Vol. 03/ 2021 Issue 01

NETL EDGE

A Publication of the U.S. Department of Energy's National Energy Technology Laboratory

NET-ZERO CARBON ELECTRICITY

Decarbonization through Integrated Energy Systems

NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL EDGE

Vol. 03/ 2021 Issue 01

NATIONAL ENERGY TECHNOLOGY LABORATORY

ON THE COVER

NETL is driving innovation and delivering solutions to reach a goal of net-zero carbon electricity. By advancing integrated energy systems that combine renewable energy, carbon-based energy production and large-scale energy storage systems with effective, affordable carbon capture systems, the Lab is enabling transformation to a sustainable energy future.

DIRECTOR'S MESSAGE

As scientists and engineers around the world focus their talent and expertise on combatting the climate crisis, NETL is at the forefront of this critical fight. Globally, now, more than ever, we face an urgent need to develop and deploy technologies that will ensure affordable, abundant and reliable energy that drives a robust economy and protects national security while enabling environmental sustainability and managing carbon across the full life cycle.

As is the case with any complex research initiative, multifaceted challenges have emerged in the battle against climate change, and NETL research continues to explore and advance multiple solutions. The following technologies are key players in this effort: Turbines; solid oxide fuel cells; solid oxide electrolysis cells; carbon capture technologies; and processes for converting energy resources and wastes from coal and natural gas production into value-added products. Just as high-impact ideas form from collaboration and diversity of thought, high-impact energy systems are enabled through leveraging many promising technologies. NETL is well position to deliver solutions. Our researchers are world-renowned experts in carbon capture, computational modeling and simulation, and other leading-edge tools to accelerate the commercialization and, ultimately, widespread deployment of the technologies required for decarbonization.

In this issue of NETL Edge, we are excited to feature work supporting integrated energy systems (IES), which serve as an important area of energy efficiency that has the potential to meet the climate goals of a carbon emission-free power sector by 2035 and a net-zero carbon economy by 2050.

IES harness multiple energy sources that work cooperatively to provide environmentally sustainable, reliable and cost-effective power and energy services. Hybrid energy systems that incorporate wind, solar, nuclear and carbon-based energy sources can effectively provide energy while meeting social and environmental objectives. Such an approach allows for the integration of clean power generation of renewable sources with the reliability of carbon-based energy conversion, which improves the electric grid's power quality, efficiency and reliability while enhancing energy security and dramatically reducing fossil fuel use and CO_2 emissions.

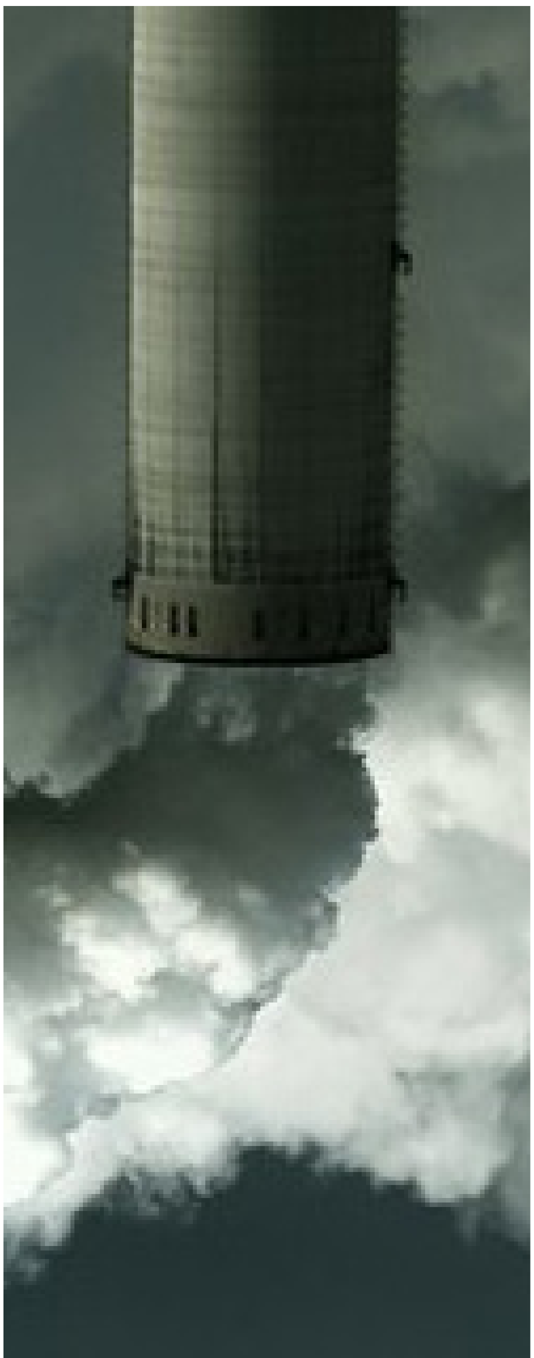
We have before us an unprecedented opportunity to take our research portfolio to a new level — ushering in a new era of clean energy production that will improve the environment and the lives of people around the world, especially those communities that have been disproportionately impacted by the climate emergency.

Sustainable energy technologies that protect the environment have long served as the foundation of our work, and NETL is now engaging on a level where the reach of our mission is more critical than ever before. I'm optimistic and extremely proud of NETL's contributions to this effort and our researchers' hard work to deliver integrated solutions to enable transformation to a sustainable energy future. As you'll read in the following pages, our researchers' world-class expertise is leading innovation in areas like carbon capture technologies, computational modeling and simulation, reaction engineering and catalysis, materials and energy conversion, to name just a few.

Saving the planet is not a trivial task, but it's a challenge NETL is well-prepared to tackle. After reading the following stories, you'll be as excited as I am that NETL is uniquely positioned for this critical opportunity to drive clean energy innovation and deliver solutions.

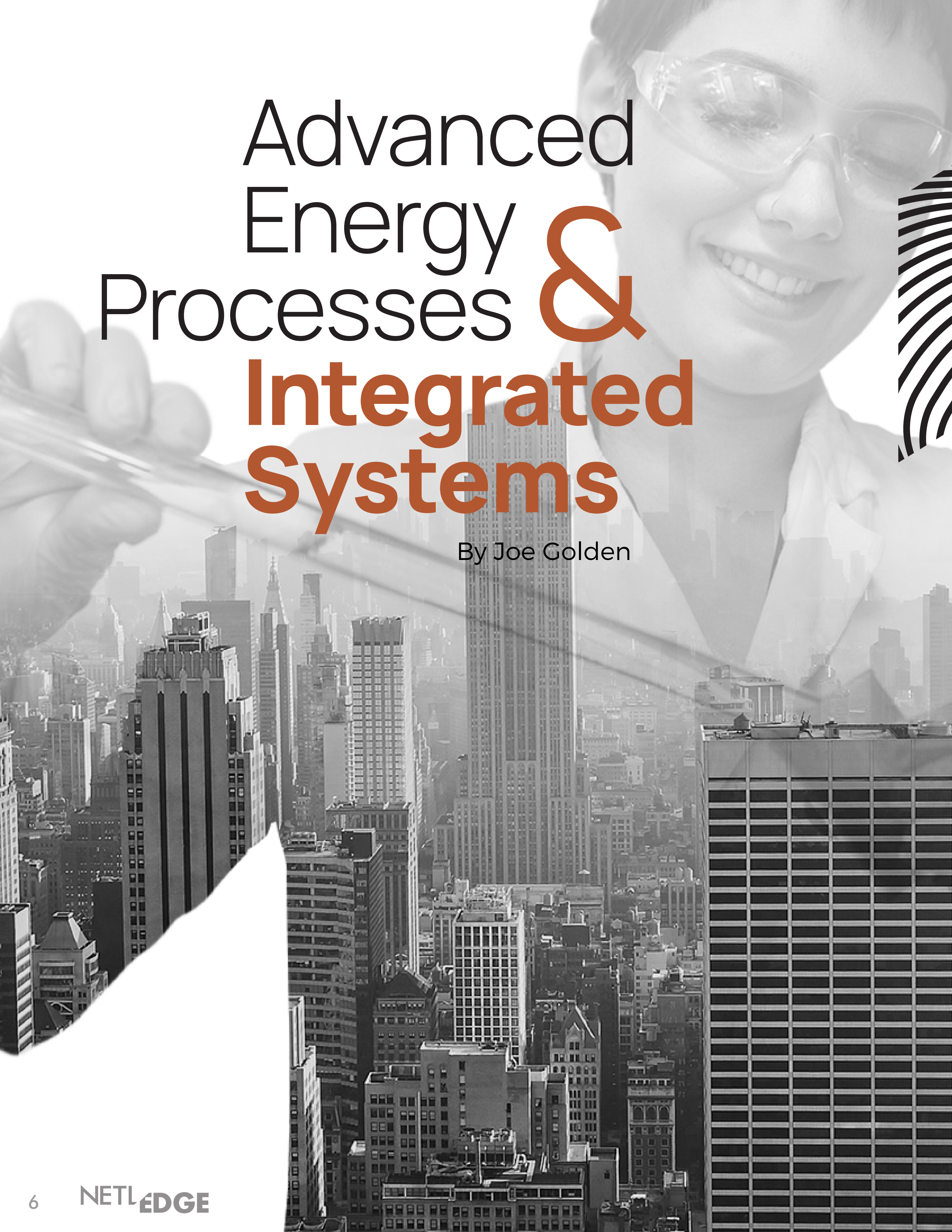
Brian J. Anderson, Ph.D.
Director, NETL

TABLE OF CONTENTS



Advanced Energy Processes & Integrated Systems

By Joe Golden



Building a Strong Foundation for Integrated Energy Systems through NETL Energy Conversion Research

With the ability to simultaneously leverage diverse energy generators and produce multiple products like heat, electricity and high-value chemicals, integrated energy systems (IES) could lead to paradigm shifts in clean energy production. However, the development of these systems will require new methods and approaches to ensure reliable and resilient energy conversion processes.

One type of future IES would couple power generation from renewable sources like solar and wind with carbon-based energy conversion systems. In such an IES, the variability of renewable energy could be partially mitigated though energy storage, but other power generation systems will likely be required to fully supplement electricity produced by renewable sources.

For example, a natural gas-fired power plant fitted with a carbon capture system could be coupled with solar and wind energy production, which would allow electricity to flow day or night, regardless of wind speed. Unfortunately, traditional high-efficiency natural gas combined cycle power plants are not designed to come online quickly and operate intermittently. Their highest efficiencies arise when running continually and at full capacity.

Frequent load cycling (i.e., switching on and off) and load following (i.e., varying output) in response to supplementing intermittent renewable energy takes a heavy toll on power plant components, which can lead to expensive repairs and shutdowns. To succeed, IES will require improved understanding of how cycling operation of one integrated component impacts the operations of the others, and what added measures — control-wise and hardware wise — are needed to reduce risk of component degradation.

Every day, NETL is working to mature advanced technologies that can offer IES the flexibility and reduced emissions required for reliable and resilient net zero carbon electricity. Research in solid oxide fuel cells (SOFCs) and solid oxide electrolysis cells (SOECs) along with various advanced turbine technologies have emerged as just a few of many possible candidates for successfully designing and building future IES. Furthermore, fuel conversion technologies such as those that convert natural gas to higher-value products will add even more value to these systems and further contribute to decarbonization.

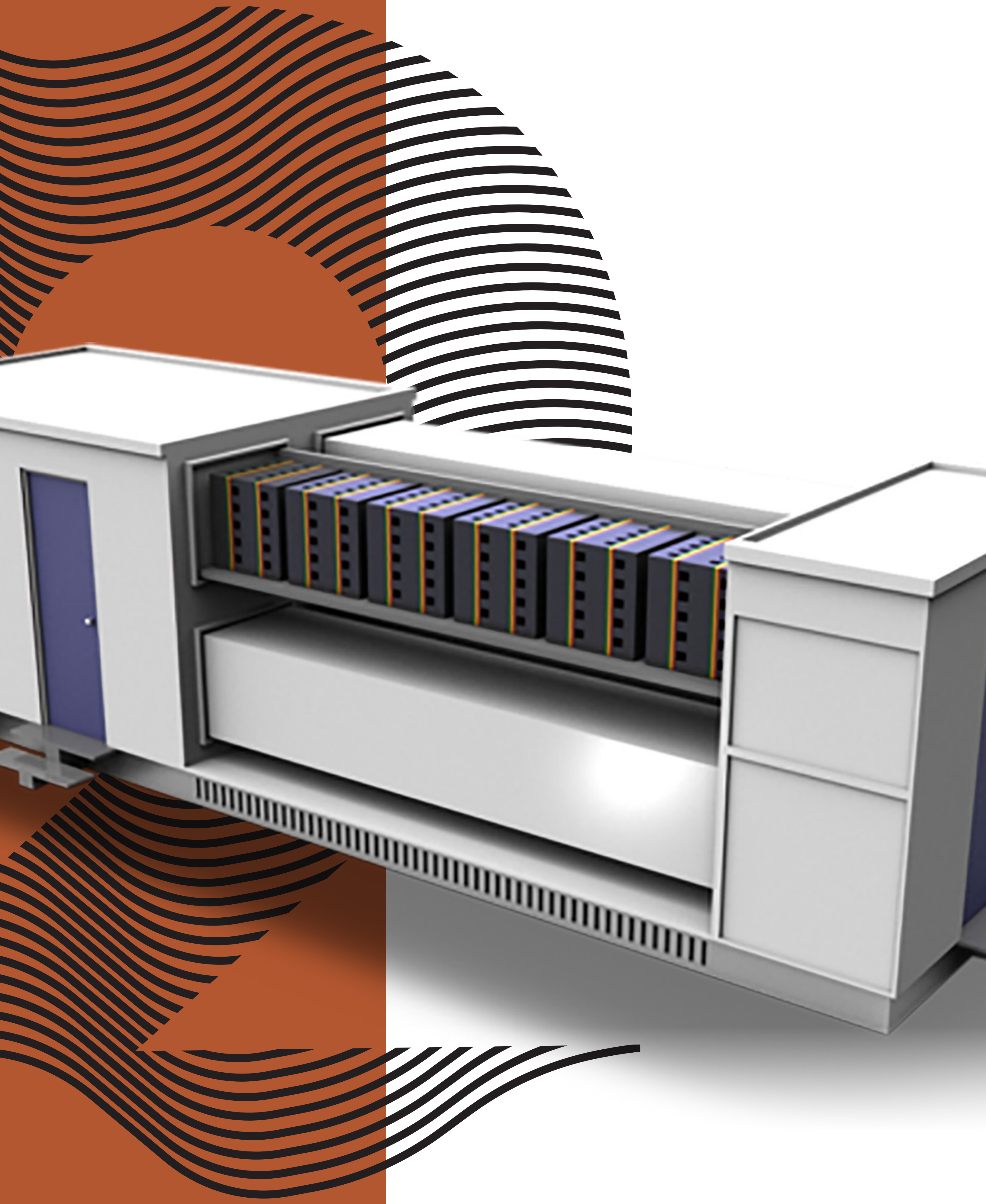
Continued on page 8

Solid Oxide Fuel Cells & Solid Oxide Electrolysis Cells

SOFCs are devices that can chemically convert the energy of a fuel and oxidant directly into electrical energy. SOFCs are well suited for IES because they are modular and designed to be fuel flexible. Since SOFCs produce electricity through an electrochemical reaction and not through a multi-step (e.g., combustion to heat to generator power) process, they are much more efficient and environmentally benign than conventional electric power generation processes. And because of their inherent chemical capacitance, they can offer fast response to power demands from the grid. These characteristics make SOFCs uniquely valuable assets for IES, offering unique generation-response capabilities to support an evolving dynamic power grid.

NETL researchers are also investigating SOECs, which produce hydrogen fuel from water and excess electricity. Hybrid SOFC/SOEC systems can increase the efficiency of power generation — resulting in decreased emissions — while the flexible operation of these systems (e.g., producing either electricity or hydrogen fuel) can further help maintain the stability and reliability of the electric grid. Importantly, these hybrid operations increase and diversify the revenue streams for electricity generators, thereby supporting the durable economic viability of these businesses and area communities.

Continued on page 10



Advanc

ced Turbine Technology

One of the fastest and most cost-effective approaches to decarbonization is to develop more efficient energy conversion systems. To this end, NETL researchers are developing revolutionary, near-zero-emission advanced turbine technologies that could one day become part of an IES. NETL's advanced turbine research accelerates turbine performance, efficiency and cost-effectiveness beyond current state-of-the-art.

For example, NETL's advanced turbine research addresses component development for turbine systems fueled with multiple fuels — including hydrogen and syngas — and natural gas in combined cycle applications with pre- or post-combustion carbon capture and storage (CCS) that could soon achieve greater than 65% combined cycle efficiency with CCS. These systems could also support load following capabilities to meet the needs of an IES and the demand of a modern grid.

NETL researchers are also investigating supercritical carbon dioxide (sCO_2)-based power cycles, which operate in a manner similar to other turbine cycles but use CO_2 as the working fluid in the turbomachinery. The cycle operates above the critical point of CO_2, so the working fluid does not change phase and thereby helps to support a highly efficient recuperated cycle. These cycles also have high power density and simplicity/flexibility of operation compared to existing steam-based power cycles. These advantages result from the ability to use small turbomachinery and the ability to be fuel- and/or heat-source neutral. Furthermore, the direct-fired version of this cycle can facilitate carbon capture by producing a high-purity stream of CO_2 at high pressure that is ready for reuse or storage.

Converting Natural Gas **to Higher-Value Products**

IES will deliver more than just electricity. In addition to heat and power, IES will produce valuable chemicals and products. For instance, depending on market demand, natural gas (which is primarily composed of methane) could be used to create power and heat. It could also be converted into higher-value products that can be used in many different industries such as plastics, pharmaceuticals, chemicals/fuels and batteries.

Creating the industrial components to manufacture these higher-value products requires an advanced understanding of reaction chemistry, and NETL has a well-developed and internationally recognized capability in this area. In addition to advancing traditional conversion routes (e.g., steam, partial oxidation or dry reforming), NETL researchers are also leading the way on a new frontier of reaction chemistry supported by microwave energy. With novel capabilities to control and enable new chemistry mechanisms and process methods, U.S. industry can monetize the nation's abundant supplies of natural gas and other carbon fuels. The microwave approach could also enable industrial decarbonization through efficient electrification of processes that would normally rely on combustion to provide heat to drive the reactions.

The groundbreaking techniques being developed at the lab will enable process-intensification for carbon conversion processes, thereby significantly cutting costs and reduce energy requirements and environmental impact while achieving higher yields and greater selectivity of products.

Microwaves provide energy at the molecular level for these chemical conversions, resulting in rapid, selective heating — a major advantage over thermal heating, which heats broadly and slowly from the outside in. NETL is well-equipped to push the boundaries of microwave chemistry research. Two microwave reactor systems have been designed and built in the Lab's state-of-the-art ReACT Facility: a 2-kilowatt 2.45 GHZ fixed-frequency, fixed-bed flow reactor and a 500-watt variable frequency reactor that spans 2-8 GHz range. The Lab continues to make new breakthroughs in this field, and this research could significantly enhance the future of IES.

These are just a few examples of NETL's cutting-edge energy conversion capabilities that can be directly applied to IES research to produce net zero carbon electricity. As the Lab continues to work toward a decarbonized energy economy, this research and many other areas of energy conversion expertise will continue to grow in significance and lay a solid foundation for these future energy systems.

Continued on page 14

NETL's **Hybrid Performance** Project

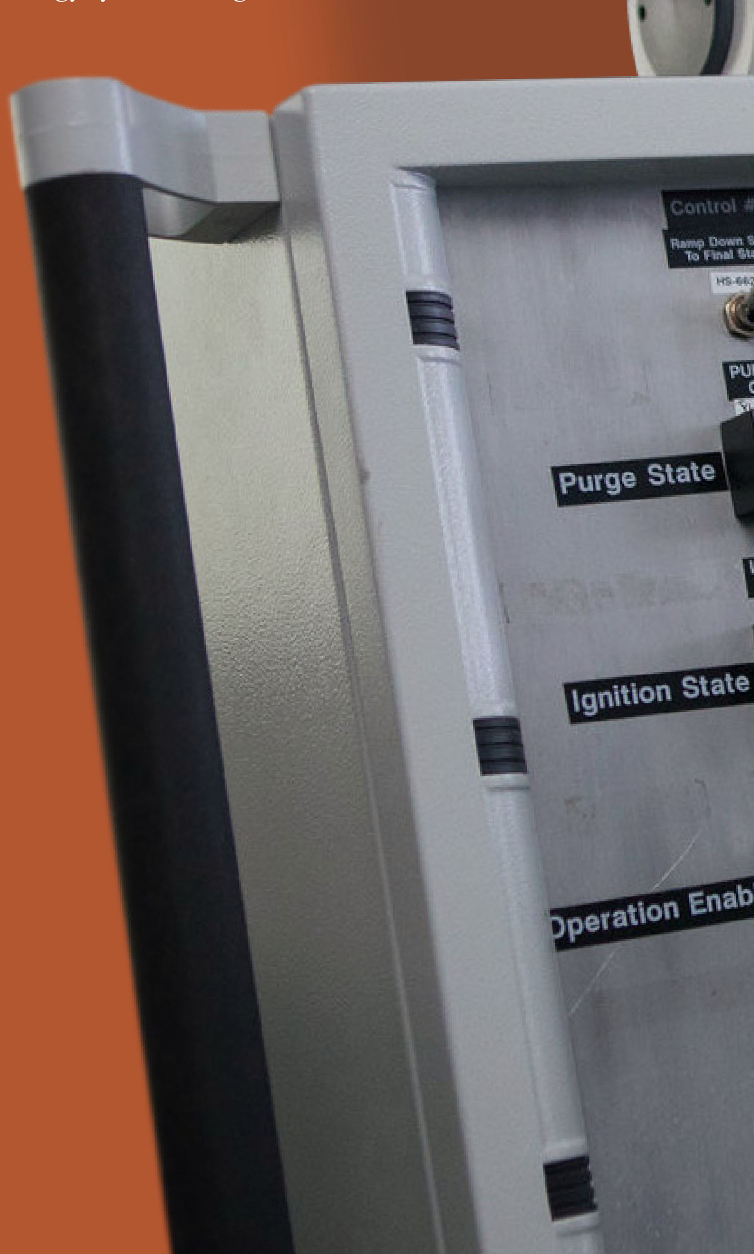
While NETL's energy conversion engineering competency continues to advance the technologies that could one day enable IES, further development will require new operational and control strategies. To this end, NETL created the Hybrid Performance (Hyper) Project to study integration of high-temperature SOFC and SOEC systems with gas turbines and fuel reformers. The scope of the Hyper project also includes support for other innovative energy technologies as a test bed for new sensors and advanced control methods.

Hyper simulates coupling technologies like SOFCs and SOECs through a combination of hardware and software known as "cyber-physical systems." The NETL cyber-physical platform embeds real-time models with power generation hardware to better capture real-time system dynamics. This approach enables higher fidelity simulation of integrated system dynamics, which is essential for development of controls needed for IES.

The cyber-physical approach allows control strategies to be developed and tested before actual implementation of the technology, reducing the risk associated with pilot-scale exploration. It also provides opportunities for feedback from the pilot scale to materials development that could impact system performance. A variety of SOFC configurations can be tested without risk to such critical system components.

For example, SOFC/SOEC hardware systems can be embedded in the platform and tested to determine how the electric grid affects the performance of IES. This research is providing valuable insights on operating strategies needed to lower cell degradation rates that extend operational lifetime and performance, as well as control strategies required to mitigate emerging grid challenges (e.g., high renewable energy variability).

Currently, Hyper has enabled valuable collaborations, such as a project with Idaho National Laboratory (INL), which is connecting test resources between the two national laboratories to create a more powerful platform for hybrid energy system controls development and demonstration. The partnership is integrating INL's digital real-time simulator infrastructure and high-performance computing resources with the simulation and hardware assets at NETL. Preliminary demonstrations have already proven the promise of such a unique capability for investigations of advanced controls development and energy systems integration.




Control #2
Ramp Up
Ramp Down
Control #3
Fan Off/On
PURGE OFF
PURGE COMPLETE
IGNITOR OFF
Flame Detected
Flame Out
ESD Armed
ESD Tripped
Key Enabled
110% Turbine Over Speed
Nominal Speed
TEST
SIL
ACK

VISUALIZING INTEGRATED ENERGY SYSTEMS:

Combining Technology and Versatility to Optimize Energy Production, Lower Emissions

By Conor Griffith

In the fight against climate change, multiple technologies and systems will have to be deployed to reach net zero emissions of carbon dioxide (CO_2) and other greenhouse gases throughout the country. Doing so is no small task, but it is a job well suited for NETL's modeling and simulation researchers.

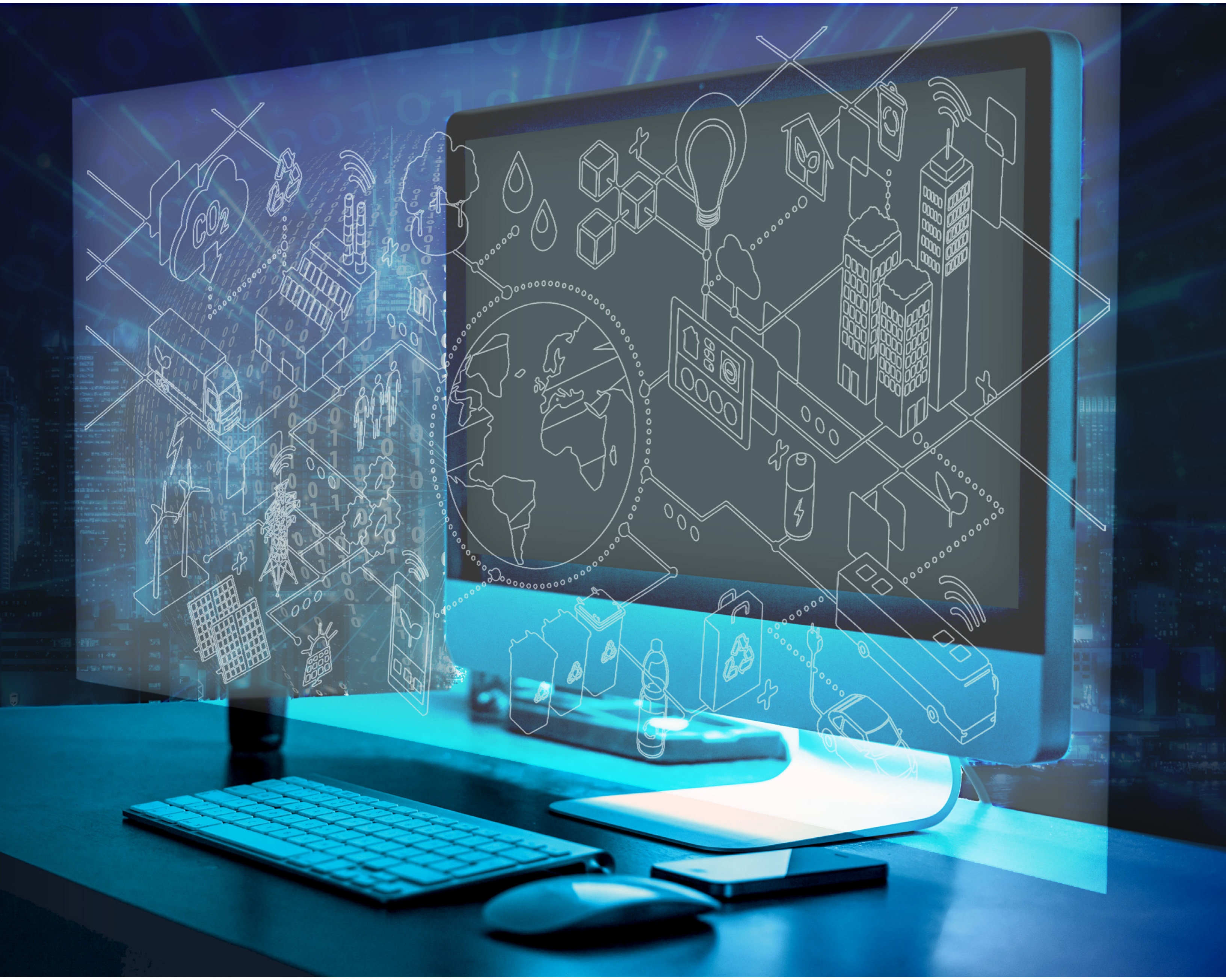
Perks of Synergizing Hydrogen, Other Assets with an Integrated Energy System

"Integrated energy systems, or IES, synergistically incorporate multiple energy sources working cooperatively to provide environmentally sustainable, reliable and cost-effective power and other energy services. We have been exploring this primarily in the context of tightly coupled hybrid systems," explained NETL's David Miller, Ph.D., senior fellow for Strategic Systems Analysis and Engineering. "Some of these ideas come out of a tri-lab effort that started in 2018 to identify opportunities for increased collaboration among the applied DOE laboratories, NETL, NREL (National Renewable Energy Laboratory) and INL (Idaho National Laboratory)."

"We typically think about energy production based on a single primary energy source such as wind, solar, nuclear or fossil. The idea of an IES is to consider ways to leverage the capabilities of diverse energy resources to more effectively provide energy services while meeting social and environmental objectives," said Miller.

NETL and its collaborators are exploring a broad range of opportunities for IES to accelerate widespread decarbonization. For example, an IES that includes renewable energy and fossil with carbon capture and storage (CCS) could produce fuels and hydrogen, while providing enhanced flexibility to meet varying electricity demand.

"There is a lot of interest in hydrogen as a carbon-free energy carrier," Miller said. "When you use hydrogen within a fuel cell or combustion turbine, you don't have any direct carbon emissions."



Much of the hydrogen produced worldwide comes from reforming of natural gas, with a secondary but significant fraction also derived from gasification of coal, petcoke and petroleum residuals. When any of these fossil fuel-based methods are combined with CCS, they can provide near-zero carbon emission hydrogen. Possibilities for gasification of blended solid feedstocks, including biomass and waste materials, emerge as carbon neutral methods when incorporating high rates of CCS. Incorporating a degree of bio-energy with CCS provides the possibility of net carbon negative hydrogen.

Producing hydrogen via electrolysis of water can also provide zero emission hydrogen if renewable energy is used. No matter how the hydrogen is produced, it is extremely versatile, and can be used for power production (solid oxide fuel cells or hydrogen turbines), chemicals and industrial processes, such as oil refining, ammonia and fertilizer synthesizing, and polymers and steel production. The hydrogen can also be stored for future use, including electricity production when power demand is high.

NETL is performing system integration studies for two energy plant concepts (i.e., IES producing net-zero carbon emission electricity and/or hydrogen) to advance the design of engineering-scale prototypes. These energy plant concepts should be capable of flexible operation to meet the needs of the grid, use components that improve efficiency, have a small size (50-350 MWe) compared to today's conventional utility-scale plants and will transform how power plant technologies are designed and manufactured.

Continued on page 18

Building up the IES Idea with IDAES

How to create these net-zero IES? That's where NETL's Institute for the Design of Advanced Energy Systems (IDAES) comes in. Formed in 2016, IDAES optimizes the design and operation of complex, interacting technologies and systems to enable the development and deployment of innovative advanced energy systems. NETL leads a diverse team of collaborators from Sandia National Laboratories, Lawrence Berkeley National Laboratory, West Virginia University, Carnegie Mellon University and the University of Notre Dame to develop these R&D 100 Award winning, open-source computational tools.

IDAES is at the heart of DISPATCHES, the Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems. It brings together the IDAES team with new collaborators at NREL and INL to create software to enable the design and optimization of IES. The project is examining how to choose among different technologies options available that will be compatible for different scenarios such as using heat, hydrogen or captured CO_2.

The goal of DISPATCHES, which is funded through the DOE Grid Modernization Initiative, is to identify flexible, dynamic designs that are responsive to grid market signals, resulting in highly efficient, cost-effective tightly coupled hybrid energy systems to provide increased flexibility and resiliency.

"IDAES is an integrated optimization platform that can represent different energy technologies in a framework that facilitates the design of an IES, including discrete choices among different technology options, which extend beyond current experience," Miller said. "In addition, it lets us represent the dynamic behavior of these systems in conjunction with unit commitment and dispatch modeling associated with the electric grid."

This means researchers can understand via advanced modeling how these new systems will be dispatched and what they will require to operate in a cost-effective manner. Essentially, IDAES can serve as a roadmap to understand systems and designs before building and testing them, saving time, money and resources.

Continued on page 20

DISPATCHES

Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems

HIGH-FIDELITY PROCESS MODELING

Elucidate complex relationships between resource dynamics and market dispatch (with uncertainty, beyond price-taker assumption)

INTEGRATED RESOURCE-GRID MODEL

Predict the economic opportunities and market impacts of emerging technologies (tightly coupled hybrid energy systems)

GRID MODELING

Guide conceptual design & retrofit to meet current and future power grid needs

Leveraging MFiX for Next-Generation Energy Reactors

A successful net zero carbon IES system model must be grounded with accurate multiscale modeling. To complement low-order plant-scale process models, NETL employs a wide range of commercial and custom computational fluid dynamics (CFD) software tools to create high-fidelity predictions of IES energy conversion reactors and associate devices.

CFD tools, like NETL's Multiphase Flow with Interphase eXchanges (MFiX) software suite, provide researchers with detailed predictions of chemical reactions, thermal characterizations and critical multiphase flow phenomena occurring within IES system reactors. Demonstrating these virtual reactors and devices, operating at full scale, allows researchers to optimize reactor design with significant cost and time savings over large-scale physical prototyping.

MFiX continuously evolves through state-of-the-art software and hardware updates. More than 36 years of NETL development has resulted in a widely accredited user-base that bridges academia, industry, national laboratories and global technical consulting entities. In fact, MFiX's open-source code and many key algorithms have been incorporated into commercial software offerings, which is a testimony to the software's cutting-edge capabilities and accuracy.

Today, MFiX continues to shape the future of CFD by offering new modeling techniques with greater precision and levels of detail required to support design of advanced IES reactors. These methods generate complex particle shapes used to model novel bio-materials, sorbents and catalysts, which, in turn, better serve reactor optimization investigations.

In addition, advances in computational power, like those afforded by NETL's highly ranked Joule 2.0 supercomputer with 74,240 central processing unit (CPU) cores and 100 graphical processing unit (GPU) nodes, establish a hardware solution for the accurate modeling of how real particles interact with one another and their environment.

As NETL moves to find ways to create an environment for integrated systems that support net-zero emissions, these MFiX advancements come at a unique time when renewable energy is in clear research focus. Leveraging decades of pyrolysis, gasification and combustion expertise, NETL computational researchers are investigating renewable biomass as an alternative to fossil fuel in IES reactors.

Biomass is a highly variable energy feedstock. Municipal solid waste and agricultural byproducts are dried (torrefaction) and compressed into briquettes of all different shapes; wood chips and shreds, pine needles and sawdust can be pelletized or used in natural form.

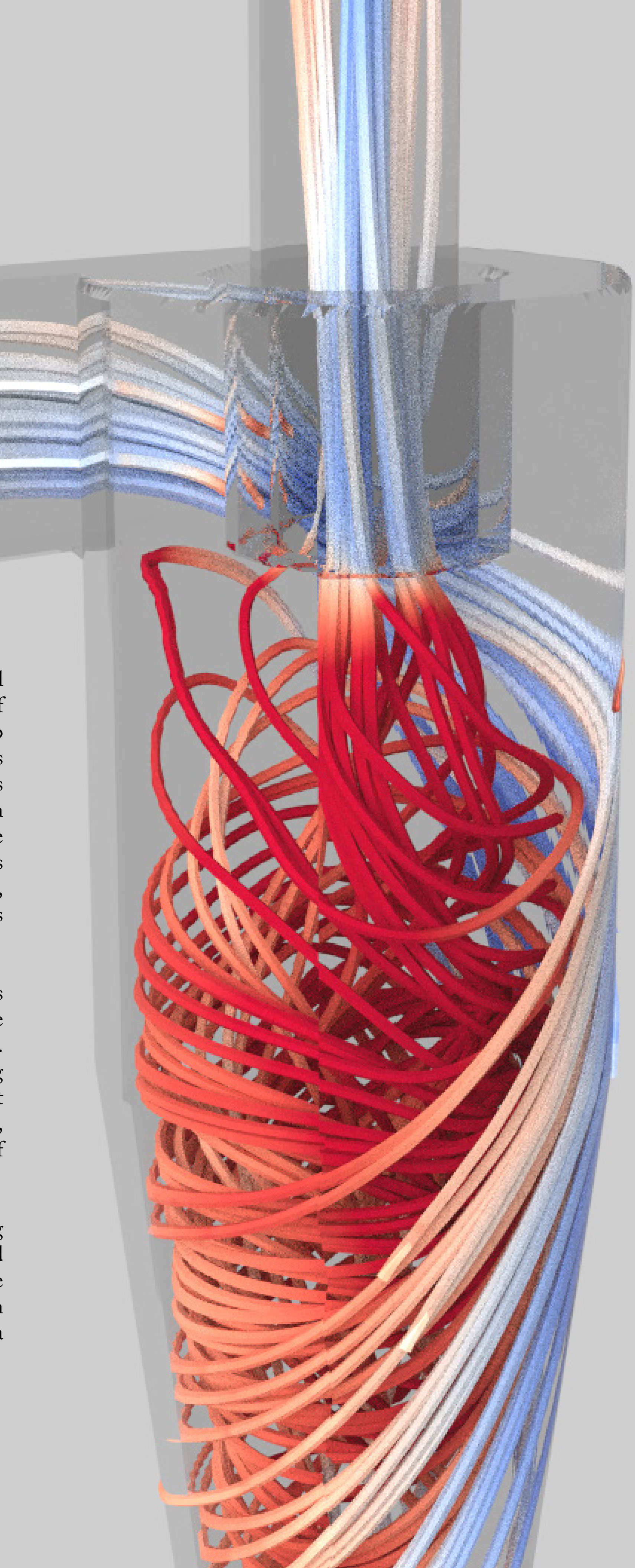
NETL researcher, Xi Gao, Ph.D., developed the MFiX-Super DEM (discrete element model) approach to solids modeling, whereby a family of geometric shapes are defined by a single formula with variable exponents. By manipulating five parameters, any MFiX researcher can make 80% of mathematically regular three-dimensional shapes, thereby making the models more closely resemble the original images. This provides greater accuracy and more reliable data than older modeling approaches.

With this capability, MFiX-Super DEM accurately accounts for particle interaction, chemical decomposition and heat transfer, thereby allowing computational simulation of realistic biomass pyrolysis and gasification. In a recent demonstration case, Gao simulated 100 million oblate (tablet-shaped) pellets in a computational fluidization experiment utilizing 6800 CPU cores on NETL's Joule 2.0 supercomputer. This represents the largest simulation of its kind and opens the door to new capabilities and possibilities. By experimenting with a variety of shapes, a wider array of scenarios can be tested, and more accurate data can be obtained. More accurate data modeling means more certainty, which minimizes project risks and expenditure of resources.

But, MFiX computational researchers have not stopped with mathematically regular shapes.

Using a recently improved mesh generation method in MFiX, developed by NETL's Jeff Dietiker, Ph.D., in concert with the glued-sphere discrete element modeling technique, researcher Liqiang Lu, Ph.D., demonstrated that any highly irregular shape that can be represented by a standard triangle language (STL) file can be converted into a glued-sphere particle assembly and subsequently visualized and simulated using MFiX-DEM.

Lu further incorporated the glued-particle assemblies into computational fluidization experiments and simulated detailed hydrodynamics, surface chemistry and heat transfer with an unprecedented level of detail. With more detailed modeling, an IES can be achieved at lower cost and achieve maximum efficiency, not to mention other potential applications such as industrial and mineral extraction operations.



The high fidelity achieved by non-spherical shape representation comes at the expense of larger computational resources required to carry out the simulations. However, NETL's Joule 2.0 supercomputer allows researchers to conduct simulations in reasonable time. In fact, Lu's ongoing research efforts indicate that MFiX-DEM may run 100-200 times faster when ported from CPU to GPU, which could vastly speed up the processes needed to optimize modern energy systems.

Ambitious research and creative solutions to America's energy challenges define the effort of NETL's researchers every day. Furthermore, recent MFiX modeling developments are paving the way for the next generation of particulate modeling tools, which will lead to better understanding of multiphase flow phenomena.

NETL's enhanced knowledge and modeling capabilities, enabled through IDAES and MFiX, will lead to breakthroughs in the design, troubleshooting and optimization of integrated energy systems needed for a reliable, sustainable, decarbonized future. ☰

Carbon Capture **Processes & Materials**

By Joe Golden

Decarbonizing Integrated Energy Systems through NETL's Carbon Capture Research

DOE is committed to achieving greater energy security, reliability and lower emissions in the energy sector, and an integrated energy approach could provide a path toward affordably reaching these goals. In future integrated energy systems (IES), carbon-based energy systems and large-scale energy storage systems could ensure a stable grid in the face of high penetration of variable renewable energy. However, to reach a goal of net-zero carbon electricity, IES will need to be equipped with effective, affordable and less energy-intensive systems to capture carbon dioxide (CO_2).

NETL possesses world-class expertise in carbon capture research, including revolutionary computational modeling and simulation tools to accurately predict costs of carbon capture technologies and accelerate the commercialization of these technologies from discovery to development, demonstration and ultimately widespread deployment. Additionally, the Lab is undertaking research and development (R&D) on promising carbon capture materials to further achieve carbon capture goals, benefit the environment and work toward enabling IES for a net-zero carbon future.

Continued on page 24

The Cost of Capture

Carbon capture systems will be critical components of IES that feature carbon-based power generation, but they must be designed and deployed affordably. NETL leverages its expansive energy analysis capabilities to model the cost of various types of carbon capture technologies across different applications. This work supports better R&D decisions to mitigate the economic challenges of carbon capture and will help stakeholders effectively evaluate the costs and reduce the risk of implementing these technologies in IES.

One way NETL is supporting this research is the development of a first-of-its-kind suite of digital tools and resources, as well as the CCSI Toolset and IDAES platforms, that can effectively evaluate technology cost and performance, including carbon capture, during each step of the value chain. The flexible design of these software tools and resources allows users to customize analyses as technologies advance, policies change or new policies are enacted.

Among the publicly available tools and resources, NETL's "Baseline Studies for Fossil Energy Plants" and its supporting series of Quality Guidelines for Energy Systems Studies establish guidelines and estimates for the cost and performance of combustion- and gasification-based power plants, as well as options for co-generating synthetic natural gas and fuels — all with and without CO_2 capture and storage.

These studies, and "Volume 1: Bituminous Coal and Natural Gas to Electricity" in particular, provide a consistent basis to compare existing and developing technologies, inform development of R&D goals and targets, and guide potential DOE investment by quantifying the prospective benefits of successful R&D of advanced technologies within the Department.

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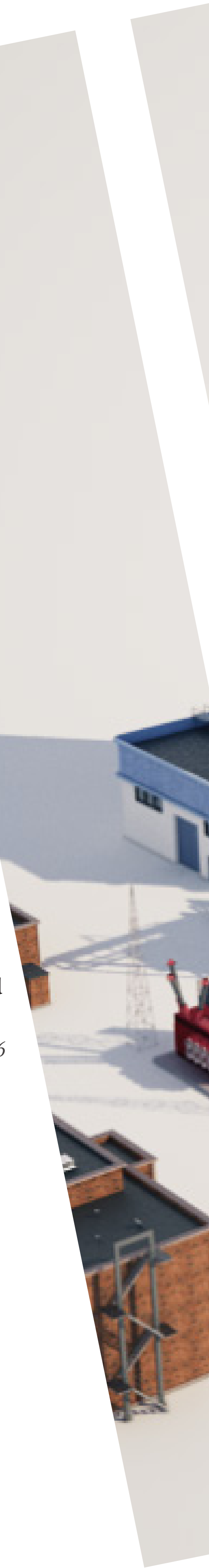


Designing & Modeling Next-Generation Carbon Capture Systems

The NETL-led Carbon Capture Simulation for Industry Impact (CCSI^2) project is a partnership among national laboratories, industry and academic institutions that is applying cutting-edge computational modeling and simulation tools specifically created to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration and ultimately widespread deployment. CCSI^2's work could be used to help to accelerate development of IES, because carbon capture is a critical element in achieving the goal of net-zero carbon electricity.

CCSI^2 is focused on developing a fundamental understanding of carbon capture technology by fully leveraging an R&D 100 Award-winning computational package called the CCSI Toolset. This toolset provides end users in industry with a comprehensive, integrated suite of scientifically validated models with uncertainty quantification, optimization, risk analysis and decision-making capabilities. In addition to custom modeling capabilities, the toolset is also designed to readily accommodate existing models and simulations created in commercial and open-source software currently in use by industry. CCSI^2 also continues to develop new software tools as necessary to fill technology gaps.

The toolset helps maximize the value of research across the entire development process. In the lab, the performance of a promising material can be simulated at the process scale using what's currently known about the material to determine the most productive research direction. As testing moves beyond the lab to more complex and expensive pilot testing, the toolset helps to select the optimal subset of test conditions that will most improve predictive capabilities on a limited budget and schedule. Doing so accelerates knowledge gain and reduces operational risk by gaining insight on potential issues that can occur at the commercial scale.

Using the toolset, NETL/CCSI^2 collaborates with industrial, academic and government partners to disseminate a rigorously quantified understanding of carbon capture systems, manage risk and reduce the barriers to technology commercialization. The results are well-informed, accelerated technology transfer processes for timely implementation of technologies that benefit the world and future IES.

Continued on page 28

CCSI^2 is led by the National Energy Technology Laboratory, partnering with Lawrence Livermore National Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, Pacific Northwest National Laboratory, Oak Ridge National Laboratory, West Virginia University, University of Pittsburgh, University of Toledo, University of Notre Dame and the University of Texas at Austin.

Advanced Carbon Capture **Materials**

One example of the many promising materials NETL is pursuing in its carbon capture materials research that could help enable IES is a novel thin film composite (TFC) membrane. Compared to conventional absorption/desorption processes used to capture CO_2, membrane technology is more compact, more efficient and simpler to operate.

To succeed, TFC membranes must achieve high gas permeance (i.e., the ability for the gas to pass through the membrane) measured in gas permeance units (GPUs), as well as CO_2 and nitrogen selectivity (i.e., how efficiently CO_2 is separated from nitrogen). To achieve this, TFC membranes are usually made up of three layers: a thicker porous support (greater than 20 microns), a thin gutter layer (less than 1 micron) and a thin selective layer (less than 1 micron) that mainly performs gas separation.

Unlike most TFC membrane research, which focuses on improving just the topmost, selective layer, the NETL work has improved all three layers to surpass their goal of achieving a scalable membrane with CO_2 permeance greater than 2,000 GPU and selectivity greater than 25.

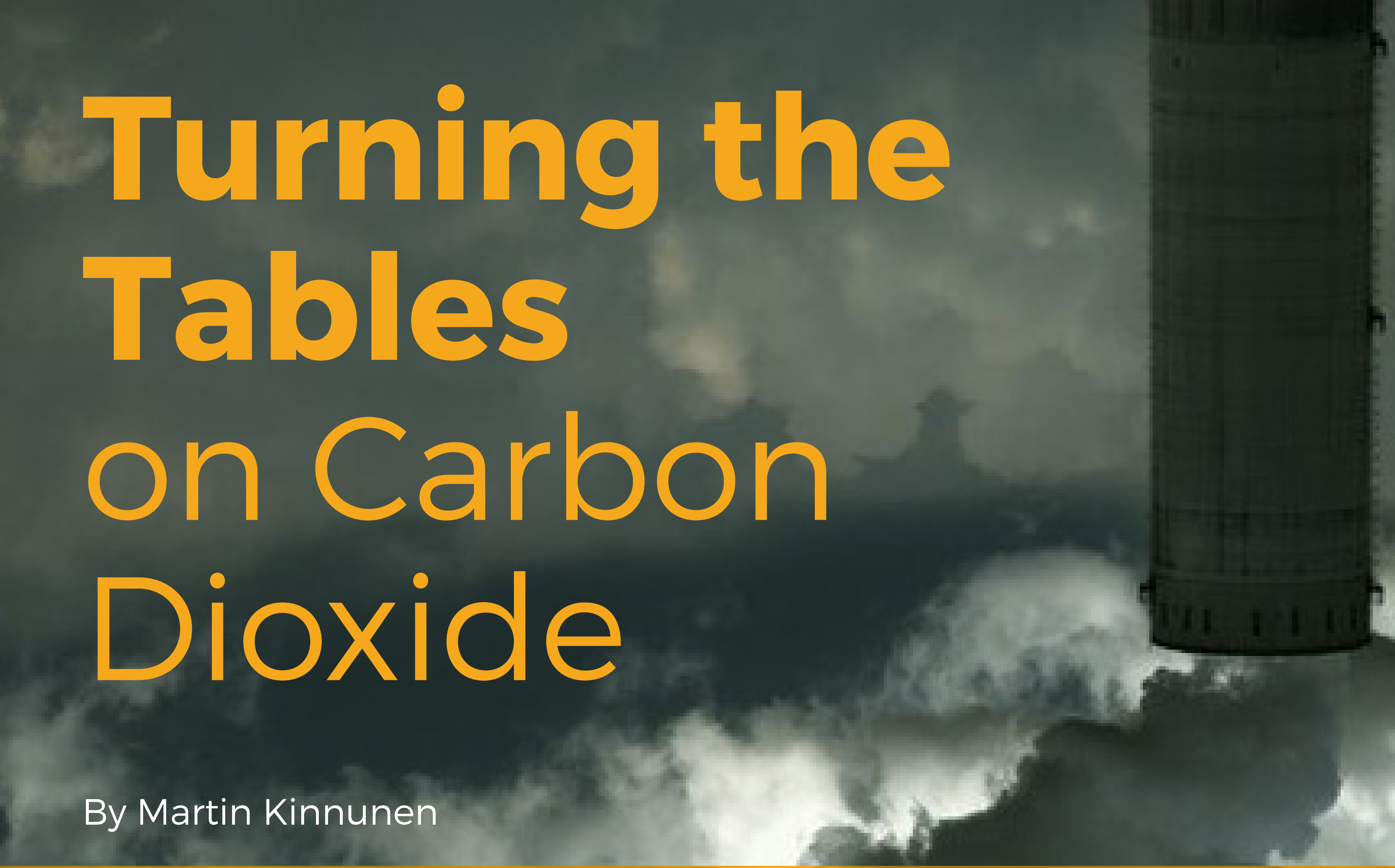
Each layer of a TFC membrane poses unique challenges to overcome. For example, the thicker bottom layer is a porous support that provides mechanical strength because the selective layer is too thin to be used on its own. Commercially available porous support layers could not provide the required physical properties to achieve program goals, so the NETL team developed their own novel and scalable nanoporous support with much greater CO_2 permeance and surface porosity, as well as better chemical stability.

The intermediate, gutter layer of the TFC membrane prevents the top layer from seeping into the pores of the bottom layer during curing of the liquid polymer solution used to create the thin film. The gutter layer also requires high gas permeance like the support layer, but it must be much thinner. The NETL team created a superior gutter layer coating that achieved record-breaking permeance when compared to commonly used gutter layer coatings of similar thickness.

The top layer of a TFC membrane is the most important, because it mainly performs the gas separation. Like the gutter layer, the selective layer must also be thin to enhance gas permeance, which is inversely proportional to the layer's thickness. Again, the NETL team exceeded current state-of-the-art in selective layer materials by developing a rubbery crosslinked polymer that exhibited high permeability and selectivity in addition to resistance to physical aging.

With breakthroughs at every level, the NETL team developed a lab-scale TFC membrane that demonstrated gas permeance of 4,200 GPU (using a pure CO_2 stream), which more than doubled their goal, and a selectivity of 30, which met the goal of greater than 25. This new technology is capable of being scaled using existing membrane fabrication equipment at the Lab and offers great potential for industrial membrane post-combustion carbon capture. Next steps include performance testing using actual flue gas at the National Carbon Capture Center in Wilsonville, Alabama.

As integrated energy systems evolve, NETL's carbon capture research will continue to work toward decarbonizing power generation processes that will help provide reliable, resilient power while protecting the environment.



Turning the Tables on Carbon Dioxide

By Martin Kinnunen

NETL researchers are developing processes to transform industrial emissions of carbon dioxide (CO_2) from an unwanted waste that contributes to climate change into the chemical building blocks to manufacture hundreds of value-added products.

Anthropogenic, or man-made CO_2 emissions, produced by power plants and other industrial processes, are well-known greenhouse gases that trap heat in the atmosphere.

What's less well known is that industrial CO_2 is also a useful feedstock that can be captured and transformed from a waste gas into a valuable commodity that can be used in the manufacturing of fuels, chemicals, building products, plastics, alcohols, carbon fibers and much more.

"At NETL, we are turning the tables on carbon dioxide," said Douglas Kauffman, Ph.D., a researcher on the Functional Materials Team in NETL's Research & Innovation Center.

"In the future, carbon emissions from power plants and other industrial sources will be recycled and used as the feedstock to make products we use daily. This will not only reduce the amount of CO_2 emitted into our atmosphere, it will generate revenues to help offset some of the costs of carbon capture and climate change mitigation while creating jobs to manufacture new products," Kauffman said.

CO_2 conversion technologies and other efforts undertaken through DOE's Carbon Utilization Program, which is managed by NETL, play critical roles in meeting goals outlined in President Biden's Executive Actions to address climate change.

Furthermore, integrating NETL's research in CO_2 conversion and carbon capture with power and industrial plants is an essential step to achieve the Biden administration's top climate change priorities — the creation of a carbon emissions-free power sector by 2035 and putting the U.S. on an irreversible path to a net-zero carbon economy by 2050.

For Kauffman, the development and optimization of new catalysts — materials that increase the rate of chemical reactions — represent a transformative technology driving revolutionary reuse of CO_2.

In the presence of electricity, CO_2 molecules react with an appropriate catalyst to form various chemicals. The type of chemical building blocks to be produced by recycling CO_2 is also determined by the catalyst's identity and characteristics. Nanometallic-based catalysts are especially effective because their high surface area, among other factors, can dramatically increase catalytic activity.

Researchers have sought efficient and affordable ways to

convert CO_2 into carbon monoxide (CO) because CO is an important industrial feedstock used in the production of chemicals ranging from acetic acid, which is used in many household cleaning products, to polycarbonate plastics and methanol, which is essential to make thousands of everyday products, including fuels, paints, adhesives, fertilizers and even windshield fluid.

Gold and silver are two of the most selective catalysts for electrochemically converting CO_2 into CO, but their cost is a factor that must be taken into account. Replacing these expensive materials with effective, affordable alternatives is essential for developing CO_2 conversion technologies.

NETL has used a variety of advanced synthetic and characterization techniques to create inexpensive nanocatalysts that rival or exceed expensive precious metals. In one case, NETL demonstrated a copper-based nanocatalyst with a unique 3D porous structure that selectively converted CO_2 into CO. In another case, NETL used its advanced surface science capabilities to develop catalysts made of iron and nickel that out-perform state-of-the-art iridium anode catalysts, at a fraction of the cost.

"NETL's goal is to discover precise catalyst recipes. Researchers want to know what types of catalysts work best to selectively and efficiently turn CO_2 into specific chemical compounds," Kauffman said.

Advancing the development of CO_2 recycling through electrochemistry has other benefits as well. Whereas traditional reaction processes often require high temperatures and pressures, the electrochemistry process can be conducted at near room temperature and ambient pressure using electricity from a renewable energy source such as wind, solar or geothermal, which makes the process more efficient and environmentally benign.

NETL also is using advanced computer modeling and simulations to identify low-cost, abundant and high-activity catalysts that can guide the reaction toward making only the desired product. Tools such as NETL's Joule 2.0 supercomputer are used as platforms to simulate experiments and develop models to identify active sites and understand how the reactions proceed.

Supercomputing helps NETL to drive innovation and deliver solutions for an environmentally sustainable and prosperous energy future. By expediting technology development through computational science and engineering, Joule 2.0 helps NETL cut costs and save time.

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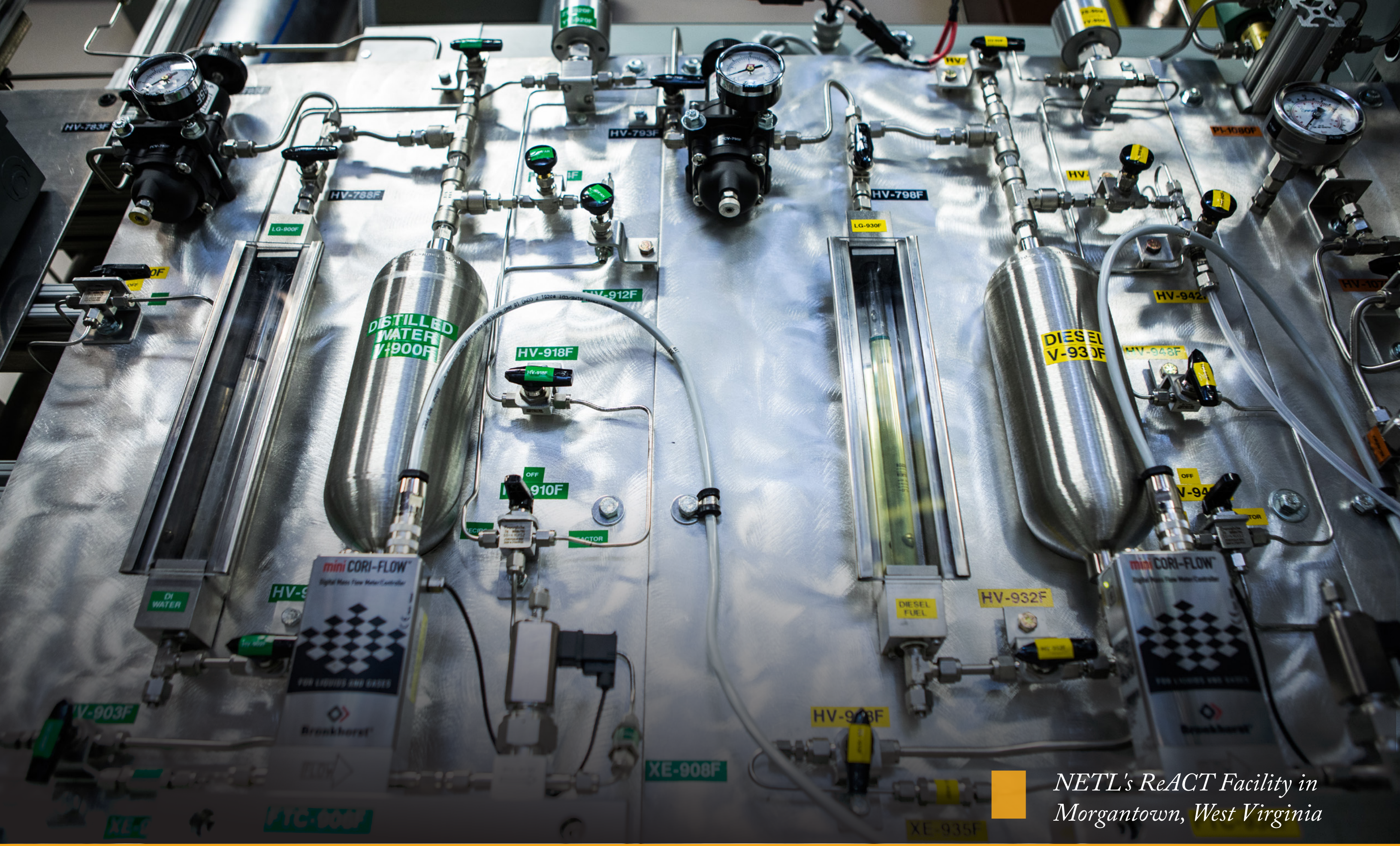


NETL's ReACT Facility in Morgantown, West Virginia

Unleashing the Power of Microwaves

When most people think of a microwave, they conjure up visions of kitchen equipment to prepare food. At NETL, microwaves have taken on a far broader connotation.

Researchers at NETL's Reaction Analysis & Chemical Transformation (ReACT) facility have unleashed the power of microwaves to advance technologies capable of providing cleaner and more affordable energy and valuable chemicals.

Many of their projects are making a profound impact. For example, NETL researchers in collaboration with West Virginia University have developed a process to produce ammonia far more efficiently than the prevailing Haber-Bosch process, which functions at high pressures and temperatures and requires a constant supply of energy.

NETL's pioneering microwave ammonia synthesis (MAS) technology, which received the 2020 IChemE Global Award in the Research Project category, is not as energy intensive as purely thermal processes due to the microwaves' targeted heating.

Furthermore, the MAS technology is also highly modular, meaning ammonia production can be shifted locally rather than relying on large-scale, centralized production facilities. The implications for agriculture and the environment are huge. Ammonia, which is largely used to make fertilizer, could be manufactured near farmers using intermittent wind or solar power, lowering production costs and the CO_2 footprint created while transporting fertilizer to farming communities.

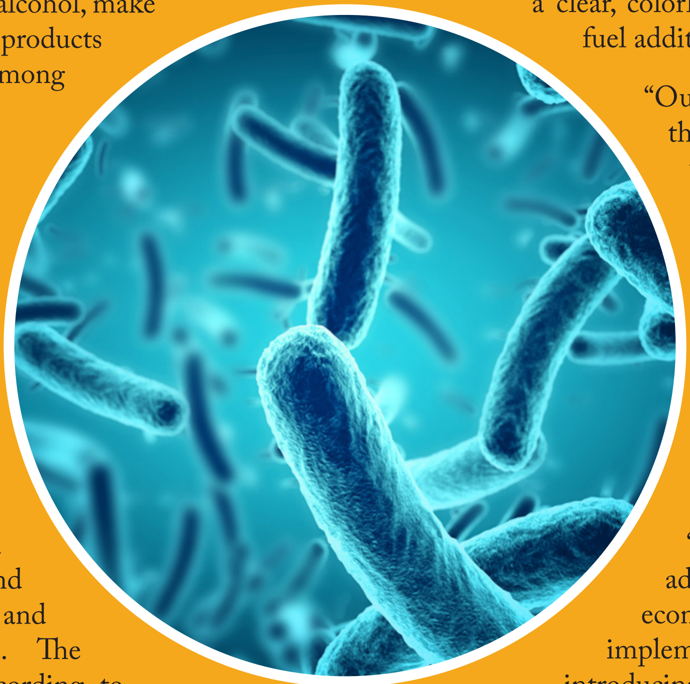
As part of another groundbreaking project, NETL researchers have reported making important strides in microwave-assisted dry reforming of methane (MW-DRM), a process that reacts CO_2, instead of water or oxygen, with methane to yield the mixture of hydrogen and carbon monoxide known as synthesis gas or syngas, a chemical building block for many products.

Microwave systems enable the high-temperature reactions the process requires because they can selectively and efficiently heat the catalyst bed in the microwave reactor without needing to heat the entire reactor volume, keeping the necessary energy efficiently directed to where the chemistry occurs.

The research also could create new markets for methane. Currently, large volumes of methane are flared off at gas wells sites, adding to global emissions.

Mighty Microorganisms for Carbon Conversion

Microbes — a diverse group of simple life-forms that are invisible to the naked eye and abound in soil, the seas and the air — ferment sugar to alcohol, make bread dough rise and produce products such as antibiotics and insulin, among a myriad of other uses.



Far within the Earth's subsurface, microbes affect the porosity, permeability, acidity and fluid chemistry of underground reservoirs. The catalytic power of these microorganisms also can be used to convert waste CO_2 into useful chemicals.

NETL is growing biocatalysts derived from environmental samples of microbes found in coalbed formation water and shale gas production fluid. The next steps in this process, according to NETL's Djuna Gulliver, Ph.D., have involved enriching the biocatalysts in electrochemical reactors and demonstrating they are capable of converting CO_2 to acetate, an inexpensive chemical that has a wide range of uses, including as a food additive and pickling agent or a laboratory reagent.

In her laboratory, Gulliver grows bacteria in electrochemical reactors to covert CO_2 into acetic acid. New capabilities have been installed to assess the production of ethanol, a clear, colorless alcohol used as solvents or fuel additives, from this biocatalyst.

"Our objective is to deliver a process that exploits microorganisms to upgrade CO_2 waste streams into a profitable product. This research can provide a tremendous boost to develop technologies that convert CO_2 into useful chemicals or functional or structural materials that can be sold to offset carbon capture costs," Gulliver said.

"Overall, the research will advance this technology into an economical process that can be implemented at an industrial scale, introducing a new commodity market to the energy industry and reducing emissions of greenhouse gas," Gulliver said. ≡

NETL Finds Answers for Carbon Storage in the Nooks and Crannies of Rock Cores

By Martin Kinnunen

By identifying and ranking geologic variables that control how carbon dioxide (CO_2) can be trapped in subterranean rock formations, NETL researchers are acquiring detailed knowledge to estimate reservoir capacities and eliminate uncertainties when selecting underground CO_2 storage sites.

"The implications of successfully ranking the factors that control CO_2 trapping are significant as we work to safely and permanently sequester larger volumes of anthropogenic carbon in the subsurface," said Dustin Crandall, research engineer on the Reservoir Engineering Team in the Lab's Geological & Environmental Systems Directorate.

NETL supports a broad portfolio of carbon storage projects. These efforts, integrated with other innovative, Lab-supported work to capture and store deep underground the CO_2 emissions from power plants and industrial sites, have the potential to reduce atmospheric levels of greenhouse gas while permitting the continued use of domestic resources to produce clean, reliable and affordable electricity for the nation.

A key to moving that strategy forward is identifying underground sites with the necessary subsurface properties and geological characteristics to store captured CO_2 in deep formations covered by caprock (a nonpermeable formation that prevents oil, gas or water from migrating to the surface). Crandall and his colleagues at NETL's geoimaging center have deployed their unique set of tools to find answers.

The center houses computerized tomography (CT) scanners, a multi-sensor core logging unit and other advanced technology to gain insights into the physical characteristics and elemental composition of rock formations from cylindrical samples extracted from thousands of feet below the surface.

By processing thousands of X-ray measurements taken from different angles, CT scans produce three-dimensional images that allow researchers to "see" inside rock samples without breaking them. Additionally, NETL's scanners are equipped with temperature and pressure controls on the core holders to enable in-situ flow testing, which can simulate subsurface conditions to evaluate how injected CO_2 would move through rock pores and fissures or dissolve with natural brines, mineralize or react with other fluids.

One of the team's current projects focuses on determining the critical components within reservoir rock that control the trapping of supercritical carbon dioxide (sCO_2), the fluid state of CO_2 when it's injected into the subsurface.

In this ongoing study, NETL's micro-CT scanner was used recently to analyze core samples of sandstone from the Vedder formation in California, the Bell Creek formation in North Dakota, the Berea formation, which spans portions of Michigan, Ohio, Pennsylvania, West Virginia, Kentucky, and the Bandera formation in Kansas.

"We used the CT scanner to focus on the smallest nooks and crannies inside the rock cores to assess their ability to trap CO_2," Crandall said. The team is conducting a pore-scale study of the samples. In a typical geological setting, pore sizes can range from a few nanometers (the equivalent to one billionth of a meter) to microns (one millionth of a meter).

Researchers hope to determine the degree to which the trapping of sCO_2 in natural pore space is impacted by pore structure, mineral composition, fluid properties, varied wettability (ability of a liquid and droplets to maintain contact with a solid surface) and other factors.

Images and measurements of sCO_2 droplet contact angles, mineral composition and trapped pore volumes were

completed in late 2020. Such data has been used to develop relative permeability curves, which describe how competing fluids, such as brine or oil and sCO_2, flow through rock.

Crandall noted that data has been shared with project partners at Virginia Tech to leverage their expertise in developing numerical models to complement the controlled experiments completed at NETL.

NETL's research to understand sCO_2 droplet behavior and the numerical simulations to expand on the applicability of that research have set the stage to complete larger field studies, develop tools to help predict and track plumes of injected sCO_2 in the subsurface and find new methods to improve storage efficiency.

Much of that future research will be addressed by the Science-informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications (SMART) Initiative. SMART is an NETL-led, 10-year, multi-organizational effort to improve the efficiency and effectiveness of field-scale carbon storage by the application of science-based machine learning and data analytics.

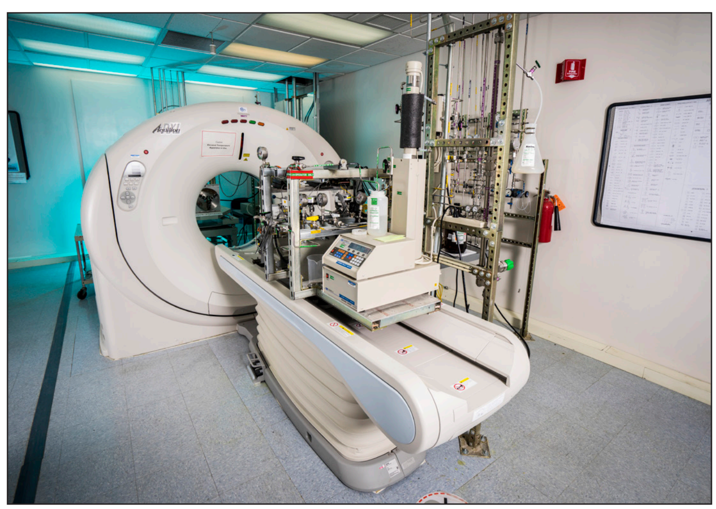
The SMART team is engaging with university, national lab and industry partners and is building off subsurface data collected from field laboratories and regional partnerships that have been part of the carbon storage program during the past 15 years.

SMART's work in carbon storage calls for transforming how people, from industry engineers to government regulators, interact with subsurface data to make well-informed decisions.

The three main goals of SMART are to enable:

- Near real-time visualization of key subsurface features and flow.
- Virtual learning for rapidly understanding the reservoir's behavior.
- Real-time forecasting of actively managed carbon storage systems.

Placing captured CO_2 underground with high confidence of permanent retention requires detailed knowledge of the subsurface structures, properties and evolutionary processes. NETL is leading the way to make that happen.



Medical CT scanner in the CT scanner lab at NETL in Morgantown, West Virginia

Optimizing the System

By Abby Humphreys

An Inside Look with Strategic Systems Analysis and Engineering Senior Fellow David Miller

David Miller, Ph.D., is the senior fellow for Strategic Systems Analysis and Engineering at NETL. Since joining the Lab in 2009, Miller has spearheaded revolutionary modeling systems that are accelerating the advancement of critical energy technologies.

Miller helped create and implement the Carbon Capture Simulation Initiative (CCSI), serving as its technical director. He also leads the Institute for the Design of Advanced Energy Systems (IDAES), which was formed in 2016 as a collaboration between several national laboratories and universities to develop new process systems engineering capabilities to improve the efficiency of fossil-based power plants while accelerating the development of other advanced energy systems. In 2020, IDAES was named a recipient of the highly prestigious R&D 100 Award, which recognizes the top 100 technology developments in the past year.

In addition to his groundbreaking work with NETL, Miller taught at the college level for 10 years. He spent the majority of his time at his alma mater, Rose-Hulman Institute of Technology, reaching the rank of associate professor. His time in academia imparted an understanding of how to mentor effectively and best utilize the research work of doctoral students.

Miller's background and unique perspectives in research are enabling continuous progress at NETL and fostering the latest breakthroughs in process systems engineering.

> **"IDAES is continuing to advance its underlying capabilities to better address energy and industrial challenges, including deep decarbonization and integrated energy systems."**

What is the goal of IDAES and its impact so far?

There are two primary goals of IDAES. The first is to develop the modeling and optimization capabilities needed to design and operate the advanced energy systems of the future, which will be more dynamic, flexible and interconnected than ever before. The second is to apply and deploy those capabilities to assist technology developers, power companies, researchers and DOE to identify the most promising concepts, understand emerging needs and opportunities, scale up new technologies and ultimately enable a sustainable energy future.

As just one example of our success, the IDAES team worked with Tri-State Generation and Transmission Association Inc.'s Escalante Generating Station, located in Prewitt, New Mexico. A single, multipurpose model within IDAES enabled an effective workflow that included data reconciliation, parameter estimation, model validation and system-wide optimization. Using operating data, the team constructed a predictive model of the entire plant and applied it to generate meaningful insights that resulted in the plant improving its minimum operating load by 44%, significantly reducing fuel cost and CO_2 emissions when demand for electricity is low.

How would you describe the capabilities within IDAES, and what makes it unique?

IDAES provides revolutionary new capabilities for process systems engineering that exceed existing tools and approaches. There are a number of capability gaps in current computational tools that limit their ability to address emerging challenges that require more dynamic analysis and optimization across multiple scales. The tremendous researchers of the IDAES technical team are achieving these goals through teamwork, collaboration and innovation across our partner labs and universities.

After years of development, IDAES has established an extensive modeling library integrated with a suite of advanced machine learning, uncertainty quantification and optimization techniques that enable process optimization, parameter estimation, advanced process control and multi-scale analysis across various levels of implementation. With its equation-oriented modeling approach, IDAES uniquely supports the process modeling lifecycle, from conceptual design to dynamic optimization and control.

What will the future of IDAES look like?

IDAES is continuing to advance its underlying capabilities to better address energy and industrial challenges, including deep decarbonization and

Continued on page 38

integrated energy systems. These tools and capabilities will help identify, design and scale up the new technologies needed to address societal challenges and understand complex interactions among industrial processes, energy generation and distribution, supply chains and markets.

Some recent advancements in IDAES include new abilities to link advanced control algorithms with grid dispatch models to enable greater flexibility while mitigating equipment damage due to thermal stress. IDAES is also exploring a way to computationally explore large design spaces to identify new hybrid energy systems to address emerging needs of the grid while also meeting environmental and sustainability imperatives.

What led you to NETL, and how did your previous experiences benefit your current research?

Over the past 30 years, I've had a number of diverse professional opportunities to apply my skill and knowledge while continuing to learn and grow. Through an internship with a major pharmaceutical company following undergrad and my first professional job with Procter & Gamble, I gained experience working in industry.

I discovered my research passion when I saw the work of a small modeling and simulation group, and I decided that was what I wanted to do. My first faculty position was at Michigan Technological University in the Upper Peninsula, where I experienced snow measured in feet and met a number of lifelong friends. During my second year there, I learned of a faculty opening at my undergraduate alma mater and decided to apply. I got an offer and pursued my dream job. I taught for eight more years, reaching the rank of associate professor with tenure before leaving to pursue my research goals at NETL.

My time at the Lab has been extremely professionally rewarding, and it has been an honor to work with such a talented and energized group of collaborators. As a national laboratory, we have the potential to make a significant difference in the lives of all people through our technology innovation.

What experiences from teaching did you bring to NETL?

One of the most important aspects of being an effective professor or mentor is two-way communication. Setting clear expectations and being able to understand how you could be misunderstood are key, as well as sharing complex information in a straightforward manner and being responsive to questions — not just the question asked, but the issues, concerns and constraints underlying the question. I've been able to apply these lessons when working with diverse, multidisciplinary research teams to help them reach their full potential.

Leveraging my diverse background has enabled me to bring together strengths and abilities of university researchers while being cognizant of their needs to conduct innovative research, publish papers and make original contributions. Among the strengths of initiatives such as CCSI and IDAES is their ability to co-develop new capabilities so they can be combined and utilized much more rapidly than being under separate projects. Thus, the contributions of Ph.D. students can be available for broader use almost instantly. The acceleration of this innovation life cycle helps make these initiatives so successful in addressing complex problems that could not be addressed only a few years ago.

What have been your most rewarding experiences as both a professor and an energy researcher?

The success of the team, both as a group and as individuals, is the most rewarding aspect of my career. For example, my first thought when learning about IDAES' R&D 100 Award win was how proud I was of the team and how happy I was to see them recognized for their hard work and accomplishments.

Additionally, mentoring students and younger researchers is important to me. I'm continually impressed when witnessing the development of close collaborations that can achieve far more than the sum of their parts — collaborations that are multiplicative in their impact, not just additive — as well as seeing students and researchers overcome technical challenges to achieve more than they thought possible. ≡

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Vol. 03/ 2021 Issue 01