_2 removed) is indicated by a blue diamond.

permeability must be paired with an MOF that is at least 10 times more permeable than the pure polymer. For an MMM with the highest permeability and selectivity, a highly permeable polymer must be paired with an MOF that is at least 100 times more permeable and 1,000 times more selective.

CALCULATING COSTS

The techno-economic analysis portion of the project estimated the CCC for about 1 million MMMs, indicating that 1,153 MMMs could achieve a CCC of less than \$50 per metric ton of CO_2 removed. In comparison, the CCC for the highly permeable PIM-1 polymer alone is estimated at \$64 per metric ton. The promising estimates highlight the potential for MMMs to meet a DOE goal to cut the CCC to less than \$40 per metric ton for pulverized coal power plants.

Design and operating conditions — such as temperatures, pressures, flow rates, etc. — were optimized for 12 distinct selectivity and permeance points. Those conditions could be adjusted to further cut costs — much like turning a knob, according to Steckel. She said flexibility and creativity can improve upon the process.

The techno-economic evaluation relied on several assumptions, including a fixed three-stage carbon-capture configuration. That means three membranes would be used for carbon capture, each with the same permeability and selectivity. Steckel noted that this configuration was selected because it has been demonstrated to be effective for post-combustion carbon capture, but it could be changed in future studies to reduce the cost further — by altering the number of membranes or using different membranes at different points in the process, for instance.

Beyond the CCC, the techno-economic analyses reiterated the importance of choosing an MOF that complements the polymer. The bottom line? "We believe that it is possible to create membranes that would bring the cost of carbon capture down dramatically," Steckel said.

FUTURE WORK

The collaborative NETL-led team is now working to narrow and refine its analyses based on the project's initial discoveries. Steckel explained that the simplest computational methods were used initially to model a vast number of possible MMMs. Now that researchers have a better idea of how to pair MOFs and polymers to create MMMs with promise, they can start with fewer MOFs — perhaps 6,000 or less — and run more complex calculations to better predict performance and cost for MMMs.

Rather than simply talking about how molecules interact, Steckel is using her background in theoretical chemistry to generate practical results that will steer investments to incorporate MOFs into polymer-based membranes for carbon capture. Several of the thick-film MMM materials created at NETL have been tested using actual flue gas at the National Carbon Capture Center in Wilsonville, Alabama, where they showed stable performance compatible to testing results from NETL's lab-based measurements. NETL is working with flat-sheet and hollow-fiber support materials to create thin-film composite materials featuring MMMs as the selective layer.

The development of MMMs with exceptional permeability and selectivity offers possibilities to cut capital costs, downsize equipment and curb emissions at coal-fired power plants. Once deployed at commercial scale, these innovative membranes will help to boost the long-term viability of the nation's abundant fossil fuel resources and ensure access to clean, reliable and affordable energy for all Americans.

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