OAK RIDGE NATIONAL LABORATORY

Review

Testing a wild theory:

Oak Ridge National Laboratory

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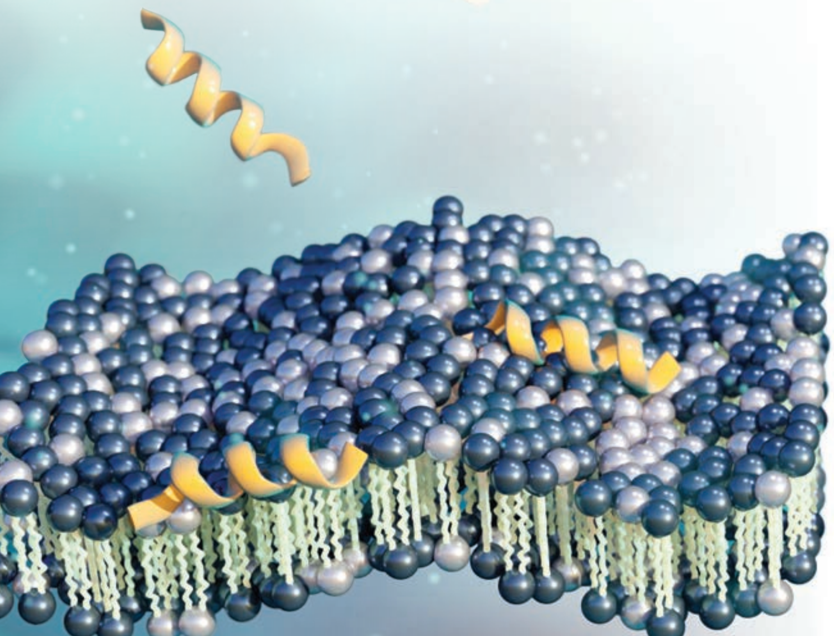
Contents



On the Cover

ORNL physicist Leah Broussard and colleagues explore the neutron lifetime puzzle. Image credit: Carlos Jones, ORNL

The uniqueness of ORNL

At the beginning of the year, I returned to Oak Ridge National Laboratory as interim director. For more than 20 years, I had the privilege to serve this institution as deputy for operations, and it is an honor to support ORNL while the search for a permanent laboratory director continues.

In my first weeks back on campus, I interacted with many staff members — new and old — to learn what has been happening since I retired in 2021. As I have gone through those conversations with colleagues from across the laboratory, I have been reminded of what a special place ORNL is — something Laboratory Director Alvin Weinberg summarized in the first issue of *ORNL Review* in 1967:

> *"Is anything really lost if a big laboratory becomes only a collection of weakly interacting little laboratories? To my mind, the laboratory's very essence is lost, both in applied research and basic research. In basic research the strength of laboratories like ORNL lies in the interdisciplinary composition of their staffs. Over and over again it has been demonstrated that the whole can be greater than the sum of its parts, that good people from diverse fields working together can make major scientific discoveries that are denied geniuses working in isolation."*

The uniqueness of ORNL lies in how our staff comes together to deliver a broad impact across basic and applied science — translating fundamental discoveries into technologies and applications that support the nation's security, energy needs and economic prosperity. Though the scientific questions have changed, it is what we have done since the days of the Manhattan Project.

Today, the challenges we address include impacts from climate change and the essential transition to sources of clean energy. Our 6,000 staff members are producing results only possible at an institution with ORNL's mix of uniquely powerful facilities, diverse expertise and mission-driven research. This issue of *ORNL Review* has multiple examples of these impressive efforts.

Our scientists used the Spallation Neutron Source to explore ways to combat rapidly evolving bacteria that does not respond to antibiotics (see "Neutrons show how promising peptide fights antibiotic-resistance bacteria" page 16).

We have developed innovative techniques using seismology to monitor the transport of nuclear material (see "Researchers use seismology, radiation detection to bolster nonproliferation efforts" page 20).

Within grid technology, ORNL researchers used new methods to stay ahead of wildfires and worked to bring independent microgrids to vulnerable areas (see "ORNL sensor research helps fight wildfires" page 22; "ORNL research to bring more reliable electricity to Puerto Rican microgrids" page 24).

It is also exciting to see the early impact and passion from some of our newest scientists and engineers (see "The best is yet to come: ORNL's Early Career Research Program award winners" page 30; "Why Science?" page 34).

Over the coming months, I look forward to continuing to have a front-row seat to the exceptional work taking place at this special institution. I am glad you have an opportunity to see a small sample of what is going on at the laboratory in this issue of *ORNL Review*.

Jeff W. Smith
Interim Laboratory Director

Energy secretary attends isotope facility event

U.S. Secretary of Energy Jennifer Granholm visited ORNL to attend an October 2022 ground-breaking ceremony for the U.S. Stable Isotope Production and Research Center. The facility is slated to receive $75 million in funding from the Inflation Reduction Act.

The facility on ORNL's main campus will produce stable isotopes on a large scale, meeting the nation's increasing demands for isotopes needed in medicine, industry, science and national security. The 64,000-square-foot facility will dramatically expand the United States' isotope enrichment capabilities, reducing dependence on foreign suppliers.

"The Biden–Harris Administration is proud to help Oak Ridge open the doors of this new center, along with the other projects receiving funding as part of the President's agenda — here and across our national labs. This funding is a down payment on our clean energy future, and we are excited to see what America will now achieve because of it," Granholm said.

East Tennessee has a rich history of producing enriched stable isotopes, generating more than 230 between 1945 and 1998 at the now-decommissioned calutron facility at the Y-12 National Security Complex. However, those stockpiles are now being depleted, and the U.S. has no existing domestic broad-scope enrichment capability.

"The construction of a new isotope production facility at ORNL is a historic milestone," said Thomas Zacharia, who retired as ORNL director at the end of 2022. "Providing isotopes that can't be made anywhere else is central to our identity as a national laboratory, and we are fortunate to have some of the most talented experts in the world advancing this capability here at a time of great international need."

ORNL has spent the past decade designing, researching, developing and prototyping the two types of isotope separation equipment that SIPRC will employ. The center will be capable of simultaneously enriching multiple stable isotopes from across the periodic table. It's also been designed with future expansion in mind. — *Kristi Nelson Bumpus*

Energy Secretary Jennifer Granholm shared the importance of producing stable isotopes on a large scale, meeting the nation's increasing demands for isotopes needed in medicine, industry, science and national security. She led the groundbreaking ceremony of the lab's new U.S. Stable Isotope Production and Research Center, or SIPRC. Image credit: Carlos Jones, ORNL

Racing company licenses ORNL battery technology

Marc-Antoni Racing has licensed a collection of patented energy storage technologies developed at ORNL. The technologies focus on components that enable fast-charging, energy-dense batteries for electric and hybrid vehicles and grid storage.

The New England–based company is exploring ways to move the racing industry away from fossil fuels while maintaining the dynamic driving experience loved by motor sports enthusiasts.

Susan Hubbard, ORNL's deputy for science and technology, and Ricardo Marc-Antoni Duncanson, founder of Marc-Antoni Racing, pose for a photograph during a licensing celebration event on Oct. 17. Image credit: Carlos Jones, ORNL

The licensed ORNL patents for battery components — anode, cathode and electrolyte solution — are based on discoveries by ORNL's Sheng Dai, Xiao-Guang Sun, Parans Paranthaman, Gabriel Veith and Craig Bridges. The members of this accomplished team are Battelle Distinguished Inventors, corporate fellows and distinguished staff scientists in chemical and materials science. They have received numerous accolades, including R&D 100 Awards.

Through new combinations of materials and design, the team has discovered components that break the barrier to fast-charging, power-dense lithium-ion batteries for electric vehicles. Additionally, the components meet a key DOE goal of reducing vehicle battery charging time to under 15 minutes, which gets EV charging closer to the time needed to refuel a gas-powered vehicle. Charging time is a major obstacle to the widespread adoption of EV technology needed to achieve the nation's goal of net-zero carbon emissions by 2050. — *Karen Dunlap*

ORNL's Humble to direct Quantum Science Center

Travis Humble has been named director of the Quantum Science Center headquartered at ORNL. The QSC is a multi-institutional partnership that spans industry, academia and government institutions and is tasked with uncovering the full potential of quantum materials, sensors and algorithms.

Humble was named deputy director in 2020, when DOE established this five-year, $115 million effort as one of five National Quantum Information Science Research Centers. Following the departure of former QSC Director David Dean, Humble began serving as interim director in January.

"I am excited to be working at the forefront of quantum science and technology with this amazing team of scientists and engineers," he said. "The QSC provides a wonderful opportunity to leverage our nation's best and brightest for solving some of the most interesting scientific problems of our time."

Travis Humble

As interim director, Humble oversaw the QSC's three primary focus areas: quantum materials discovery and development, quantum algorithms and simulation, and quantum devices and sensors for discovery science. In his new role, he will continue collaborating with QSC partner institutions including ORNL, Los Alamos National Laboratory, Fermi National Accelerator Laboratory, Purdue University, Microsoft and IBM.

Humble joined ORNL as an intelligence community postdoctoral research fellow in 2005, then became a staff member in 2007. He received a bachelor's degree in chemistry from the University of North Carolina, Wilmington, and a master's degree and doctorate in theoretical chemistry from the University of Oregon.

As QSC director, Humble will prioritize the development of quantum materials for quantum computing and quantum sensing, as well as the application of these technologies to aid scientific discovery, improve the nation's security and energy efficiency and ensure economic competitiveness. Other goals include demonstrating the advantages of early quantum computers and advancing methods for probing the fundamental physics of quantum matter. — *Elizabeth Rosenthal*

Existing water pipes are an untapped power source

Millions of miles of pipelines and conduits across the United States make up an intricate network of waterways used for municipal, agricultural and industrial purposes.

In a new report, ORNL researchers have found potential opportunities in all 50 states to efficiently utilize existing infrastructure to harvest this otherwise wasted energy.

A hydropower turbine is installed into an existing drinking water distribution system in Palmdale, California. Image credit: Canyon Hydro

In a first-of-its-kind analysis, ORNL estimates that conduit hydropower, which uses water from structures such as water supply pipelines and irrigation canals, has the potential to add 1.41 gigawatts of electricity to the country's power grid — enough to power more than a million homes.

"You can think of conduit hydropower as low-hanging fruit, and what has been started is a mere drop in the bucket," said Shih-Chieh Kao, water power program manager at ORNL. "For all its benefits, the biggest barrier is a general lack of awareness of conduit hydropower's potential."

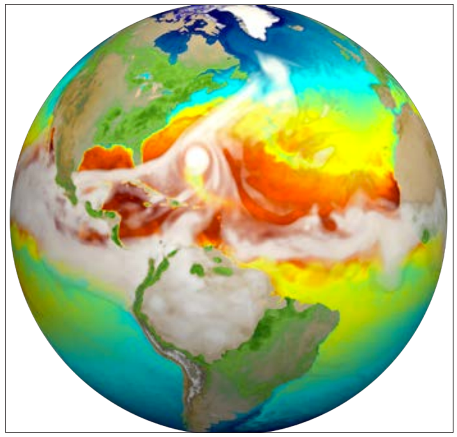
The process for municipalities and other stakeholders to develop conduit hydropower would be relatively easy. Without the need to build new dams, facility operators could install hydropower generators at locations with excess hydraulic head — the height of water needed for hydropower generation. This could be coordinated with planned facility upgrades that replace aging infrastructure with more energy-efficient systems. Rural communities may benefit by adding small hydropower generation to their existing infrastructure for net metering, making them less dependent on the external grid.

Because conduit hydropower taps into existing infrastructure with minimal environmental impacts, the permitting process is streamlined. Through the Hydropower Regulatory Efficiency Act of 2013 and its amendments in America's Water Infrastructure Act of 2018, the federal regulatory approval process can be completed in 45 days. To date, more than 350 conduit hydropower projects have been permitted or constructed, with more to come. — *Kim Askey*

For more information:
https://bit.ly/3DEp5uu

Earth system coalition to boost data speed, ease

The Earth System Grid Federation, a multiagency initiative that gathers and distributes data for top-tier projections of the Earth's climate, is preparing a series of upgrades that will make using the data



A simulation of the planet from the DOE Energy Exascale Earth System Model, one of the large-scale models incorporated in the Earth System Grid Federation led by DOE's Oak Ridge, Argonne and Lawrence Livermore national laboratories. Image credit: LLNL

easier and faster while improving how the information is curated.

The federation, led by ORNL in collaboration with Argonne and Lawrence Livermore national laboratories, is integral to some of the most important, impactful and widely respected projections of the Earth's future climate: those made by scientists working with the Coupled Model Intercomparison Projects for the World Climate Research Programme.

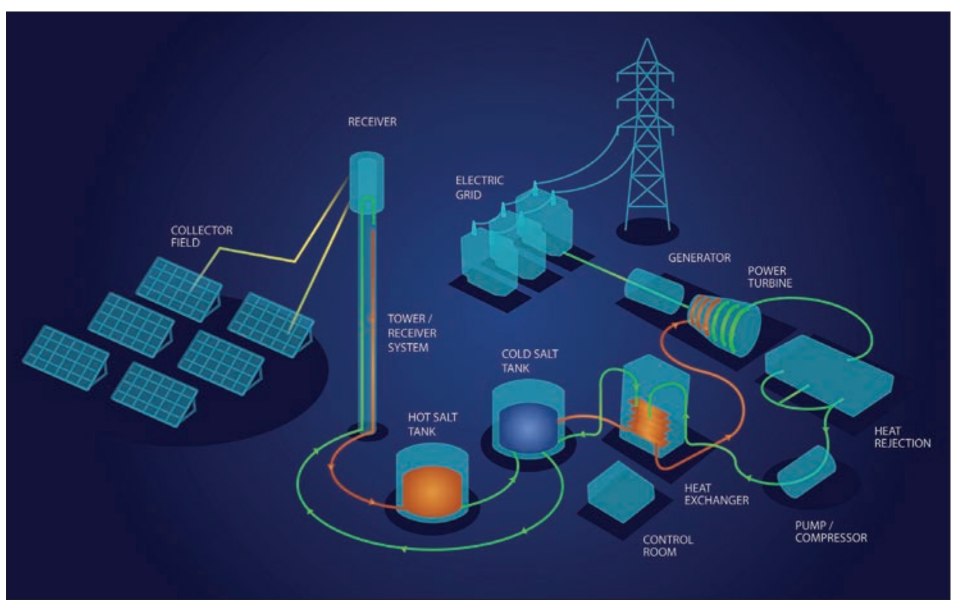
"ESGF data are about the future of life on Earth," said Forrest Hoffman, lead for ESGF and the Computational Earth Sciences group at ORNL. "By providing scientists easy access to the full collection of international models, ESGF enables them to make the very best guess about the future trajectory of our climate."

A key ESGF mission is to support the data needs of scientists who prepare the United Nations Intergovernmental Panel on Climate Change's comprehensive climate assessments released every six to seven years. ESGF data underpins IPCC landmark reports such as the recent Sixth Assessment Report, AR6, and its working group findings. The data also informs IPCC special reports focused on climate vulnerabilities, adaptation scenarios and mitigation strategies. — *Stephanie Seay*

Scientists develop method for purifying molten salts

ORNL scientists recently demonstrated a low-temperature, safe route to purifying molten chloride salts that minimizes their ability to corrode metals. This method could make the salts useful for storing energy generated from the sun's heat.

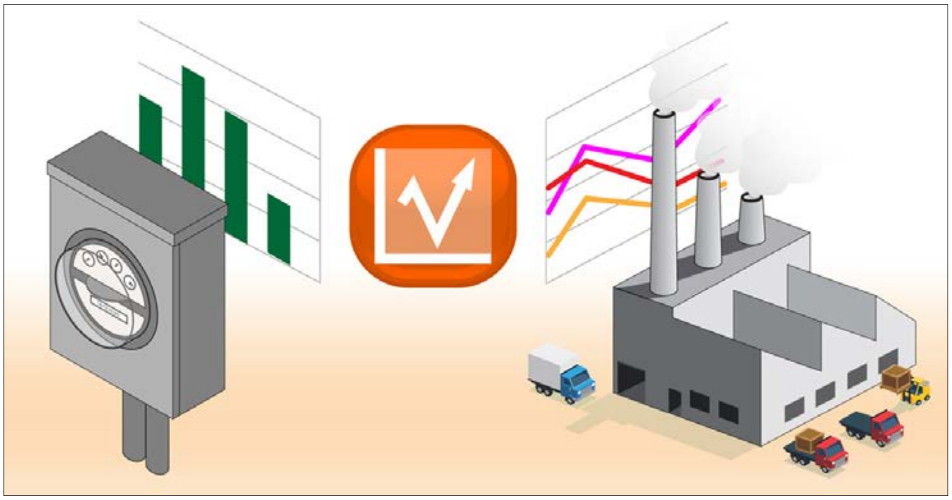
The experiment, detailed in *Frontiers of Chemical Engineering*, involved using thionyl chloride to remove corrosion-causing impurities from the salts. Without



This diagram demonstrates how a concentrating solar-thermal plant could use molten salts to store solar energy that could later be used to generate electricity. Image credit: Jaimee Janiga, ORNL this purification, the salts corrode pipes and storage tanks.

The team melted a commercial carnallite — an abundant mineral being considered for solar-thermal energy storage — and put it in contact with inert gas saturated with thionyl chloride to cause a reaction. The scientists monitored reaction conditions by measuring salt temperature and by analyzing the off-gas through infrared spectroscopy.

"Using high-temperature molten salts to store energy as heat could be key in making solar energy a consistent source of electricity, replacing fossil fuels," said ORNL's Joanna McFarlane, who led the team that performed the experiment. — *Kristi Nelson Bumpus*



A new online tool called VERIFI, developed by ORNL researchers, provides an easy-to-use dashboard for plant managers to track carbon emissions produced by industrial processes. Image credit: ORNL

Moss genome study identifies two new species

A team from ORNL, Duke University and other institutions studying *Sphagnum* moss have identified two new species in North America, and they are learning how evolution may affect the species' role in carbon storage.

Researchers looking at moss samples from far-flung habitats used genome sequencing and advanced computation to identify differences within the *Sphagnum magellanicum* complex. So far, they have discovered *S. magni* and *S. diabolicum*, which differ in geographic distribution and may have evolved in response to climate.

"By understanding their evolution and genetic diversity, we can start to link some of the traits of these organisms to their impact on carbon cycling," said ORNL's Bryan Piatkowski.

Sphagnum is the chief engineer of peatlands in the Northern Hemisphere, where one-third of terrestrial carbon is stored. The moss's response to warmer temperatures can inform predictions about how much carbon will stay locked away in soils or be released to the atmosphere. — *Stephanie Seay*

Scientists used genome sequencing and computational biology to tease out the genetic profile of a new moss species, Sphagnum magni, typically found in the southeastern United States. Image credit: Blanka Aguero, Duke University

Online tool helps firms track carbon emissions

ORNL researchers have developed an online tool that offers industrial plants an easier way to track and download information about their energy footprint and carbon emissions.

Visualizing Energy Reporting Information and Financial Implications, or VERIFI, is a tool that uses an open-source framework with a utility dashboard. It allows energy coordinators and plant managers to monitor and improve their understanding of energy- and water-use patterns, including the amount of carbon emitted from industrial processes. Users can generate automatic reports, too.

"Industries want to know how to conserve and improve efficiency while reducing costs but often don't know how to begin or lack the time to track it," ORNL's Kristina Armstrong said. "VERIFI provides a user-friendly platform for monitoring energy efficiency benchmarks and baselines and allows for the visualization of energy and utility bills."

ORNL is testing VERIFI for the Department of Energy's Better Plants Program. — *Jennifer Burke*

ORNL's Sheng Dai named DOE Distinguished Fellow

ORNL Corporate Fellow and section head Sheng Dai has been selected by the DOE Office of Science as a 2023 Distinguished Scientist Fellow. The competitive award recognizes exceptional scientists from the national laboratories with strong records of academic and university collaborations. The opportunity provides each fellow with $1 million over three years to support activities that develop, sustain and promote scientific and academic excellence in Office of Science research.

Sheng Dai

Dai received the award for "pioneering advances in development of functional materials for separation science, energy storage, catalysis and other energy-related applications and for excellence in leading team science and mentoring the next generation of researchers."

"This award is further evidence of Sheng's talent as both a scientist and a leader," ORNL Director Thomas Zacharia said. "He has long exemplified the quality and impact we seek for our research at Oak Ridge, and it is a well-deserved honor that the Office of Science has selected him for this fellowship."

At ORNL, Dai leads the Separations and Polymer Chemistry section of the Chemical Sciences Division. He oversees diverse team projects on carbon and composites, chemical separations, nanomaterials chemistry and soft matter. His research interests include ionic liquids and porous materials and their applications for separation sciences and energy storage as well as catalysis by nanomaterials. He also holds a joint faculty appointment in the Department of Chemistry at the University of Tennessee, Knoxville. — *Ashley Huff*

ORNL report addresses hydropower sustainability

ORNL has provided hydropower operators with new data to better prepare for extreme weather and shifts in seasonal energy demands caused by climate change.

For the new report, ORNL researchers used downscaled global climate projections to simulate future hydrologic conditions at 132 federal hydropower facilities across the United States. The resulting projections will enable hydropower operators and policymakers to plan for changing climate conditions and reduced water availability by shifting their operational schedules and their use of water each season as part of an overall mitigation strategy.

"The intensification of future extreme events, including both floods and droughts, is one of the most critical issues threatening the resilience of U.S. hydropower systems and infrastructure," said Shih-Chieh Kao, water power program manager at ORNL. "This new normal requires us to think differently about current operational practices to adapt to a changing climate."

In addition to extreme events, a growing conflict in water availability versus energy demand is a looming challenge for hydropower operators. Earlier-than-expected snowmelt seasons in the western United States likely will impact water runoff. This scenario may result in less water for hydropower generation in the summer months, just as energy demand grows. Increased evaporation because of rising temperatures is also putting a strain on water needed for flood control, navigation, municipal water supplies and industrial and agricultural use.

Better understanding of these changes is important to future energy planning. Hydropower provides 35 percent of renewable energy and nearly 7 percent of all electricity produced in the U.S. — *Mimi McHale*

Commercial partners using ORNL building models

Two years after ORNL provided a model of nearly every building in America, commercial partners are using the tool for tasks ranging from designing energy-efficient buildings and cities to linking energy efficiency to real estate value and risk. International companies like Google and SmithGroup are sharing the benefits by making the resulting data publicly available. Because the buildings sector accounts for 40 percent of American energy consumption, increasing its efficiency is vital to national decarbonization goals.

ORNL is studying how climate change may impact water availability for hydropower facilities such as the Shasta Dam and Lake in California. Image credit: U.S. Bureau of Reclamation

Dozens of companies have requested data from ORNL's Automatic Building Energy Modeling software suite, or AutoBEM, said project leader Joshua New. He and his team developed AutoBEM using high-performance computing to process layers of imaging data with information about individual buildings, such as their size, use, construction materials and heating and cooling technologies.

"The unifying theme is to create a digital twin of our nation's buildings," New said. "We can simulate market-relevant ways to reduce energy use and offset with renewable sources."

The software has simulated energy use for 123 million structures, representing 98 percent of U.S. buildings. New's team has been updating the software in 2022 for even greater building detail and accuracy.

Google is using AutoBEM to improve its free Environmental Insights Explorer tool, which launched in 2018 to help cities worldwide recognize sources of greenhouse gas and reduction opportunities. Saleem Van Groenou, product manager for Environmental Insights Explorer, said Google wants to incorporate more precise energy efficiency simulations for buildings.

"Oak Ridge has much deeper expertise in building energy systems and modeling management and action than we do," Van Groenou said. "We can now help cities focus more on what changes should be made, then track the impact of those changes over time."

Most users of AutoBEM focus on existing buildings, but SmithGroup, an international architecture and engineering firm, takes the approach of incorporating efficiency from the first blueprint.

"Our interest in AutoBEM and working with the lab stems from a dramatic need to scale the work we're doing in response to climate change," said Stet Sanborn, who oversees the ORNL collaboration for SmithGroup. "The number of buildings we need to touch, and the pace we need to do it, exceeds what an individual could do in their lifetime. And we need to do that in the next five years." — *S. Heather Duncan*

ORNL's software suite AutoBEM is being used in the architecture, city planning, real estate and home efficiency industries. Users take advantage of the suite's energy modeling of almost all U.S. buildings.
Image credit: ORNL

ORNL's Rama Vasudevan named APS Fellow

ORNL research scientist Rama Vasudevan has been elected a Fellow of the American Physical Society. The honor recognizes members who have made significant contributions to physics and its application to science and technology.

Vasudevan was cited by the APS Topical Group on Data Science for "pioneering and visionary development of open-sourced physics-based machine learning methods in atomic-scale and mesoscopic imaging, and their application in physics."

Rama Vasudevan

At ORNL, Vasudevan leads the Data NanoAnalytics group at the Center for Nanophase Materials Sciences, which is a DOE Nanoscale Science Research Center. His research connects microscopy with machine learning and artificial intelligence to advance materials science. Vasudevan is part of an emerging effort to build smart, "self-driving" instruments and develop new techniques to accelerate the design and discovery of new materials. As a materials scientist, he focuses on oxide, ferroelectric, and memristive materials with unique functional properties for computing and electronic applications.

Vasudevan received a doctorate in materials science from the University of New South Wales. He first joined ORNL as a postdoctoral researcher in the Scanning Probe Microscopy Group and was hired as ORNL staff in 2016.

He sits on the editorial board of the IOP journal *Machine Learning: Science and Technology*. In 2019 Vasudevan and his colleagues were awarded a *Microscopy Today* Innovation Award by the Microscopy Society of America. — *Ashley Huff*

Frontier study

could uncover new cures, treatments

by Matt Lakin
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The world's fastest supercomputer could help discover the next great cure hiding in plain sight.

ORNL researchers used Frontier, the world's first exascale computer — capable of more than a billion billion calculations a second — to scan hundreds of thousands of biomedical concepts from millions of scientific publications in search of potential connections among symptoms, diseases, conditions and treatments. The effort began as part of the fight against COVID-19 but could become as essential to basic diagnosis and treatment as Google is to an online search.

"We're connecting dots at high speed," said Ramakrishnan "Ramki" Kannan, the study's lead author and an ORNL computational scientist. "We want to take these medical concepts, connect them and show how they relate to each other."

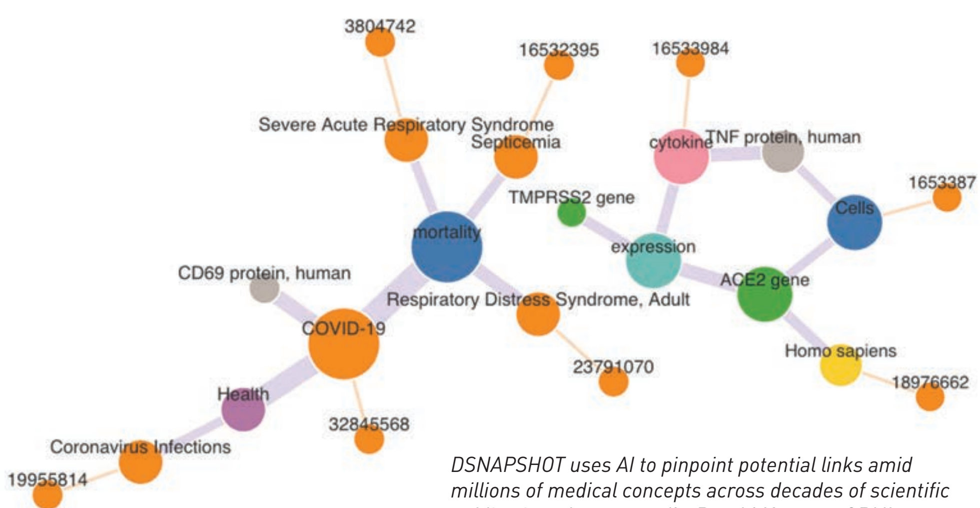
The study earned the team a finalist nomination for the Association of Computing Machinery Gordon Bell Prize, which recognizes outstanding achievements in applying high-performance computing to challenges in science, engineering and large-scale data analytics.

The project seeks to push the fast-forward button on drug discovery to streamline exploration. The inspiration came in early 2020 during the COVID-19 pandemic, when scientists around the world focused on searching for potential treatments.

Kannan and fellow scientist Tom Potok of ORNL's Computer Science and Mathematics Division led a team that developed the Distributed Accelerating Semiring All-Pairs Shortest Path algorithm, or DSNAPSHOT, a method using AI to pinpoint potential links amid millions of medical concepts across decades of scientific publications. The team aimed the algorithm at a dataset drawn from more than 800,000 papers on COVID-19 and associated coronaviruses.

"What do we already know, and where can it lead us?" Kannan said. "For example, patients with COVID-19 often have fevers. Can a drug that treats other kinds of fever help treat this disease?"

The team used DSNAPSHOT and another algorithm — the Communication-Optimized All-Pairs Shortest Path, or COAST — to plot each concept already identified by scientists across a graph and



DSNAPSHOT uses AI to pinpoint potential links amid millions of medical concepts across decades of scientific publications. Image credit: Ramki Kannan, ORNL

ORNL computational scientists Tom Potok, left, and Ramki Kannan.
Image credit: Carlos Jones, ORNL

draw virtual paths between the various points. They sought to expand the digital dragnet from that dataset to a graph of concepts pulled from the U.S. National Library of Medicine's PubMed database and used Summit, Frontier's predecessor, to power the search.

"Some of these connections will be obvious, some will be unworkable, and some will be promising," Potok said. "Can we narrow the results to what's promising?"

Even Summit could process only about a sixth of the graph, which spanned more than 35 million PubMed citations. The team turned to Frontier, fresh from its spring 2022 debut as the world's fastest supercomputer at 1.1 exaflops, or more than 1 quintillion calculations per second.

"We knew we needed a next-generation computer of this caliber to achieve what we wanted," Kannan said. "Frontier solved the problem we couldn't solve on Summit."

The team used 9,200 of Frontier's more than 9,400 nodes to perform an initial search across a graph drawn from PubMed and the Scalable Precision Medicine Open Knowledge Engine, or SPOKE, a comprehensive index of medical databases maintained by the University of California, San Francisco. The run took only 11.7 minutes to search more than 7 million data points drawn from 18 million publications.

"The next steps require further studies such as clinical trials to validate," Kannan said. "There may be connections we would never discover otherwise. We want to index and understand the relationships between all of these — the diseases, symptoms, treatments, complications — so during the next pandemic we can have potential answers closer at hand."

Accelerating drug discovery with AI

by Coury Turczyn
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A team of ORNL computational scientists has designed a machine-learning software stack called TwoFold that predicts how strongly a given drug molecule will bind to a pathogen, as well as the 3D structure of how it will attach to the target. This vital information can greatly shorten the trial-and-error process of lab experimentation usually needed to find viable drug candidates, especially for novel viruses like COVID-19, the structures of which are yet unknown.

"Together, these two representations — binding strength and structure — give pharmaceutical researchers more information to decide whether a molecule is worth pursuing as a drug candidate. This will reduce the amount of time, effort, and money spent on the experimental side," said project team leader Jens Glaser, a computational materials scientist at the National Center for Computational Sciences.

A finalist for the 2022 Gordon Bell Special Prize for HPC-Based COVID-19 Research, TwoFold was inspired by the ORNL team's previous efforts early in the pandemic to identify candidates for new COVID-19 therapeutics. The virtual screenings conducted on ORNL's Summit supercomputer used AI to help identify molecular candidates that could more efficiently bind with the virus's proteins and potentially disrupt them. But they found that this methodology alone wasn't informative enough to effectively narrow the field of drug options.

"It's not sufficient to only predict the single number that characterizes how strongly a molecule will bind against its viral target, because 90 percent of drugs fail in clinical trials," Glaser said. "Even with in vitro experiments, it's realistic to expect that only 1 percent of compounds are active against the target.

"So, we asked ourselves, what is holding us back from routinely producing good predictions? And we found that the big factor is a lack of efficient, reliable and accurate structure prediction for novel, unseen targets."

> *In our case, once we have the protein's amino acid sequence — which can be easily obtained way before the crystallization that allows you to determine the target structures — you can already start the drug development process. By simply inputting the target sequence, TwoFold gives you a head start — it shortens your time to solution for proposing possible candidates.*
>
> — Postdoctoral research associate **Darren Hsu**

Without a map of a virus's structure and its possible protein targets — which is a very likely shortcoming in the case of a new disease like COVID-19 — researchers face a slow, hit-or-miss effort to identify drug candidates. Protein structures are usually mapped through the process of crystallization, in which a protein is dissolved in an aqueous solution until it reaches a supersaturated state and its molecules align themselves in a crystalline lattice. The resulting pattern can then be analyzed to determine the protein's 3D structure. This laborious process may take anywhere from a month to a year or more. That means any

TwoFold team members, from left, Michael Matheson, Darren Hsu, Feiyi Wang, John Gounley, Hao Lu, Jens Glaser and Aditya Kashi.
Image credit: Genevieve Martin, ORNL

methodology that requires protein structures to effectively identify drug candidates will be on hold until the crystallization is completed and analyzed. Not so with TwoFold.

"In our case, once we have the protein's amino acid sequence — which can be easily obtained way before the crystallization that allows you to determine the target structures — you can already start the drug development process," said team member Darren Hsu, a postdoctoral research associate at the NCCS. "By simply inputting the target sequence, TwoFold gives you a head start — it shortens your time to solution for proposing possible candidates."

The ORNL team achieved this predictive twofer by devising a new methodology that computes its results in two steps conducted on two supercomputers, Frontier and Summit, both of which are managed by ORNL's Oak Ridge Leadership Computing Facility.

First, a neural network — an AI component trained to recognize patterns in datasets — was trained by the team on Summit with experimental data for drug-target interactions and receptor-bound structures. Second, this deep learning model produced a matrix of millions of equations that was solved on the even more powerful exascale-class Frontier supercomputer.

With its unprecedented speed and accuracy, TwoFold could help make supercomputers an integral tool in drug research, thereby greatly accelerating the discovery process.

For more information: https://bit.ly/3k7ExI4

Computational tools promote children's mental health

by Leo Williams
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Computational researchers from ORNL are working with a Cincinnati children's hospital to better predict and address mental health disorders in children.

The five-year collaboration between the lab and Cincinnati Children's Hospital Medical Center will leverage ORNL's strengths in high-performance computing, health data analysis and artificial intelligence to improve the hospital's approach to predicting and treating childhood mental illness, focusing first on anxiety, then on depression and finally on suicidal thoughts and self-harm.

The collaboration comes at an important time. The Centers for Disease Control and Prevention estimates that nearly 6 million children from 3 to 17 years old suffered from anxiety between 2016 and 2019, while nearly 3 million experienced depression. The agency says both conditions are on the rise.

According to ORNL computational scientist Greeshma Agasthya, the project aims to develop mental health trajectories for children who visit the hospital, correlating information ranging from medical diagnoses to the children's home environments with the likelihood that they will develop mental illnesses.

"You've seen growth charts for children," Agasthya said. "Just like growth charts can help predict the expected height and weight of a child at different ages, we aim to build similar charts for pediatric mental health trajectories that can help predict the occurrence of mental health disorders in children."

> *You've seen growth charts for children. Just like growth charts can help predict the expected height and weight of a child at different ages, we aim to build similar charts for pediatric mental health trajectories that can help predict the occurrence of mental health disorders in children.*
>
> — ORNL computational scientist **Greeshma Agasthya**

Electronic health records data from CCHMC covers children and young adults from birth to age 25. It includes young people both before and after they develop mental health disorders, as well as those who don't develop any mental health disorders.

The project kicked off at the end of 2021, with CCHMC delivering a hard drive of anonymized patient data to the lab, where it was uploaded to a secure computer server within ORNL's Knowledge Discovery Infrastructure.

Agasthya noted that ORNL has created several secure infrastructures to house and work with sensitive health data from agencies such as the National Cancer Institute and the Department of Veterans Affairs.

The first challenge was to get the CCHMC data into a format that could be used in deep learning models. Agasthya said the researchers are looking at three types of data. The first, known as tabular data, consists of information such as blood pressure, test results and diagnoses as well as the child's age, sex, race, ethnicity and language of preference.

The second source of data comprises notes taken by doctors, nurses and other health care providers. To process this information, researchers employ natural language processing methods to automate the search both for specific keywords and for the contexts in which they are used.

Finally, the project looks at data on environmental factors experienced by the patients, such as family income, education levels of the parents, air pollution in the child's neighborhood and neighborhood crime rates.

Agasthya noted that ORNL is an ideal collaborator for this undertaking. Not only does the lab's Oak Ridge Leadership Computing Facility house two of the world's four most powerful supercomputers — No. 1 Frontier and No. 4 Summit — the lab is also home to world-leading experts in machine learning, artificial intelligence and quantum information science.

The outcomes from the Cincinnati project will enable early intervention in clinics by helping health care providers identify children who are likely to develop mental health disorders before they manifest and disrupt patients' lives.

"We have information for both patients with and without mental health illness," Agasthya said. "Using this information, we will create computational models to determine, given a child's baseline, what is the probability of the child developing a mental health disorder in the next six months, one year, five years, 10 years and so on. We can also identify the most important factors that influence a person's mental health in the first 25 years of their life."

Physicists confront

the neutron lifetime puzzle

by Dawn Levy
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To solve a long-standing puzzle about how long a neutron can live outside an atomic nucleus, a team of physicists entertained a wild but testable theory positing the existence of a right-handed version of our left-handed universe.

They designed an experiment at ORNL to try to detect a particle that has been speculated but not spotted. If found, the theorized "mirror neutron" — a dark-matter twin to the neutron — could explain a discrepancy between answers from two types of neutron lifetime experiments and provide the first observation of dark matter.

"Dark matter remains one of the most important and puzzling questions in science — clear evidence we don't understand all matter in nature," said ORNL physicist Leah Broussard, who led the study.

Neutrons and protons make up an atom's nucleus. However, they also can exist outside nuclei. Last year, using the

ORNL's Leah Broussard shows a neutron-absorbing wall that stops all neutrons but in theory would allow hypothetical mirror neutrons to pass through. Image credit: Genevieve Martin, ORNL

ORNL's Matthew Frost and Leah Broussard used a neutron scattering instrument at the Spallation Neutron Source to search for a dark-matter twin to the neutron. Image credit: Genevieve Martin, ORNL

Los Alamos Neutron Science Center, physicist Frank Gonzalez, now at ORNL, led the most precise measurement ever of how long free neutrons live before they decay, or turn into protons, electrons and anti-neutrinos.

The answer — 877.8 seconds, give or take 0.3 seconds, or a little under 15 minutes — hinted at a crack in the Standard Model of particle physics. That model describes the behavior of subatomic particles such as the three quarks that make up a neutron. The flipping of quarks from down to up initiates neutron decay into protons.

To measure the lifetime of a free neutron, scientists take two approaches that should arrive at the same answer. One traps neutrons in a magnetic bottle and counts their disappearance. The other counts protons appearing in a beam as neutrons decay. It turns out neutrons appear to live nine seconds longer in a beam than in a bottle.

The ORNL-led team performed the first search for neutrons oscillating into dark-matter mirror neutrons using a novel disappearance and regeneration technique at ORNL's Spallation Neutron Source. A beam of neutrons was guided to SNS's magnetism reflectometer, which applied a strong magnetic field to enhance oscillations between neutron states. Then the beam struck a sheet of boron carbide, called a "wall" because it is a strong neutron absorber.

If a neutron does in fact oscillate back and forth between regular and mirror states, the scientists theorized, when the neutron in its normal state hits the wall, it will interact with atomic nuclei and get absorbed into the wall. If it is in its theorized mirror state, however, it is dark matter that will not interact.

So only mirror neutrons would make it through the wall to the other side. It would be as if the neutrons had gone through a portal to some dark sector — a figurative concept used in the physics community.

Yet, the press reporting on related work has had fun taking liberties with the concept, comparing the theorized mirror universe Broussard's team is exploring to the "Upside Down" alternate dimension in the TV series "Stranger Things." To be clear, the team's experiments were not exploring a literal portal to a parallel universe.

The conclusion: The team saw no evidence of mirror neutrons. "One hundred percent of the neutrons stopped; zero percent passed through the wall," Broussard said. Regardless, the result is still important to the advancement of knowledge in this field.

With one particular mirror–matter theory debunked, the scientists can turn to others to try to solve the neutron lifetime puzzle.

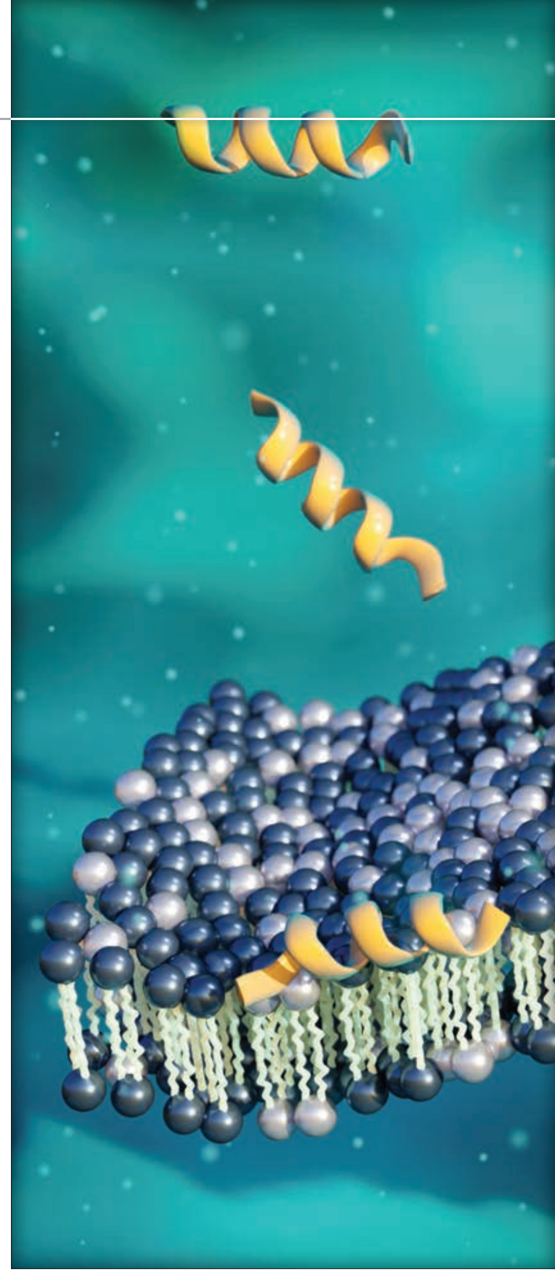
"We're going to keep looking for the reason for the discrepancy," Broussard said, noting that her team will move the search to ORNL's High Flux Isotope Reactor, where ongoing upgrades will enable more sensitive searches.

If it seems sad that the neutron lifetime puzzle remains unsolved, take solace from Broussard: "Physics is hard because we've done too good a job at it. Only the really hard problems — and lucky discoveries — are left."

For more information: https://bit.ly/3Ojuw44.

Neutrons show how promising

peptide fights antibiotic-resistant bacteria



by Olivia Trani
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Since the advent of penicillin more than 90 years ago, antibiotic drugs have saved countless lives by preventing and treating bacterial infections. However, bacteria are rapidly developing new ways to resist antibiotics, making some of modern medicine's most powerful drugs less effective against life-threatening infections.

One potential strategy for combating antibiotic resistance involves developing strings of amino acids, called peptides, that have a penchant for neutralizing bacterial invaders.

Neutron experiments led by ORNL scientists have produced new insights into a promising group of peptides known as antimicrobial peptides, or AMPs. Given the ability of AMPs to quickly identify and take down a wide range of pathogens, they are considered promising therapeutic candidates for treating bacterial infections where antibiotics fall short.

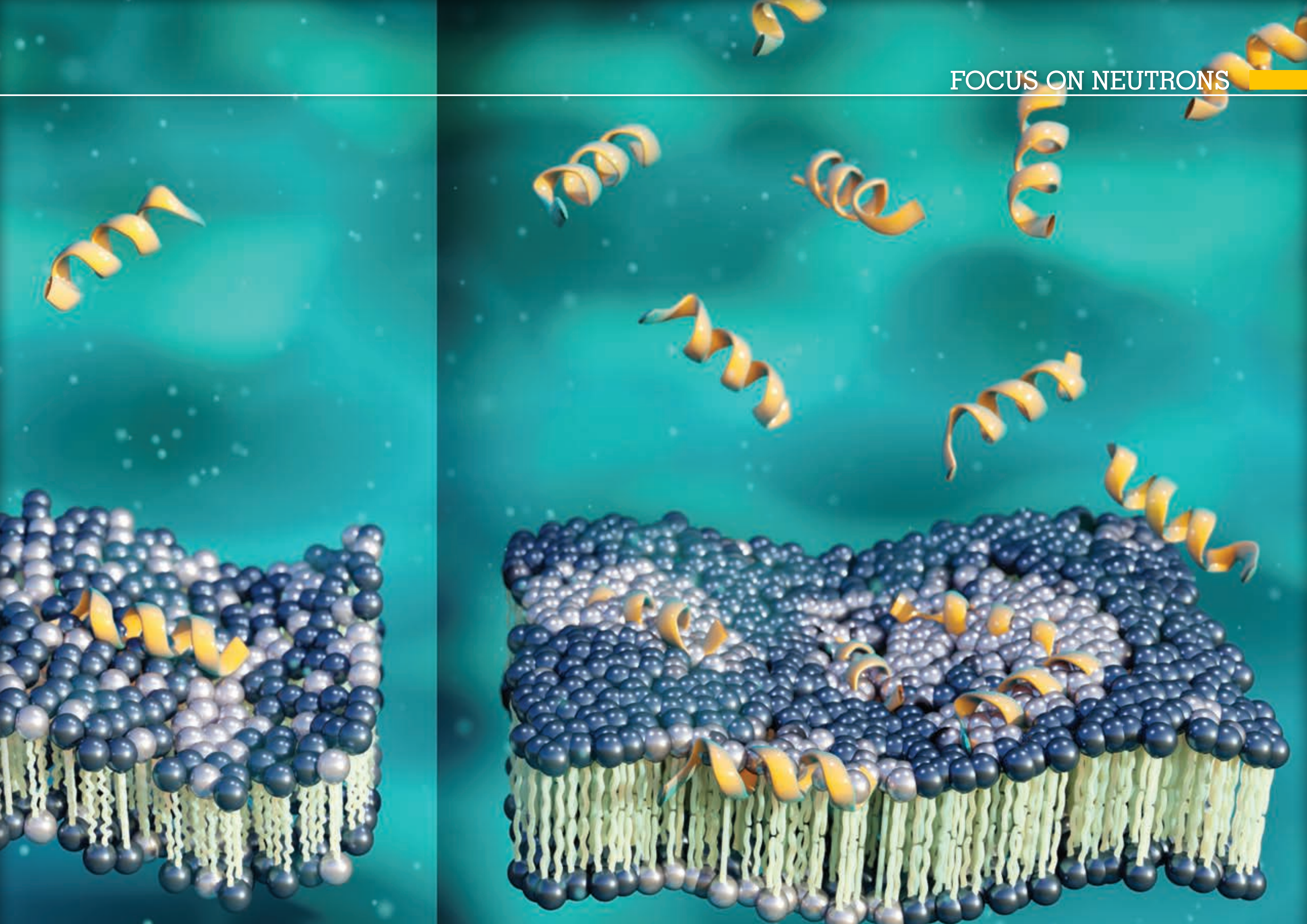
By studying an effective AMP called aurein 1.2, the team pieced together the molecular mechanics behind the peptide's ability to deal significant damage to bacterial cells, even when used in small quantities. Their findings, published in *BBA Advances*, could help pharmaceutical experts develop drugs that attack antibiotic-resistant bacteria more efficiently and effectively.

"AMPs fight bacterial cells by targeting their membranes with the help of electrostatic and hydrophobic forces," explained Shuo Qian, the ORNL neutron scattering scientist who led this research.

"The fundamental structure of a cell membrane is a double layer of lipid molecules. Many of the lipid molecules making up the surface of bacterial cell membranes are negatively charged, so the bacteria become highly attractive for positively charged AMPs. Once bound to an intruding bacterial cell, the hydrophobic peptides will often embed themselves within the membrane to avoid exposure to water."

When present in great enough numbers, AMPs bore deep holes within bacterial membranes. This action disrupts the membrane's structure and leaves the invading bacterial cells weakened, but the approach is potentially expensive and may introduce side effects. Drugs that effectively kill antibiotic-resistant bacteria without needing a high peptide count would be both more beneficial and more cost-effective. This is where the team's aurein 1.2 studies provided insights.

Made up of just 13 amino acids, aurein 1.2 is one of the shortest AMPs found in nature. Synthetically generated versions of this peptide — first discovered in Australian tree frogs — have proven to be potent against various bacteria. However, the molecular mechanism behind its



Scientists used neutrons to better understand how an antimicrobial peptide known as aurein 1.2 kills antibiotic-resistant bacteria by attacking their membranes. As the peptide concentration increases (yellow), aurein 1.2 induces lipid molecule clusters (white) within the membrane, making it thicker, more rigid and more susceptible to breaking down under stress. Their findings could inform new strategies for treating infections where antibiotics have fallen short.
Image credit: Jill Hemman, ORNL

pathogen-fighting capabilities has largely remained unknown.

Previous neutron experiments led by Qian provided some initial clues to the peptide's mystery mechanism. These studies showed that, instead of puncturing holes in bacterial membranes as other AMPs do, aurein 1.2 interferes with the membranes' electrostatic balances. At low concentrations, the positive charge of the peptide causes lipid molecules to slow their lateral movement and form clusters with other similarly charged lipid molecules within the membrane.

In his latest study, Qian teamed up with ORNL neutron scattering scientist Piotr Zolnierczuk to better understand how the peptide-induced lipid clusters disrupt bacterial membrane behavior. They utilized two neutron scattering instruments at ORNL's Spallation Neutron Source.

Using the EQ-SANS instrument to measure peptide penetration within the membrane, Qian found that aurein 1.2 remained embedded near the membrane's surface, even at high concentrations. Zolnierczuk then performed experiments on the Neutron Spin Echo Spectrometer to examine aurein 1.2's impact on membrane flexibility and compressibility.

"Membrane fluctuations occur on the order of tens or hundreds of nanoseconds, and neutron spin echo spectroscopy is the only technique capable of measuring dynamical behaviors at that length and timescale," said Zolnierczuk. "By analyzing neutron spin echo data through mathematical models, we can then infer information about a membrane's mechanical properties, such as how soft or stiff the membrane becomes."

The results suggest that, through its lipid-clustering mechanism, aurein 1.2 peptides can make bacterial membranes thicker and more rigid.

In this state, the bacterial membrane cannot recover from stresses as quickly, its structural integrity is weakened and it's less able to carry out normal functions. This combination of adverse effects makes the bacterial cell more likely to break down under stress.

The data obtained from this research will help scientists better understand the intricacies of AMP-based defenses against bacteria and could inform future therapeutic strategies for fighting infections in an increasingly antibiotic-resistant world.

Neutrons shed light on

methane-to-methanol conversion

by Paul Boisvert
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Naturally occurring methane, or natural gas, is an abundant and valuable fuel, used to power vehicles, heat homes and operate industrial systems. However, methane, also known by its chemical formula as CH_4, can also be dangerous and expensive due to the difficulties of extracting, transporting and storing it.

Methane gas is also harmful to the environment when it is released or leaks into the atmosphere, where it is a potent greenhouse gas. Fossil fuel production and use, forest fires, agricultural waste, landfills and melting permafrost are all sources of atmospheric methane.

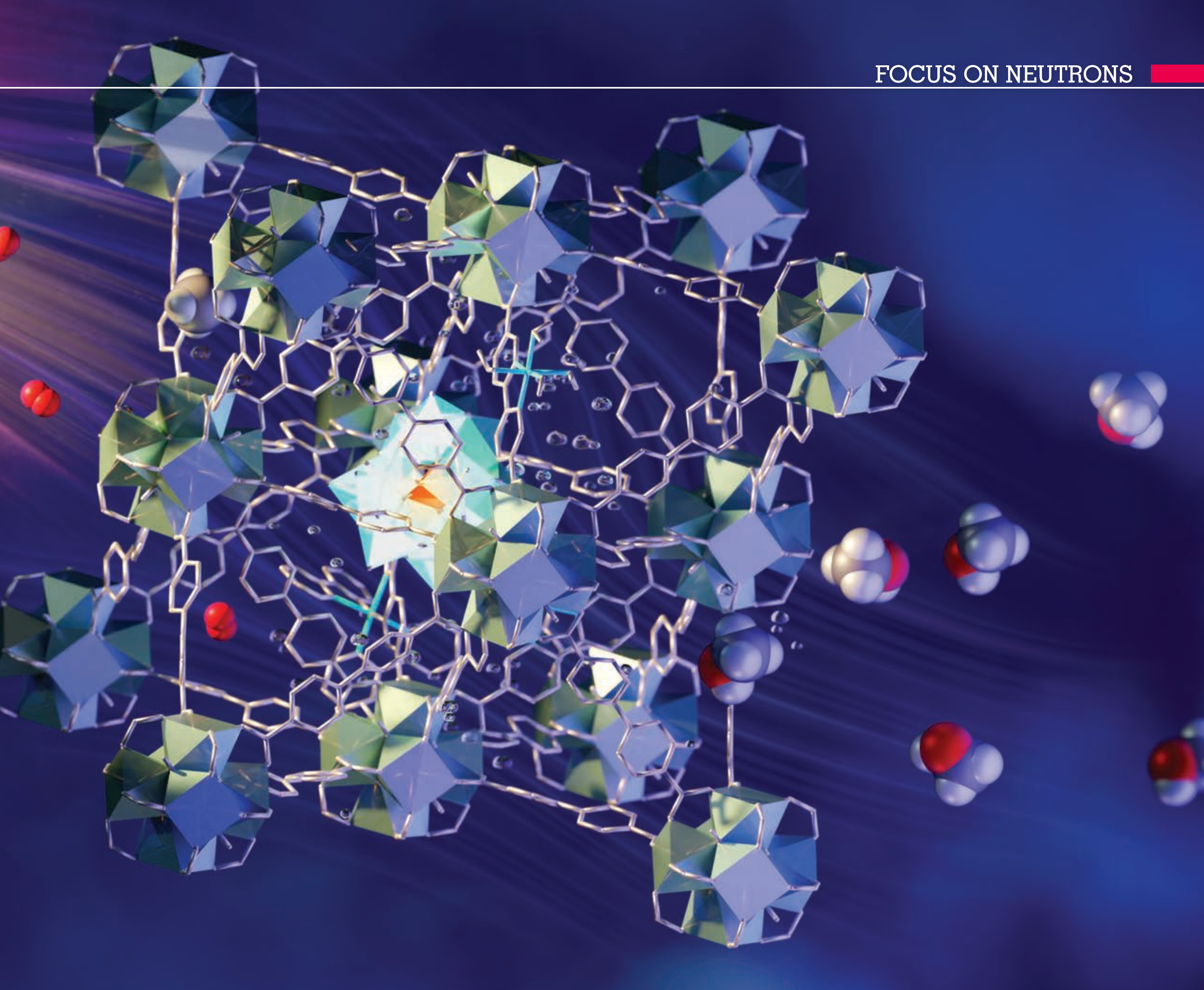
Industry has long sought an economical and efficient way to convert methane into methanol, a safer, highly marketable and versatile feedstock used to make a variety of consumer and industrial products. Such a conversion process would not only help reduce methane emissions; it would also provide an economic incentive to do so.

Scientists at the University of Manchester in the United Kingdom have developed a fast and economical method of converting methane into liquid methanol at ambient temperature and pressure. The method takes place under continuous flow over a novel, functional metal–organic framework, or MOF, catalyst using visible light to drive the conversion.

To help observe how the process works and how selective it is, the researchers used the neutron scattering capabilities of the VISION instrument at ORNL's Spallation Neutron Source. Using neutron scattering to take "pictures" of the chemical conversion confirmed the strong interactions between CH_4 and the mono-iron-hydroxyl sites in the MOF that weaken the carbon–hydrogen chemical bonds.

Methanol is a more versatile carbon source than methane and is a readily transportable liquid. It can be used to make thousands of products such as solvents, antifreeze, plastics, plywood, pharmaceuticals and agrichemicals. The conversion of methane into a high-value fuel such as methanol is also becoming more attractive as petroleum reserves dwindle.

A primary challenge of converting methane — CH_4 — to methanol — CH_3OH — has been the difficulty of breaking the C–H bond in order to insert an oxygen atom to form the COH bond in methanol.



University of Manchester scientists have developed a fast and economical method of converting methane, or natural gas, into liquid methanol, used for many consumer and industrial products, at ambient temperature and pressure. Image credit: Jill Hemman, ORNL

Conventional methane conversion typically involves industrial-scale processes that are energy-intensive, costly and inefficient, and that require high temperatures and pressures.

"To greatly simplify the conversion process, when methane gas is exposed to the MOF material, activated oxygen molecules and energy from a light source promote the activation of the C–H bond in methane to form methanol," said Sihai Yang, a professor of chemistry at Manchester. "The process is 100 percent selective, meaning there is no undesirable byproduct."

The researchers demonstrated that the solid catalyst can be isolated, washed, dried and reused for at least 10 cycles, or approximately 200 hours of reaction time, without any loss of performance.

"This process has been termed the 'holy grail of catalysis.' Instead of burning off methane as a waste product, it may now be possible to convert the gas directly to methanol, a high-value chemical that can be used to produce biofuels, solvents, pesticides and fuel additives for vehicles," said Martin Schröder, vice president and dean of faculty of science and engineering at Manchester. "This new MOF material may also be capable of facilitating other types of chemical reactions by serving as a chemical test tube in which we can combine different substances to see how they react."

By eliminating the need for high temperatures or pressures and using the energy from light to drive the photo-oxidation process, the new conversion method could substantially lower equipment and operating costs. The higher speed of the process and its ability to convert methane to methanol with no undesirable byproducts will facilitate the development of in-line processing that minimizes costs.

Researchers use seismology,

radiation detection to bolster nonproliferation efforts

by Alexandra DeMarco
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An ORNL team has tackled the challenge of detecting nuclear materials in vehicles by combining radiation detection with seismology, typically used to study earthquakes.

Putting these two detection methods together, they were able to not only detect radioactive materials in passing vehicles but also determine what direction those vehicles were traveling. This unique combination of data could provide authorities with a crucial tool for enhancing nuclear safety.

This project grew out of a previous experiment at ORNL's High Flux Isotope Reactor. In that project, Monica Maceira, seismology portfolio manager in the National Security Sciences Directorate, noticed that vehicles generated enough energy at certain points around the facility to produce seismic signals — for instance, when encountering a large metal plate.

This observation planted an idea: What if seismology could be used to detect all vehicles driving around a facility, regardless of contact with an obstacle? So, Maceira and her team set out to prove that seismic sensing could be used for nonproliferation efforts that account for vehicle movement.

For 11 days, including a two-day targeted experiment, researchers deployed 24 three-component seismic sensors along roads around HFIR. Sensors detected vibrations from vehicles' engines and the force of tires hitting the road.

"Those signals are very small," Maceira said. "They are part of the background noise recorded by your sensor, and it's nothing compared to an earthquake."

Such small seismic signals could become lost among the heterogenous noise of a facility like HFIR. Despite this hurdle, the seismology team successfully monitored vehicle movement and verified results with GPS sensors and video surveillance.

> *The different nuclides emit photons with different energies, and so they deposit in different portions of your spectrum. You have more counts in some parts of the spectrum than in other parts of the spectrum, and based on that you can fingerprint the nuclide.*
>
> — Nuclear Science and Advanced Technology Section Head **Dan Archer**

"You still can see the vehicles throughout the HFIR facility where you don't have a metal plate or a speed bump or anything like that in the road," Maceira said.

Polarization indicated vehicle direction; about every 0.5 seconds, the three-component sensors mathematically

Monica Maceira. Image credit: Carlos Jones, ORNL

rotated. The angular change between each rotation indicated the direction a detected vehicle was traveling, explained Omar Marcillo, an ORNL geophysicist who works alongside Maceira.

"That is a huge advantage," Marcillo said. "The level of resolution is not great, but it gives you enough information to hint the direction of movement."

On its own, the ability to detect and monitor a traveling vehicle is a valuable asset for high-security situations — so Maceira's efforts were only strengthened by a collaboration with Dan Archer, section head for Nuclear Science and Advanced Technology in the Physics Division.

Traditionally, radiation detection systems travel while searching for radioactive material, but in Archer's team's system, the radiation detectors remain stationary to monitor moving vehicles.

"If your source is moving and your detector's moving, there's a low probability of overlap," Archer said.

Six two-sensor radiation systems around HFIR detected moving vehicles, charted their trajectories and detected radioactive materials — including nuclides such as actinium-225, a rare cancer-fighting isotope that ORNL produces — among cargo.

As vehicles pass by, sensors record gamma radiation photon-by-photon, allowing researchers to identify both the radioactive material and the speed and distance of the vehicle. The captured photon energy histogram is then used to denote the specific radioactive nuclide.

"The different nuclides emit photons with different energies, and so they deposit in different portions of your spectrum," Archer said. "You have more counts in some parts of the spectrum than in other parts of the spectrum, and based on that you can fingerprint the nuclide."

The data volume accumulated during this experiment was so large — researchers dedicated a full petabyte of storage to the project — that the team plans to analyze the data for additional, unnoticed patterns.

"It's a data-rich set," Maceira said. "It would be great for us to keep looking [for more information]."

Researchers are planning additional experiments to further characterize the detection method's potential.

ORNL sensor research helps fight wildfires

by S. Heather Duncan
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As climate change leads to larger and more frequent wildfires, ORNL researchers are using sensors, drones and machine learning to prevent fires caused by electrical arcing and to remotely sense the direction of spreading fires.

The need is urgent. Last fire season, DOE targeted two wildfire projects at ORNL headed by Peter Fuhr, who leads the lab's Grid Communications and Security Group.

"The work ORNL is doing with sensor technology on drones that can go beyond line of sight is unique and very critical, because it allows us to be several steps ahead of issues that can put the grid at risk, making it unreliable and less resilient," said Stewart Cedres, a senior DOE technical lead and strategist. Last summer, the White House cited research being conducted by Fuhr's team in a list of ways the Biden Administration is tackling the wildfire threat.

Preventing wildfires

Sensors placed near power lines or in power electronics equipment can register variations in power flow that lead to superheated sparks. ORNL senior researcher Ali Ekti is developing an algorithm for rapidly recognizing and classifying these electrical arcing events, which occur when electricity jumps through the air between two conductors.

His algorithm separates traces of arcing, represented by spikes in voltage or current that are visible in wave form signatures provided by utilities and universities. Next steps will involve training a software program to recognize these patterns and pinpoint where the arcing is happening. The technology could instantly alert a utility's command center so staff could check the location — if it's accessible.

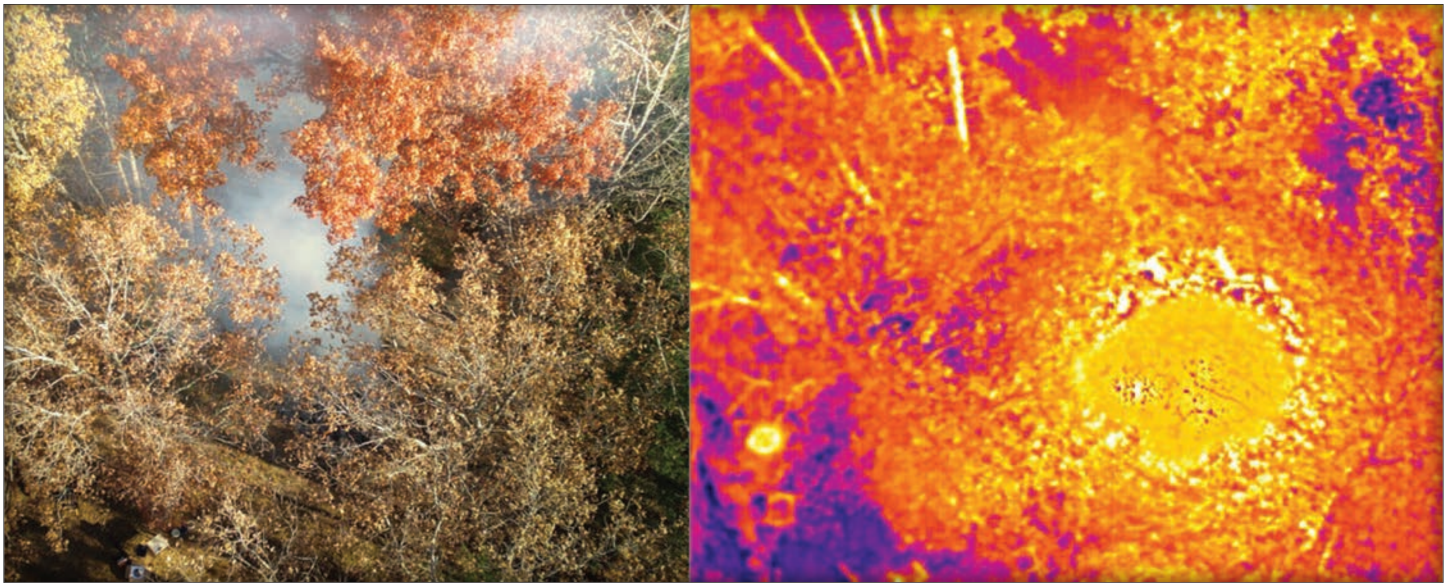
This is where drones come in: Arcing often happens in rugged areas that are tough to reach. ORNL's experience with operating drones beyond visual line of sight allows for transmission line inspection over a much larger distance. The Federal Aviation Administration recently cleared Fuhr's team to fly drones throughout the U.S., and up to 1,500 feet with special permission.

Drone-mounted audio sensors face a challenge distinguishing the crackling noise of arcing from the buzz of the drone propeller. Ekti has resolved this issue with an approach that uses math to extract the audio signature of arcing from background noise.

Directing fire suppression

Fuhr's team incorporated their drone-mounted sensing method into another demonstration in October for the U.S. Forest Service, the primary agency for fighting wildfires. In Montana, ORNL

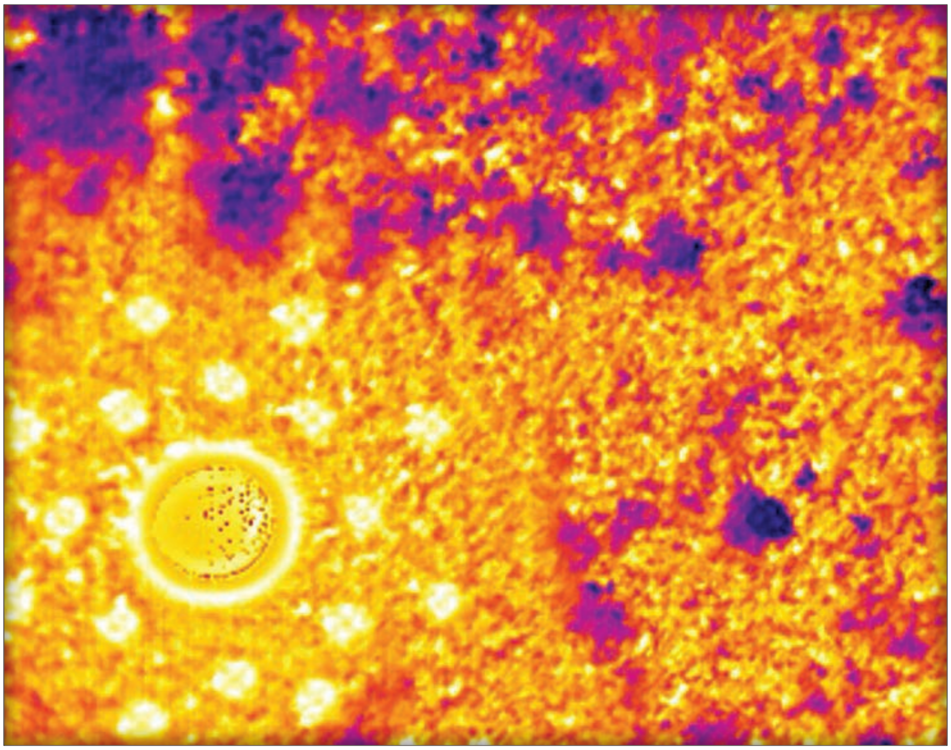
ORNL researchers are exploring ways to use drones to check remote parts of the electric grid for dangerous electrical arcing that could start wildfires. Image credit: ORNL



ORNL researchers have demonstrated that thermal imaging sensors mounted on drones can sense the presence of fire under tree cover and indicate its size, even when there is little to no smoke. In this image, heat and smoke under tree cover (left) are revealed in remotely sensed thermal images (right). Image credit: ORNL

researchers showed how they can use drones to thermally detect tiny sparks that start new fires, which might otherwise be difficult to sense in the presence of a large blaze.

This could be a game-changer, said Marva Willey, a member of the team that develops tools and technology for the Forest Service. "Heat-detecting sensors have so many applications that can increase our situational awareness and knowledge of where heat and fire are," she said. "It's all about knowing what's going on before you put people out there."



Drones could also be used to locate hot spots remaining in a burned-over area — a task that has long been performed by hand. And drones are currently the only technology that can sense heat under a canopy of trees, where smoke isn't visible.

Fuhr's team has performed initial investigations of other ways to use drone-mounted sensors to prevent fire risks from the electrical grid. For example, when a 2021 wildfire caused by downed power lines burned through Wears Valley, situated near Great Smoky Mountains National Park in Tennessee, Fuhr and his team used drones to monitor heat in transmission lines and transformers. This could help identify where equipment should be replaced.

"New Mexico was on fire earlier this year, and when you see the devastation that happened with the Camp Fire [in California] and the resulting bankruptcy of the utility — if our activities can reduce those kinds of outcomes, it's good for everyone," Fuhr said.

ORNL researchers demonstrating drone-mounted imaging sensors can recognize the presence of small fires even near a larger one, as shown by bright dots surrounding a larger dot at bottom left. Image credit: ORNL

ORNL research to bring

more reliable electricity to Puerto Rican microgrids

by S. Heather Duncan
duncansh@ornl.gov

When Hurricane Maria battered Puerto Rico in 2017, it killed residents, destroyed homes and knocked out power for months. This past September, Hurricane Fiona left most of the island in the dark again, underscoring the weaknesses remaining in the island's electric grid five years later.

To provide more reliable service to underserved communities, scientists from ORNL are developing a technology that will build resilience into independent microgrids powered by renewable energy. The technology will manage groups of small microgrids as a cluster, enhancing their reliability even when damaged.

ORNL engineers Ben Ollis and Max Ferrari lead a team developing a microgrid orchestrator that will deploy as a test case in the Puerto Rican town of Adjuntas. A community microgrid project is already being developed in this mountain town through a partnership between local nonprofit Casa Pueblo and the Honnold Foundation.

Honnold, which funds solar projects to reduce global energy poverty, is investing $1.7 million to build two microgrids, said Honnold project coordinator Cynthia Arellano. They will generate electricity with solar arrays linked to batteries, keeping the power on when the broader utility network fails.

Interconnected grid

This is where ORNL steps in, creating a tool to connect and manage a cluster of microgrids so they work together.

"I don't know of a microgrid controller anywhere that can communicate and coordinate with another controller," Ollis said. "We're designing an architecture for multimicrogrid controls, so any number of microgrids can operate independently but share information to an orchestrator that will predict when switching, routing and connecting should happen."

That isn't just a matter of convenience. "A lot of people died after [Hurricane Maria], and many of the deaths were related to power failures," said Arturo Massol-Deyá, executive director of Casa Pueblo, a project partner that promotes fair and sustainable development around Adjuntas. "Energy security being interrupted is about quality of life,

Solar panels are installed on commercial buildings to create independent microgrids in Adjuntas, Puerto Rico. ORNL researchers are developing technology that connects the microgrids to make them more resilient. Image credit: Fabio Andrade, University of Puerto Rico, Mayaguez

The mountain town of Adjuntas, Puerto Rico, lost power for four months after Hurricane Maria. The microgrids, funded by the Honnold Foundation through local partner Casa Pueblo and slated for connection via ORNL-developed novel technology, will make critical electrical service more reliable. Image credit: Isabela Zowistowska, Honnold Foundation

and there were long-term consequences in the community."

Collective benefits

For the project, solar panels were installed on the roofs of 13 businesses, and soon they will be linked to each other and to batteries through microgrids. Business owners agree to provide critical services like medicine, refrigeration and cell phone charging to residents during long power outages. In return, the businesses will save money on electricity and can avoid the use of expensive diesel generators during natural disasters. Microgrid profits will fund future expansion as well as solar arrays for the most vulnerable residents.

Fabio Andrade, a visiting scientist at ORNL and professor at the University of Puerto Rico, Mayaguez, is collaborating on the Adjuntas project. His students model strategies, tools and algorithms for sharing solar power among microgrid users. Data from this and other UPRM research projects is incorporated into ORNL's simulations, which are being tested live with microgrid hardware at ORNL's Grid Research Integration and Deployment Center, or GRID-C.

Solar panels funded by the Honnold Foundation are installed in Adjuntas, Puerto Rico. Image credit: Fabio Andrade, University of Puerto Rico, Mayaguez

The technology will be deployed in Adjuntas next year. It holds broad potential for incorporating renewable energy into the electric grid to increase flexibility and resilience while supporting vital decarbonization efforts.

"The orchestrator includes a framework of algorithms that can be expanded and deployed to many microgrids at any site," Ollis said. "They could provide more reliable electricity to many rural communities at the grid edge. I want to see a future where we have hundreds of microgrids working together to protect critical infrastructure."

ORNL's work on the Adjuntas project is funded through DOE's Solar Energy Technologies Office. Much of the microgrid orchestrator design, configuration and testing is being carried out in the network microgrid test bed called COMMANDER, for Coordination of Multi-Microgrids and Networked Distributed Energy Resources, which is part of the GRID-C facility funded largely by the DOE's Office of Electricity.

Predicting climate change

in vulnerable neighborhoods

by Stephanie Seay
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A new capability to assess urban neighborhoods vulnerable to climate change could help ensure that mitigation and resilience programs reach the people who most need them.

Ensuring that vulnerable populations benefit from climate change mitigation measures is a key aspect of environmental justice. The method developed at ORNL takes into account infrastructure and population down to the block and building levels in historically disadvantaged neighborhoods.

Project lead Nagendra Singh said climate modeling in the past has mostly focused on "where factors like a one-degree temperature increase will happen, or where there's going to be more heat waves in our climate models. But we have not stressed the fine details of those impacts — how climate events will disproportionately impact different communities. Applying this geodemographic data to the model outputs is a good approach to generating the information needed by decision-makers."

"We have to think about where the people are," said team member Christa Brelsford. "Most of the world's population lives in cities. In order to analyze climate risk, we have to think about impacts and vulnerability — and there's a lot of vulnerability in an urban environment."

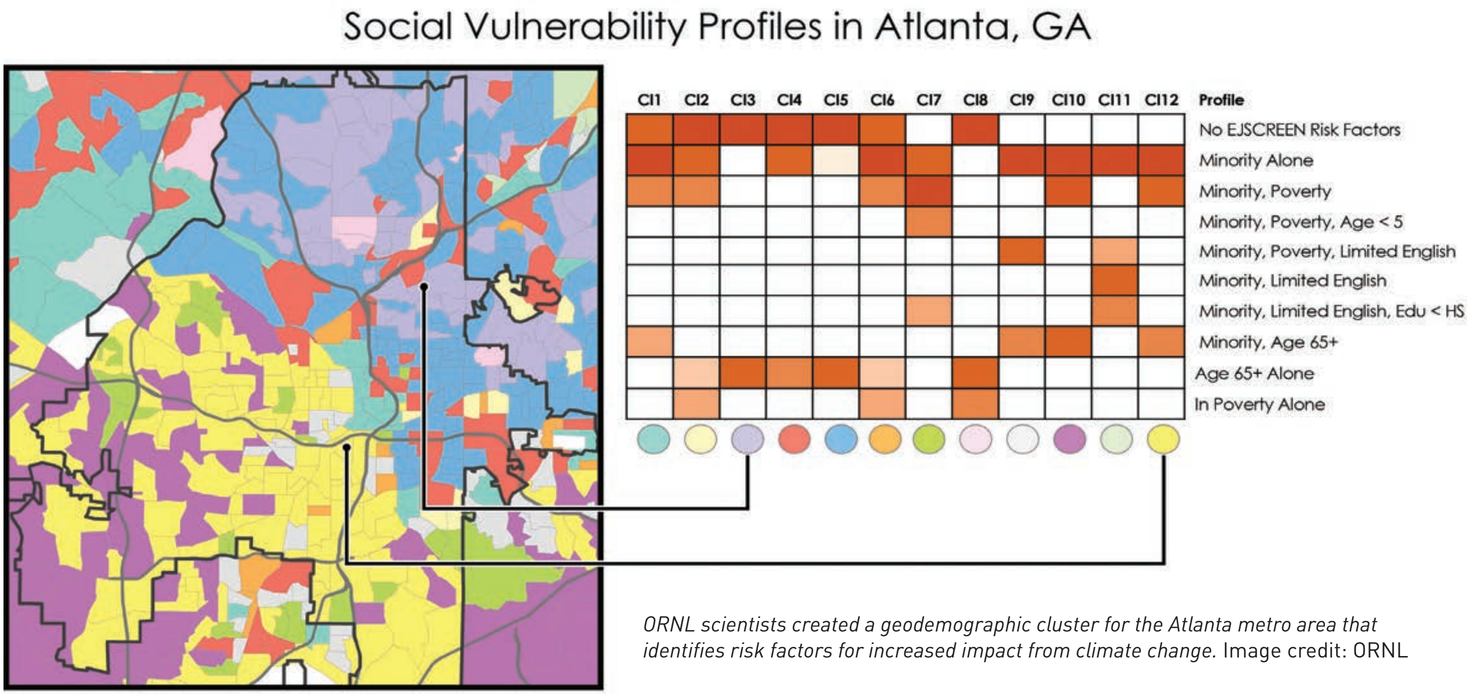
Team member Joe Tuccillo described how the team used microdata from the U.S. census to create a synthetic population, approximating the individual makeup of urban communities to assess the vulnerability of individual neighborhoods to climate events and their ability to adapt.

The team gleaned demographic information such as income level, age, gender, ethnicity and housing from the census databases. Team members then generated building characteristics data to determine whether a structure was an office, store, apartment building or other type of structure by applying machine learning techniques to satellite imagery. The combined data generated a high-resolution analysis of differential impacts across socioeconomic groups down to the household level.

The work is detailed in an ORNL report, "An Environmental Justice Lens for Measuring Neighborhood Scale Vulnerability," which is available at bit.ly/3TFeCUC.

Getting down to the individual household level is important, said team member Taylor Hauser. If there's an environmental risk, is it because people are living in the same at-risk physical structure such as an apartment building, or is it because the people living in that structure have different socioeconomic characteristics? Such an analysis can help scientists understand the similar or differing risk to individuals who may occupy the same neighborhood but have different demographics, he explained.


Atlanta, Georgia



ORNL scientists created a geodemographic cluster for the Atlanta metro area that identifies risk factors for increased impact from climate change. Image credit: ORNL

ORNL scientists developed and tested the platform using data from the Atlanta metropolitan area to characterize neighborhoods and then evaluated the potential impacts from urban heat islands across different demographically defined groups.

The methodology builds on ORNL's long-standing expertise in measuring populations and environmental change, including the lab's Climate Change Science Institute and human dynamics modeling tools developed as part of its national security science research.

"A better understanding of where people are and the infrastructure and environment around them can help us provide better science-based answers as to how specific neighborhoods might be affected by new projects," Singh said.

Environmental and energy justice is a key aspect of the federal government's strategy for infrastructure development and policy implementation, he noted. However, there are no robust tools for measuring the socioeconomic consequences of future climate events and new infrastructure. The ability to incorporate individual information into neighborhood profiles will help to provide targeted support for resource allocation and policy interventions, he said.

One of the roles of the DOE national labs is "making sure that the most vulnerable among us are equally, fairly and accurately represented in science, and we don't get to that when we only look at urban aggregates. We have to look at neighborhood-scale differences in order to do that well," Brelsford said.

For more information:
https://bit.ly/3fMsTjT

Listening in on soil conversations with rhizosphere-on-a-chip

by Stephanie Seay
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To better understand the belowground environment that determines plant health and soil carbon storage, scientists have created a miniaturized version of the ecosystem to eavesdrop on important interactions among microbes, chemicals and plant roots.

The rhizosphere-on-a-chip research platform builds on ORNL's history of constructing lab-on-a-chip devices, in which tiny channels and chambers are etched on a microscope slide so that fluids can be introduced and studied for biochemical separations research and testing.

In this case, scientists are mimicking soil on the chip, sprouting poplar trees in the fluid and studying the environment around their roots, known as the rhizosphere. Scientists observe how microbes are interacting with chemicals within the artificial soil to influence plant health and gain a better understanding of the processes governing carbon storage.

The rhizosphere is one of the most complex systems in the world, in which plant roots take up water and nutrients, create a unique physical and biogeochemical environment for microbes and emit atmospheric carbon into the soil. There may be hundreds of different bacteria that grow near plant roots or are influenced by the rhizosphere. ORNL scientists are particularly interested in how microbes such as bacteria and fungi interact with plant roots to help plants grow faster and survive threats like drought, wildfire, disease and pests.

"It's very difficult to see inside soil to observe those processes, as the particles are very dark," said ORNL analytical chemist Jack Cahill.

Rhizosphere-on-a-chip allows scientists to create model systems and then use techniques including mass spectrometry to identify chemicals and their distribution around plant roots. That

ORNL scientists have created a rhizosphere-on-a-chip research platform, a miniaturized environment that enables them to study the ecosystem around poplar tree roots for insights into plant health and soil carbon sequestration. Image credit: Carlos Jones, ORNL knowledge informs analysis of chemical interactions in the ecosystem, such as chemical signals sent out by plants to attract or repel microbes. Using the chip system also conserves samples by removing only a tiny amount of the liquid from the platform and allowing plants to continue growing.

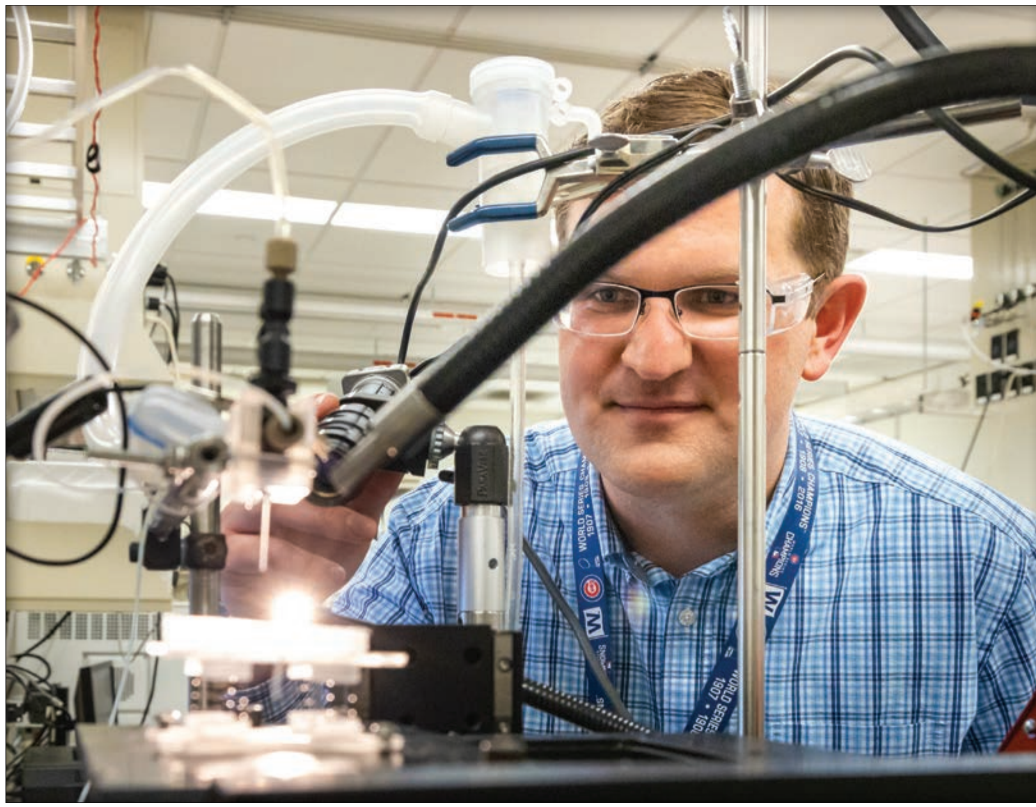
"Using mass spectrometry, we're able to eavesdrop on the conversation between these living systems of plants, fungi and microbes to figure out how and why they do the crazy things they do," said ORNL distinguished staff scientist Scott Retterer. He co-developed the platform using the nanofabrication facilities within the Center for Nanophase Materials Sciences at ORNL.

"I describe it as a fancy fishbowl," Retterer said. "Except our fishbowl is the size of a microscope slide, and the tools we use to shape that environment are the same kinds of tools Intel uses to make microchips. We throw a dinner party in the fishbowl for bacteria, plants and fungi. We set the table with food and watch how that influences the party."

ORNL scientists using the platform have found, for instance, high concentrations of amino acids very close to plant roots — a phenomenon that had previously gone unseen. While those compounds were once thought to move and dilute across the soil structure, that is not the case, Cahill said.

"The fluid dynamics in these chip systems are confined, so it lets us see concentrations of molecules that you wouldn't necessarily anticipate without being able to directly measure it using the chip platform," he added.

For ORNL's bioenergy research, the impact is "a better understanding of how plants, microbes and their chemical states relate to each other. If we can predict and control this, we can use that knowledge to develop plants that are environmentally resistant, that grow faster, are cheaper to produce and are therefore more suited for economical production of sustainable biofuels," Cahill said.



ORNL analytical chemist Jack Cahill positions a rhizosphere-on-a-chip slide for imaging by mass spectrometry at ORNL. Image credit: Carlos Jones, ORNL

A poplar tree grows from a microfluidic channel as part of the rhizosphere-on-a-chip platform developed at ORNL. Image credit: Carlos Jones, ORNL

The best is yet to come

ORNL's Early Career Research Program award winners

by Jim Pearce
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Since 2010, DOE's Office of Science has helped to expand and invigorate the nation's scientific workforce by supporting 785 young scientists at universities and national laboratories through its Early Career Research Program.

This year, three ORNL scientists were among the 83 selected to receive ECRP awards. Each will be awarded $500,000 annually for the next five years to cover their salary and research expenses. Awardees were selected based on peer review by outside scientific experts.

"These ORNL researchers exemplify the groundbreaking work done by DOE to advance clean energy technologies and scientific discovery," said Susan Hubbard, ORNL deputy for science and technology. "Supporting these scientists as they begin their careers will have a lasting impact on ORNL's and the nation's research efforts in critical fields."

ORNL's ECRP award recipients are:

- **Trey Gebhart**, a research and development staff member in the Fusion Energy Division, who was selected by DOE's Fusion Energy Sciences Program for his proposal "Solutions for a More Efficient and Economical Fusion Fuel Cycle."
- **Elizabeth Herndon**, a senior R&D staff member in the Environmental Sciences Division, who was selected by DOE's Biological and Environmental Research program for her proposal "Biogeochemical Controls on Phosphorus Cycling in Urban-Influenced Coastal Ecosystems."
- **Guannan Zhang**, a computational mathematician in the Computer Science and Mathematics Division, who was selected by DOE's Advanced Scientific Computing Research Program for his proposal "Advanced Uncertainty Quantification Methods for Scientific Inverse Problems."

"Supporting America's scientists and researchers early in their careers will ensure the U.S. remains at the forefront of scientific discovery and develops the solutions to our most pressing challenges," said U.S. Secretary of Energy Jennifer M. Granholm. "The funding announced today will allow the recipients the freedom to find the answers to some of the most complex questions as they establish themselves as experts in their fields."

Read the profiles that follow to learn more about the ORNL researchers who won DOE ECRP awards this year and the research their awards will help fund.

Profiles of ECRP award winners from previous years, including information about how the program bolstered their research and careers, can be found at https://bit.ly/3Dyem5i.

Pushing fusion energy technology forward

Trey Gebhart

by Jim Pearce
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Trey Gebhart traces his interest in fusion energy back to his experiences as an undergraduate engineering student at Virginia Tech.

"When I was an undergrad, my senior design project was to build a Farnsworth fusor, a benchtop-scale device for generating nuclear fusion reactions," he said. "That sort of opened my eyes to fusion and the possibility that it holds for generating clean energy to curb our pending climate crisis."

His latest foray into fusion energy is his research proposal "Solutions for a More Efficient and Economical Fusion Fuel Cycle," which received an ECRP award from DOE's Office of Science. His studies will be focused on improving the handling of tritium, a rare isotope of hydrogen that is needed, along with deuterium, to fuel fusion reactors.

"Tritium is very expensive," Gebhart said, "about $30,000 per gram, and that price is only going to go up. So, in order for a fusion power plant to truly be economical, the tritium inventory of the plants must be kept as low as possible."

He noted that the groundbreaking ITER fusion device currently under construction in France is designed to send tritium-containing exhaust through an extensive, external recovery and separation process before feeding recovered tritium back into the device's fuel system. Future fusion power plants will not need to isotopically separate their fuel stream as long as the isotope ratios can be monitored in real time.

"My research is focused on developing a direct, internal recycling loop that will separate both tritium and deuterium from fusion exhaust and send it immediately back into the fueling system," Gebhart said. "If we can largely bypass the tritium plant in future power plants, we can minimize power plants' size and increase their economic viability and overall safety."

Gebhart plans to reach that goal by developing a series of cryogenic pumps that can handle these separations.

"The exhaust from fusion devices has a handful of impurities that are pretty well known," he said. "We have the background needed to develop pumps that can separate impurities from the fuel to make the fusion fuel cycle more efficient."

"We could just design these pumps and determine whether they would be efficient enough to reduce the overall tritium inventory of the plant," Gebhart said, "but the real deliverable isn't just knowing whether or not this approach is viable; it's developing the tools and hardware that makes it possible at reactor-relevant conditions."

Promoting healthy river deltas

Elizabeth Herndon

by Jim Pearce
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Elizabeth Herndon has already worked in a variety of environments, focusing her research on how soil minerals affect the storage or release of organic matter and nutrients in various ecosystems. That pattern holds true for her Early Career Award–winning proposal "Biogeochemical Controls on Phosphorus Cycling in Urban-Influenced Coastal Ecosystems." This study will investigate how the nutrient phosphorous is cycled in ecosystems on the Gulf Coast of Louisiana.

"I've worked in stream systems, I've worked in temperate forests and I've worked in the Arctic tundra," Herndon said, "but coastal systems are completely new to me. Fortunately, the science doesn't really change depending on the environment."

Louisiana's Gulf Coast has experienced significant land loss as a result of urban flood prevention measures. These measures often include channelizing rivers — thereby disconnecting them from their floodplains — and diverting fresh water away from urban areas and toward less-developed coastal areas. These redirections change sediment supply to deltas, altering their susceptibly to flooding but changing the amount of nutrients, like phosphorus, flowing to coastal ecosystems.

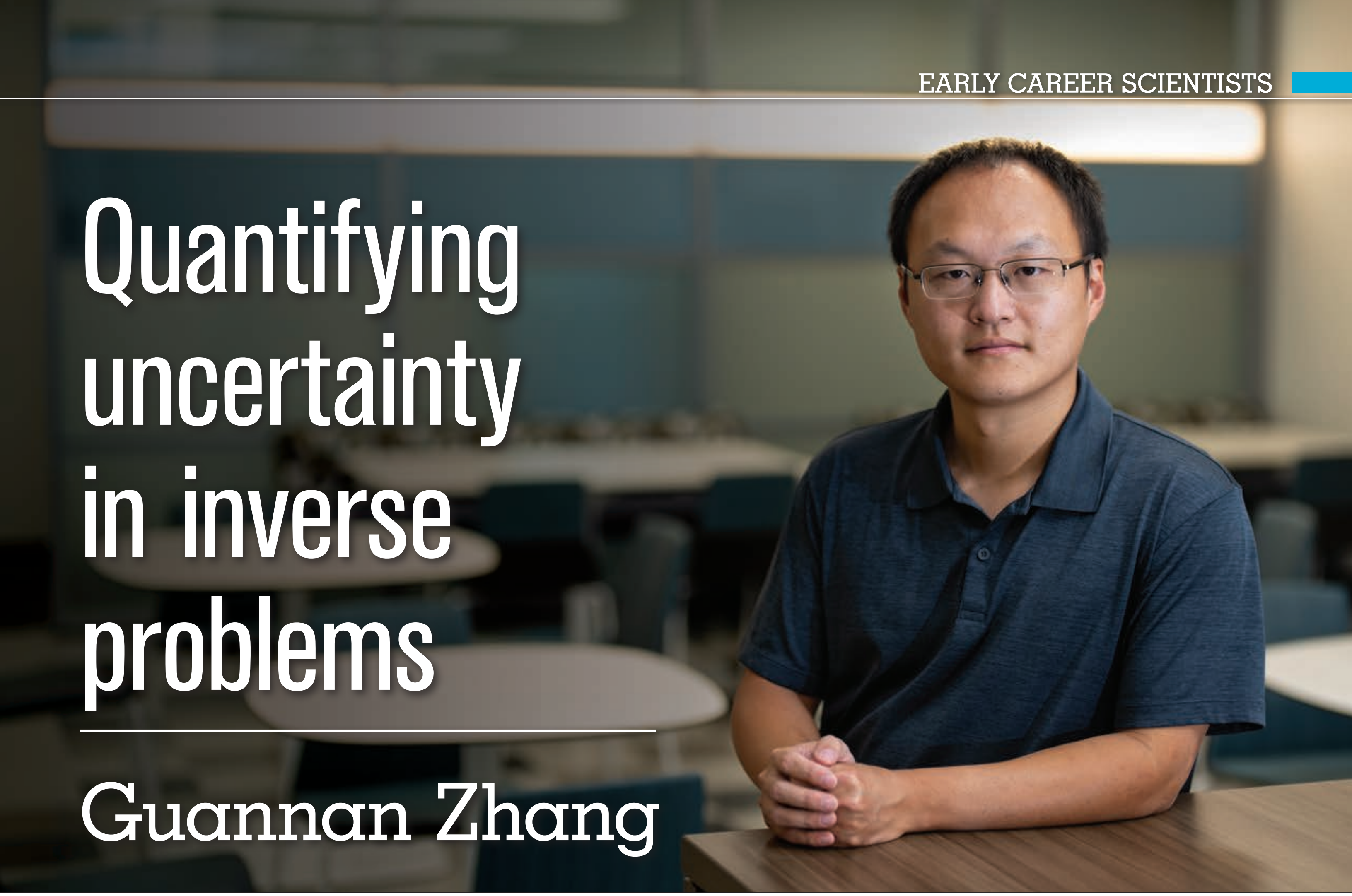
Phosphorus is an important nutrient for all ecosystems. Sometimes too much can limit plant growth or microbial activity or cause "nutrient pollution" — think algae blooms that can produce toxins that are harmful to humans and animals.

"How bioavailable phosphorous is to plants and microorganisms depends a lot on how it's interacting with minerals in the soil," Herndon said, "so my study is looking at the interactions between phosphorus and soil minerals. Some of the factors that can affect whether phosphorus is bound to minerals include how much oxygen is available in the soil or the salinity of the water in the soil."

Her studies will compare those interactions in two different coastal delta ecosystems — one that is growing and one that is shrinking.

"The growing delta is increasing in elevation relative to sea level, because it's receiving fresh water that also contains a lot of sediment," Herndon said. "But the rivers have been diverted away from the shrinking delta, so it's no longer receiving sediment, and it's starting to sink below sea level. This means that the delta is getting flooded with seawater. When that happens, it increases the salinity and decreases the oxygen that's available. This disrupts the interactions between nutrients and soil minerals."

Herndon's research will examine how being flooded with seawater affects interactions among phosphorus, iron and manganese in coastal river deltas to improve predictions of the future carbon storage and ecological health of these areas.



Quantifying uncertainty in inverse problems

Guannan Zhang

by Jim Pearce
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"When I was an undergraduate, my major was mathematics," Guannan Zhang said, "but when I went to graduate school, I got into programming and other aspects of computing, so it was very natural for me to pursue a Ph.D. in computational mathematics."

His ECRP proposal, "Advanced Uncertainty Quantification Methods for Scientific Inverse Problems," continues in a similar vein, focusing on developing better ways to determine the reliability of scientific inverse problems — the process of looking at the effects of an occurrence and calculating its causes through a process called inverse sampling.

"A scientific inverse problem uses measurements that are obtained from experiments to infer unobservable quantities that we are interested in," Zhang said. "For example, when scientists at the laboratory's Spallation Neutron Source conduct a neutron scattering experiment on a sample of material, they often try to determine its unobservable structure by analyzing the observable neutron scattering patterns that are produced when a beam of neutrons passes through the sample. That's a scientific inverse problem."

Inverse sampling can have an advantage over measurements taken in experiments that are subject to data noise and uncertainty; however, the sampling technique also presents the challenge of data uncertainty. Zhang's research will address this and other inverse sampling–related challenges by building deep neural networks, a kind of artificial intelligence. The networks will learn to conduct inverse sampling more efficiently and accurately while solving inverse sampling problems in a range of disciplines.

"There are a lot of methods that can give you an answer to inverse problems," Zhang said, "but because you don't have enough prior knowledge to verify whether or not this answer is right, the biggest question is, should you trust this answer or not? The main idea of my proposal is to develop methods that will enable us to quantify the confidence you can have in the answer to an inverse problem. When the scientists use my method to solve an inverse problem, they will not only get an answer, but they will also get the confidence level of that answer. This will help them make more reasonable and informed decisions."

Zhang noted that his five-year project will concentrate on fundamental research aimed at improving uncertainty quantification. Scalable implementation will be follow-on work.

"In five years, we will be able to develop deep neural networks. After that, we hope to accelerate their performance on bigger computers," Zhang said. "We need to use AI to determine the best way to go from the observable to the unobservable. If we didn't use AI, we would have to try all the possible solutions, which is not computationally affordable. Even with the biggest supercomputer, you couldn't really do this by brute force. You have to search for the most likely solutions in a smart way. That's where AI can help."

ORNL is proud of its role in fostering the next generation of scientists and engineers. We bring in talented young researchers, team them with accomplished staff members, and put them to work at the lab's one-of-a-kind facilities. The result is research that makes us proud and prepares them for distinguished careers.

We asked some of these young researchers why they chose a career in science, what they are working on at ORNL and where they would like to go with their careers.

Elizabeth Piersall

Graduate student, Electrification and Energy Infrastructure Division
Ph.D. student, Data Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Fredericksburg, Virginia

What are you working on at ORNL?

My research focuses on examining approaches to using signal processing and data science tools to combine noisy data from collaborative sensor systems measuring ambient parameters. We hope to be able to better interpret and predict measured parameters — for example, to use measured incident sunlight to predict power generation from solar panels.

What would you like to do in your career?

What I have enjoyed most so far, and believe I will continue to enjoy, is finding ways to contribute what I've learned to address existing needs, whether applying data science to technical challenges in energy or through science outreach and mentorship of future scientists.

Why did you choose a career in science?

I have always enjoyed the process of learning how things work. Part of the appeal of data science to me was that it can be applied to many fields and problems, giving me the opportunity to continue learning new things and contributing what I know to new challenges.

Zachary Tener

Postdoc, Materials Science and Technology Division
Ph.D., Inorganic Chemistry, Florida State University
Hometown: North Liberty, Iowa

What are you working on at ORNL?

I work in the Advanced Processing Laboratory, researching the effects of thermomagnetic processing on materials. I utilize convection or induction heating inside a static magnetic field, up to 9 Tesla and 2,000°C. My primary project involves miniaturizing this technology to create an in situ sample environment for neutron beamlines.

What would you like to do in your career?

I am inspired to utilize magnetism to solve a breadth of issues in manufacturing and environmental, energy and critical materials sciences. I want to develop new technology and solutions to address challenges in these fields towards sustainable science. I am also passionate about promoting scientific interest in students.

Why did you choose a career in science?

I was given encouragement by a mentor early in life, along with a childhood fascination of NASA and astronauts. Though this never passed, my attraction to magnetism at the interface of chemistry, physics and materials science developed during my undergraduate studies and continues to my present research.

Sara Sultan

Graduate student, Buildings and Transportation Science Division
Ph.D. student, Energy Science Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Haripur, Pakistan

What are you working on at ORNL?

I am working on thermal energy storage integrated with heat pumps. I work on designing control strategies to reduce peak energy and carbon emissions associated with air conditioning in residential buildings.

What would you like to do in your career?

I am interested in pursuing a career in climate change policy. I want to communicate with a wider audience and use my knowledge and experience to influence technology.

Why did you choose a career in science?

I loved physical sciences. I was curious to learn about the working phenomena behind simple equipment we use in daily life. I was most interested in optics, climate studies and fluid dynamics. I studied physics during my undergrad and then chose energy studies for research.

Rinkle Juneja

Postdoc, Materials Science and Technology Division
Ph.D., Computational Materials Science, Materials Research Centre, Indian Institute of Science, Bangalore, India
Hometown: Punjab, India

What are you working on at ORNL?

My research focuses on advancing a comprehensive view of heat transport properties of materials for energy applications such as thermoelectrics, barrier coatings, cooling electronics and spintronics. Besides being relevant to ORNL's mission of energy solutions, our work would be useful for the broader community focused on designing energy-efficient devices.

What would you like to do in your career?

I want to build a cutting-edge research team in the area of heat management to bring transformative changes and clean, innovative solutions in global energy resources. Along with my research work, I am very enthusiastic about mentoring and sharing my knowledge with the next generation of scientists.

Why did you choose a career in science?

Being curious about everything around me made me choose science. Learning at least one new thing every day is the beauty of science for me. The potential to make direct impact on the community and the opportunity to address challenging problems in a team spirit keep me excited as a researcher.

Xun Li

Postdoc, Materials Science and Technology Division
Ph.D.: Mechanical Engineering, University of Pittsburgh
Hometown: Yichang, China

What are you working on at ORNL?

My research at ORNL focuses on vibrational and transport properties of quasiparticles in quantum materials for energy-related applications. I calculate phonons and their interactions among themselves and with spins from first principles, which are crucial to understanding emergent phenomena in quantum materials.

What would you like to do in your career?

I want to be a computational materials scientist focusing on materials properties such as thermal and magnetic properties. I hope to provide fundamental understanding of the physics and apply them to practical applications for various materials.

Why did you choose a career in science?

I have always been fascinated by how things work. I believe that science and technology are primarily productive forces, and fundamental understanding leads to applications. I chose energy engineering in college, as energy is the future, and then got interested in thermal science to study how materials transfer heat.

Lynnicia Massenburg

Graduate student, Neutron Scattering Division
Ph.D. student, Biochemistry, Microbiology and Molecular Biology, Penn State
Hometown: Aston, Pennsylvania

What are you working on at ORNL?

I am researching the protein structure of a plant cellulose synthase, a membrane protein that makes cellulose used in biofuel production. I use small-angle X-ray and neutron scattering techniques complemented with cryo-electron microscopy to describe cellulose synthase oligomerization and provide rational insights in biofuel crop improvement.

What would you like to do in your career?

I am fascinated by the pursuit of membrane protein structural biology research in the bioenergy field. I seek to mentor future scientists in structural biology and give technical consulting in membrane protein purification and structural biology to other groups as well to open the field for more discovery.

Why did you choose a career in science?

I was interested in pursuing an art degree in college until I realized that there is art in science. I appreciate the creativity and serendipity in the scientific process. A research experiment is the canvas, and my pipette is the paint brush.

Libby Johnson: On the frontier for nuclear safety

by Sumner Brown Gibbs
gibbsss@ornl.gov

ORNL physicist Libby Johnson demonstrates a new control panel at ORNL's Bulk Shielding Facility in 1957. Among the first females to operate a nuclear reactor, Johnson blazed trails for women. Image credit: ORNL

ORNL physicist Libby Johnson, one of the world's first nuclear reactor operators, standardized the field of criticality safety with peers from ORNL and Los Alamos National Laboratory.

Johnson worked for more than a decade as a senior experimenter in the lab's Critical Experiments Facility. As evidence of the facility's successes developing criticality standards, there hasn't been a criticality accident — that is, an accident involving a sustained nuclear chain reaction — on U.S. soil since 1978.

"The experiments that you and your colleagues conducted over these years were crucial to the whole business of nuclear energy," former ORNL Director Alvin Weinberg told facility director Dixon Callihan, Johnson's colleague and mentor, in 1996 during a historic group interview.

"All of us owe you a great debt for your having pioneered in this ever-so-important enterprise and shown the way."

The Oak Ridge Critical Experiments Facility was established in 1950. This isolated facility, now slated for demolition, is nestled in the hills between ORNL and the neighboring Y-12 National Security Complex. The facility had been constructed for uranium storage and was remodeled to support studies underpinning safety standards. Years later, Callihan would recall his unsuccessful efforts to get a women's restroom included in the remodeling plans — a request that was later granted. His advocacy for this amenity contrasted sharply with the overall scientific environment of that time, which was organized by and optimized for men.

"Johnson trod the silent path of women's history in the nuclear industry," said Nuclear Regulatory Commission historian Thomas Wellock. The NRC appointed Johnson to the Atomic Safety Licensing Board in 1975 as its first full-time female technical expert.

Johnson was a graduate student in physics at Vanderbilt University in 1944, when at age 23 she was recruited to work on the Manhattan Project at Columbia University. She came to Oak Ridge in 1948 to work as a research assistant at the K-25 uranium enrichment plant in Oak Ridge. From 1950 to 1961, she worked as a supervisor and senior reactor operator at ORNL's Bulk Shielding Facility, where she oversaw fuel loadings and reactor maintenance, trained reactor operators and coordinated experimental programs. She also taught students from ORNL's pioneering Oak Ridge School of Reactor Technology how to assemble reactor fuel safely.

In 1954, Johnson became a charter member of the American Nuclear Society, where she served in numerous leadership roles, chairing the society's Nuclear Criticality Safety Division, speaking at national standards meetings, forming standards subcommittees, contributing immeasurably to standards writing groups as both member and secretary and mentoring incoming professionals.

Johnson also helped found ORNL's ANS chapter. The society made her a fellow in 1982, recognized her with an achievement award in 1985 for her work in nuclear criticality safety and posthumously awarded her with its Standards Service Award in 2013. Upon her appointment in 1975 to the Atomic Safety Licensing Board, Johnson contributed to open hearings that included legal and technical experts to answer questions from the public and discuss concerns before construction licenses were issued. When Johnson retired in 1994 as the longest-serving female in the board's history, she remained its sole female technical expert.

Johnson also helped open doors for women in nuclear science — including for her granddaughter, Autumn Higgins, who joined the Nuclear Navy in 1995, a year before Johnson's death. In 2022, Higgins earned her senior reactor operator license for the Tennessee Valley Authority's Sequoyah Nuclear Plant.

"If I could talk to her today, I would want her to know her struggle meant something for me and other women," Higgins said. "Not only her scientific contributions, but also her personal contributions. They meant something."

Welcome to Research Insights

Toward a Carbon Neutral Future, Part II: Technologies for a more carbon-friendly future

ORNL Review is pleased to present the fourth issue of *Research Insights*, a collection of research articles from our scientific and technical staff. *Research Insights* was created to showcase the world-leading work being performed at ORNL, with each issue addressing an overarching theme.

This issue highlights recent advances by ORNL staff to support the United States' ambitious and achievable goal to reduce net greenhouse gas (GHG) emissions by 2030. Achieving the nation's 2030 GHG goals will place the United States firmly on a path to reach net zero by 2050.

In recent years, ORNL has developed a substantial fundamental and applied research program as part of our *Transformational Decarbonization Initiative*. An integral part of this effort is ORNL's drive toward improvements in carbon dioxide management in the nation's infrastructure through development of intelligent tools and processes. Along this theme, articles in this issue of *Research Insights* address technologies to create a more resilient electric power grid; tools for monitoring grid interconnections, developing smart traffic routing regimes, and helping consumers make informed fuel economy choices; analysis of high-temperature alloy selection for future hydrogen-based energy applications-tools for improving solid-state battery design-and discussions of opportunities and challenges associated with floating nuclear power plants and novel technologies in advanced fission and fusion power production.

The articles presented in this issue of *Research Insights* represent a small fraction of the ORNL research portfolio dedicated to support the nation's net-zero emission goals. We hope that you enjoy the sampling of the exceptional work being performed by the ORNL research community.

Toward A Resilient All Power Electronics Grid

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INTRODUCTION

According to the US Environmental Protection Agency [1], the electricity sector contributes 25% of total US greenhouse gas emissions. The electric power grid is evolving, with renewable power and clean energy sought after as the "holy grail" of decarbonization and climate change. Reforming and stabilizing the future of a decarbonized power grid, power electronics technologies play indisputable roles in capturing and converting the intermittent and highly fluctuating power associated with renewable energy—direct current in many cases—into the regulated alternating current used by residential, commercial, and industrial customers and the electrified transportation sector.

An All Power Electronics Grid (APEG), as illustrated in Figure 1, is an electric power grid in which all the generating resources and loads are connected to the electric power network via power electronics. Power electronics encompass the technologies or devices (i.e., converters or inverters) that use electronics or semiconductors to control power flow and convert electricity from one form to another. Such a scenario represents the future of power systems, with revolutionary changes on the horizon for both grid architecture and grid dynamics. Using power electronics improves energy efficiency and power controllability [2]. On top of these, additional benefits [2,3] of adopting an APEG include acute fault tolerance, simplified grid operation, and inherent grid resilience leveraging grid architectures that incorporate design-for-resilience principles, fast and robust inverter controls, and dynamical multiphysics decoupling. Nevertheless, planning and operating an APEG presents unexpected complexity and uncertainty requiring novel technical advancements.

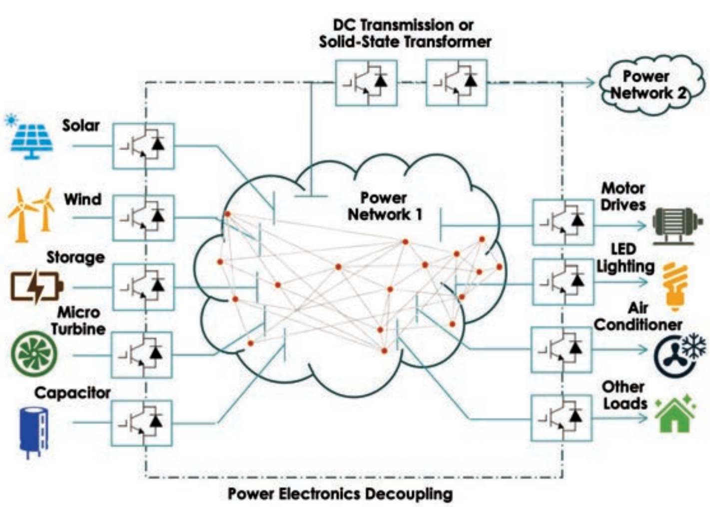

Figure 1. APEG architectural vision. (Credit: Y. Xue, ORNL)

Oak Ridge National Laboratory's (ORNL's) APEG research project, which is sponsored by the US Department of Energy (DOE) Office of Electricity, Advanced Grid Modeling Program, Resilient APEG Modeling and Operation, explores new modeling capabilities and analysis methods that could help utilities predict new grid instability issues potentially introduced by power electronics and develops grid-friendly power electronics control design to handle increasing complexity. The project's short-term objectives are to establish modeling methodologies and operational principles for APEG systems and develop best practices for grid architecture design for resilience, which will be both instructive and constructive as the US power grid improves resilience and evolves to an APEG. The project's long-term goals are to eliminate technical barriers for 100% renewable integrations and establish power electronics as viable grid resilience tools.

BACKGROUND

Today's US power grid evolved from Nikola Tesla's work in the late 19th and early 20th centuries. While emerging technologies have surged and the world's socioeconomic structure has changed dramatically since Tesla's time, the vertical and centralized power grid structure has not changed significantly. With global climate change, extreme natural events, and increasing electricity consumption and consumer expectations, resilience becomes a major risk management measure for power grids, as attention to national critical infrastructure, building a better power grid [4] that is more resilient to the impacts of climate change, and increasing access to affordable and reliable clean energy all become vital.

A recent report [5] identified seven social, technical, and economic forces driving change in future US power systems. Technical forces include development of grid-edge technologies such as distributed generation, storage, and microgrids and grid stability challenges due to high-penetration renewables, distributed energy resources (DERs), and/or inverter-based resources (IBRs). There exist emerging trends and systemic issues [6] associated with today's and future grid changes. For example, so-called power electronics converter–driven stability [7,8] was introduced by the Institute of Electrical and Electronics Engineers and the International Council on Large Electric Systems and included in the definition and classification of power system stability. The findings in [5] point out major needs for the future electric power system, including (1) new tools and different grid architectures for large-scale grid simulations to better understand how the system is evolving; (2) new power electronics and control technologies to ensure clean, sustainable, reliable, and resilient electricity services; and (3) innovations to enable deploy-

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ment of tens of millions of IBRs/DERs and operation of these "intelligent" nodes or control points at tens to hundreds times faster than today's grid controls.

Power electronics, the key to enabling many future grid architectures, is tied to many of these change drivers and needs and, hence, can be viewed as the main ingredient in many state-of-the-art power grid visions. However, the potential future system instability mechanism is quite different from today's synchronous machine-predominant power grid, which is still not clearly understood and has not been thoroughly investigated by the research community. Existing power system modeling and simulation tools also fall short, due to either being too simple and not capturing power electronics dynamics or being too detailed and computationally challenging for large-scale systems. As a result, the present techniques become the bottleneck preventing us from efficiently quantifying the risks of system instabilities and resonances under high-penetration power electronics, not to mention systemwide stability analysis and grid stabilization control, which may require approaches different from conventional practices.

These gaps and needs have motivated the APEG work. The future power grid will be characterized by more decentralized architecture with increased control complexity, fast electromagnetic transient dynamics adopting small-footprint power electronics devices, and more resilient operation to meet increasing public expectations. We seek to address needs with forward thinking that leads to solutions allowing us to adapt to evolving grid changes with technological breakthroughs that deliver maximized benefits from the future power grid.

RESEARCH PROBLEMS AND METHODOLOGY

The APEG project focuses on grid resilience and grid stability and develops proactive and design-oriented modeling, analytical, and control approaches to address the challenges of planning and operating high-penetration power electronics grids. Some of the research problems we are tackling include:

- How can we design a grid with inherently resilient architecture?
- How are fast grid dynamics modeled to capture harmonic oscillations and to judge system instability?
- How is a large-scale, multitimescale power electronics grid simulated in a computationally efficient way?
- Can robust stability become a performance metric for power electronics devices?
- What system functions should power electronics devices provide?
- Can future power grids be operated and controlled in a distributed manner?

In this project, fundamental R&D pillars are systematically laid out. Both short-term incremental solutions and long-term breakthroughs or radical concepts are pursued to steadily "push the technology envelope" on three tasks: Resilient Architecture; Modeling, Analysis, and Simulation; and Operation and Control.

RESULTS

Major outcomes under the three R&D tasks are summarized in this section.

Resilient Architecture: Establishing power electronics as grid resiliency tools. Resilience is a property of any ecological system that measures the persistence and ability to absorb change and disturbance and still maintain the same relationships between populations or state variables, as first defined in [9]. While the framework of power system resilience and its quantitative metrics to measure both power transmission and distribution levels are still evolving, various short-term operational approaches have been adopted by utilities. Nevertheless, developing an intrinsically resilient grid requires a multidimensional and long-term vision coupled with technological advances. While existing resilience approaches focus more on resource optimization and system recovery strategies, the APEG work envisions long-term grid resilience integrating grid hardware strength, operation performance, and architectural- and control-enabled grid elasticity. New architectural- and control-enabled grid resilience is substantiated by five design-for-resilience principles [3] utilizing the joints, buffers, decouplers, and decentralized controls, based upon which specific technical approaches [2] are derived.

Modeling, Analysis, and Simulation: Solutions to model and analyze harmonic stability. The power grid, already complex, becomes even more complicated [10] with nonlinear and fast dynamics, renewable uncertainties, granular structures, and ultralarge-scale interconnections. Analyzing and simulating a large-scale APEG with existing simplified phasor or detailed switching modeling methods and commercial tools creates either approximation or computation bottlenecks. A computationally efficient and physically meaningful modeling and analysis framework is needed to simulate and capture the potential resonance or instability phenomena at the frequency range of hundreds to kilohertz levels; this is the so-called "harmonic stability" distinguished from the ~60 Hz or below level, known as "subsynchronous oscillations," observed in traditional power grids. To fill this technical gap, the APEG project developed frequency-domain multifrequency averaging approaches using harmonic state-space [11,12] and dynamic phasor [13,14] models based on linear time-periodic theory. In addition, a design-oriented harmonic resonance identification and location method [15] was developed that utilizes an impedance-based stability criterion and network decomposition theory and is applied to a 140-bus, 48-inverter, 7-area large-scale APEG system. Figure 2 shows analysis results for an example APEG system.

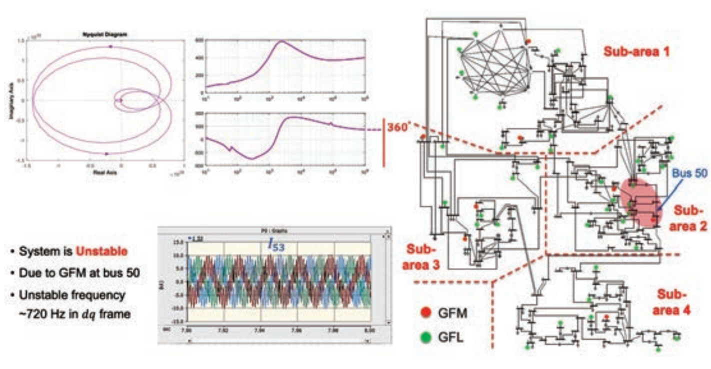

Figure 2. Large-scale harmonic stability analysis and identification results for an example 140-bus, 48-inverter, 7-area APEG system. (Credit: Y. Xue, ORNL; F. Wang, ORNL/UTK; L. Qiao, UTK; L. Kong, UTK)

Operation and Control: Distributed power system stabilizer. With high penetrations of relatively small-scale renewables and energy storage, power system operation and control can be expected to undergo a paradigm shift—from centralized to decentralized, from dispatched to autonomous, from top-down structured to bottom-up fractal, and from fully planned to more adaptive and self-optimizing. One project goal involves developing decentralized APEG control philosophy and strategies and advancing state-of-the-art power electronics control technologies for grid integrations. This has been achieved by grid-friendly power electronics control designs that handle increasing uncertainty and complexity, leapfrogged smart inverters with integrated system functions [3], and distributed power system stabilization [16] at each power electronics converter node.

As mentioned above, stability is a major challenge for the future power grid. This task emphasizes stability enhancement solutions. For the first time, stability is defined as an inverter performance metric and a type of grid service that can be offered to damp system oscillations. This requires passivity-based control design. A system is said to be passive if it can only dissipate, without generating, the energy stored initially (e.g., a resistor). The electrical subsystem is typically passive, but external disturbances can lead to instability. Therefore, injecting additional damping capabilities via a virtual resistor into controls can make the subsystem strictly passive, and thus it can obtain global stability. Several linear and nonlinear passivity-based control methods [17,18] were developed for power electronics converters and tested in an example 6-inverter 2-area APEG system. Figure 3 shows the new energy pumping and damping control, and the hardware testing results under two different uncertainty scenarios.

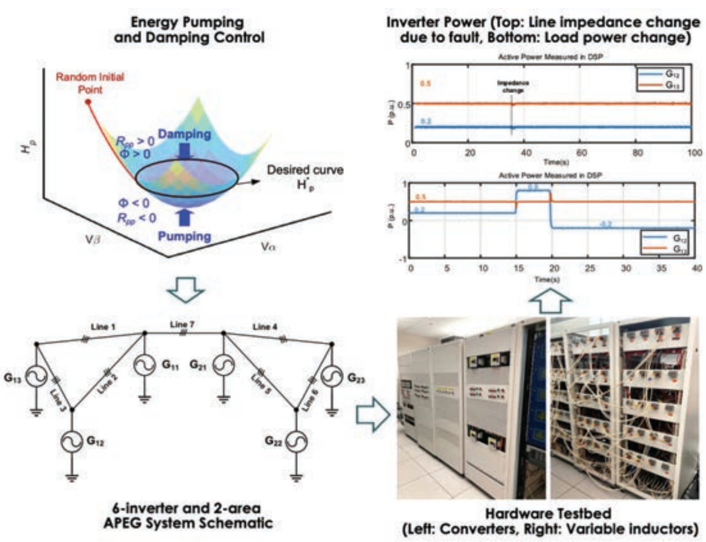

Figure 3. Novel control and validation in the hardware test bed for an example APEG system. (Credit: Y. Xue, ORNL; F. Wang, ORNL/UTK; L. Kong, UTK; L. Qiao, UTK)

The new inverter control provides advanced functions of distributed power system stabilization and grid forming in addition to basic power conversion and regulation. Ultimately, the whole system is guaranteed to be stable regardless of the number of power electronics and other components, if they are all designed to be passive.

CONCLUSIONS

Decarbonization and resilience are transforming power grids from traditional "machine age" systems into power electronics–based "silicon age" systems. Like any new technology, unforeseen uncertainties and systemic issues can be expected to occur. The APEG work initiates research that models and analyzes these concomitant changes and innovates the design and operation of the modernized power grid. Our initial results have been verified in small-scale APEG test systems. Future work will involve demonstration of a large-scale APEG system and field implementation of the novel grid controls and stabilization.

IMPACT

This work provides timely support to the Biden–Harris Administration's goal of achieving 100% carbon pollution–free electricity by 2035 and, more importantly, addresses national needs [5] for future US electric power systems based on better grid architectures, large-scale grid simulations, and grid control technologies and strategies to meet new stability challenges and enable significant deployment of DERs and IBRs.

The APEG project has provided the technical foundation for other ongoing projects and initiatives, has developed new R&D capabilities for ORNL and DOE to establish technical leadership among professional societies and the scientific community, explores new distributed grid stabilization methods, and pushes the envelope on science and technology that will help solve future grid problems.

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REFERENCES

1. US Environmental Protection Agency. "Inventory of U.S. Greenhouse Gas Emissions and Sinks." April 14, 2022. https://www.epa.gov/ghgemissions/inventory-us-greenhouse-gas-emissions-and-sinks.
2. S. Xu, Y. Xue, et al. *IEEE Open J. Power Electron.* 2, 88–105 (2021).
3. Y. Xue et al. "On a Future for Smart Inverters with Integrated System Functions." In *Proceedings of the 9th IEEE International Symposium on Power Electronics for Distributed Generation Systems*, Charlotte, NC, June 25–28, 2018, pp. 1–8.
4. US Department of Energy, Grid Deployment Office. "Building a Better Grid Initiative." https://www.energy.gov/gdo/building-better-grid-initiative.
5. National Academies of Sciences, Engineering, and Medicine. *The Future of Electric Power in the United States.* Washington, DC: The National Academies Press (2021).
6. Y. Xue et al. *Emerging Trends and Systemic Issues Influencing Today's U.S. Electric Grid.* Grid Modernization Labo-

ratory Consortium Report no. GMLC-1.2.1/ORNL Report no. ORNL/TM-2022/2372 (February 2022).

7. N. Hatziargyriou et al. *IEEE Trans. Power Syst.* 36 (4), 3271–3281 (July 2021).
8. L. Kong, Y. Xue, et al. *IEEE Open Access J. Power Energy* 9, 29–41 (2022).
9. C. S. Holling. *Annu. Rev. Ecol. Syst.* 4, 1–23 (1973).
10. Y. Xue. "Computational Challenge of Large-Scale Power Electronics Grid Analysis." Presentation at DOE Workshop on Computational Mission Needs for Clean Energy and Manufacturing, Oak Ridge, TN, June 28–29, 2021.
11. J. K. Motwani, Y. Xue, et al. "Analysis of Inter Converter Interactions Using Harmonic State Space Modeling." In *Proceedings of the 6th IEEE Workshop on the Electronic Grid (eGRID)*, Nov. 8–10, 2021.
12. J. K. Motwani, Y. Xue, et al. *IEEE Open J. Power Electron.* 3, 689–704 (2022).
13. A. Nazari, Y. Xue, et al. "Dynamic Phasor Modeling of Three Phase Voltage Source Inverters." In *Proceedings of the 6th IEEE Workshop on the Electronic Grid (eGRID)*, Nov. 8–10, 2021.
14. A. Nazari, Y. Xue, et al., "Dynamic Phasor Modeling of Multi-Converter Systems." In *Proceedings of the IEEE Energy Conversion Congress and Exposition (ECCE)*, Oct. 10–14, 2021, pp. 2716–2721.
15. L. Qiao, Y. Xue, et al. "Nodal Admittance Matrix Based Area Partition Method for Small-Signal Stability Analysis of Large-Scale Power Electronics Based Power Systems." In *Proceedings of the IEEE Applied Power Electronics Conference and Exposition (APEC)*, June 14–17. 2021, pp. 687–693.
16. K. Divya and Y. Xue. US Patent no. 9,640,997 (May 2, 2017).
17. L. Kong, Y. Xue, et al. *IEEE Trans. Power Electron.* 37 (12), 14141–14156 (Dec. 2022).
18. L. Kong, Y. Xue, et al. "Angle Droop Design for Grid-Forming Inverters Considering Impacts of Virtual Impedance Control." In *Proceedings of the IEEE Energy Conversion Congress and Exposition (ECCE)*, Oct. 10–14, 2021, pp. 1006–1013.

GridEye: A Situational Awareness Tool for Facilitating the Decarbonization of the US Power Grid with a High Penetration of Renewable Energy

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INTRODUCTION

Electricity generation in the United States is undergoing a significant change: carbon-free renewable energy–based sources such as wind and solar are replacing fossil energy–based power plants. The success of this transition is critical to achieving the goal of a carbon-free US power grid by 2035. However, because of the volatility of renewable resources and the challenges inherent in replacing large mechanical generators by lightweight power electronics devices, the transition to decarbonized energy production will require versatile solutions. To ensure a reliable power supply to the US economy during decarbonization, we need a situational awareness tool that will provide real-time monitoring and analytics for the power grid.

BACKGROUND

Developed by a team of researchers at Oak Ridge National Laboratory (ORNL) and the University of Tennessee–Knoxville (UTK), GridEye won an R&D 100 Award in 2022 and is the first nationwide GPS-synchronized power grid monitoring system to provide US power grid situational awareness capabilities to aid decarbonization. The GridEye system consists of hundreds of quickly deployable GPS-synchronized GridEye sensors (Figure 1), communication, and data centers located at ORNL and UTK. Approximately 300 GridEye sensors are operating in real time to monitor five North American power grid interconnections (Figure 2), while more than 70 GridEye sensors are monitoring power grids in other countries worldwide. As a multifunctional instrument, a GridEye sensor can measure frequency, voltage phase angle, voltage magnitude, power quality, and instantaneous power grid

Figure 1. GridEye sensor. (Credit: ORNL, UTK)

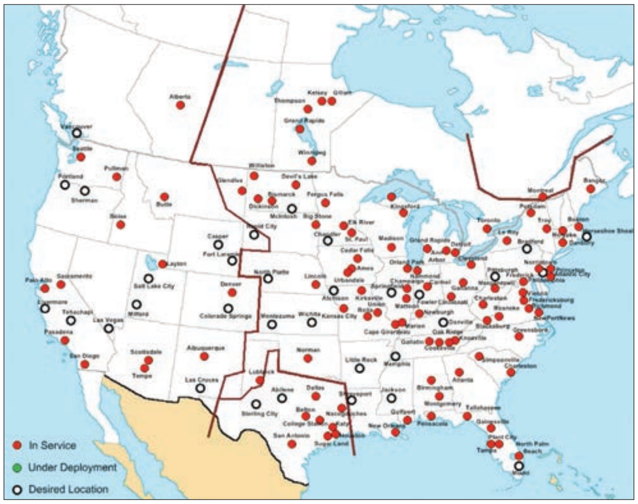

Figure 2. GridEye deployment in North America. Red dots represent GridEye sensor locations. (Credit: ORNL, UTK)

waveforms, providing unprecedented visibility of North American and worldwide power grids since it was first introduced in 2004. GridEye has many advanced situational awareness applications that are operating online for power grid monitoring and analysis. GridEye provides real-time alerts to industry consortium members, utilities, the US Department of Energy, the North American Electric Reliability Corporation (NERC), the Federal Energy Regulatory Commission, and others. Based on analysis results drawn from GridEye data in the Eastern Interconnection oscillation event on January 11, 2019 (Figure 3), NERC has published the *Eastern Interconnection Oscillation Disturbance* report, which provides key findings and recommendations to the industry for proactive mitigation of potential future oscillation events [1].

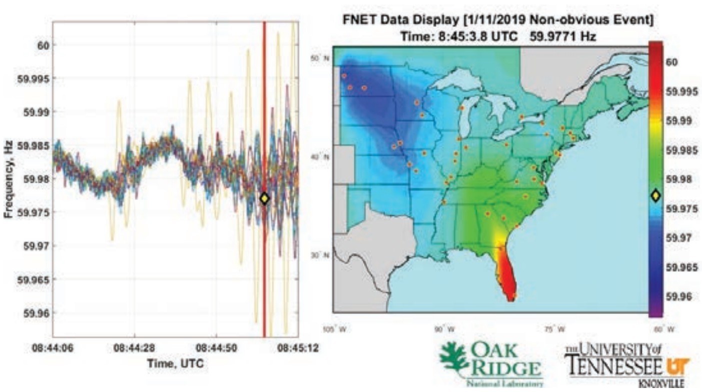

Figure 3. GridEye monitoring output for the Eastern Interconnection event on Jan. 11, 2019. (Credit: ORNL, UTK)

GRIDEYE APPLICATIONS

Real-time visualization. Real-time visualization of wide-area power grid measurement data is one of GridEye's most important applications. Power grid operators need real-time grid measurements for power systems situational awareness. Some utilities have their own real-time visualization system, but they access only the utilities' own data, and utilities have very limited access to data outside their own system. In contrast, with the easy deployment of its sensors, GridEye provides full coverage of the North American power grid, thus providing system operators with a complete picture of the power grid. Figures 4 and 5 show samples of a real-time power grid frequency map and a phase angle contour map of the North American power grid, respectively, as generated by GridEye.

Figure 4. GridEye real-time frequency gradient map. (Credit: ORNL, UTK)

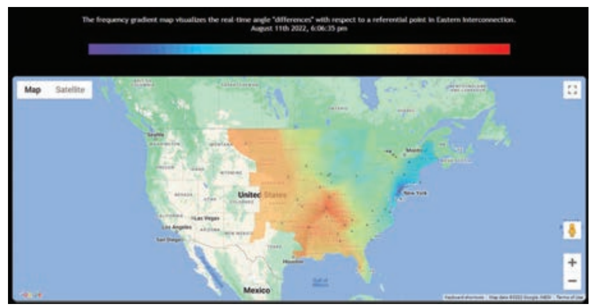

Figure 5. GridEye real-time angle gradient map. (Credit: ORNL, UTK)

Inertia estimation and alert. One of the most complicated challenges presented by a high-renewable power grid is the low inertia problem introduced by renewable resources. The inertia in power grids mainly refers to the energy stored in large generators, and it can help stabilize the power grid by providing stored energy during system dynamics. Utilities are concerned about the problem because it could cause frequency instability, potentially forcing power plants to go offline and resulting in blackouts. GridEye provides event measurements–driven and ambient measurements–driven machine learning–based inertia estimation solutions. Verified by NERC data, GridEye provides accurate inertia monitoring with 98% accuracy. Figure 6 shows the inertia estimated by using GridEye sensor data and the measured inertia. The mean absolute percentage error is ~1% for both heavy and light load seasons.

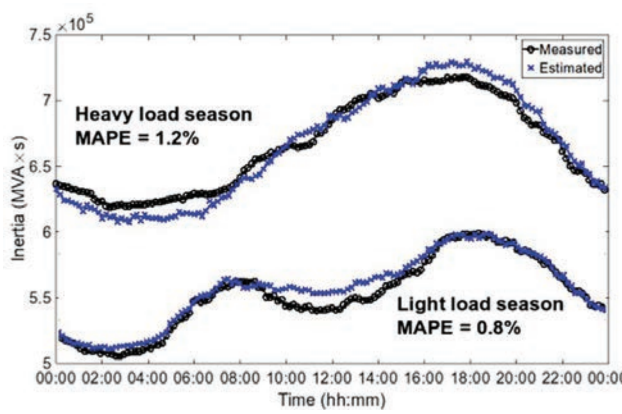

Figure 6. Performance of the machine learning–based inertia estimation using ambient frequency measurements. (Credit: ORNL, UTK)

Real-time oscillation detection and location. One of the major threats to a high-renewable power grid is low-frequency (<1 Hz) oscillations. Low-frequency oscillation could cause instability of the power grid, resulting in power outages. As the proportion of electricity provided by renewable resources increases, oscillations can occur more frequently. Using both event and ambient data, GridEye can help utilities detect, locate, and assess potential risks of oscillations. Figure 7 shows three oscillations detected by GridEye in the US power grid, on January 11, 2019 (left), April 7, 2020 (middle), and April 28, 2020 (right). Working with Tennessee Valley Authority, ORNL has used GridEye to successfully detect and locate several additional oscillations in recent years.

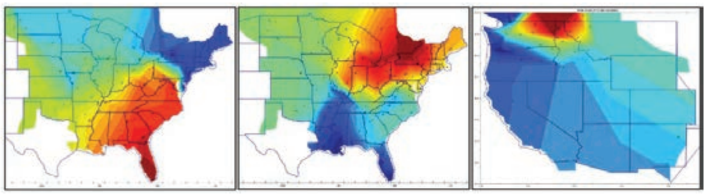

Figure 7. Forced oscillations detected by the GridEye system. (Left to right) Oscillations occurred on January 11, 2019, April 7, 2020, and April 28, 2020. (Credit: ORNL, UTK)

Islanding detection. Renewables are expanding in distribution systems as microgrids—local electrical grids with defined electrical boundaries acting as a single controllable entity—gain market share. Microgrids can operate in grid-connected mode or island mode, which is disconnected from the power grid. Islanding detection of microgrids will become more important for system operators, with increasing penetration of renewables in distribution systems. GridEye can detect the disconnection of a microgrid from the power grid (i.e., islanding detection) and can distinguish the islanding events from other events, such as generation trip events. Figure 8 shows two examples of islanding detection of microgrids in the Eastern Interconnection (left) and Western Electricity Coordinating Council (right) power grids, two major electric power grids in North America.

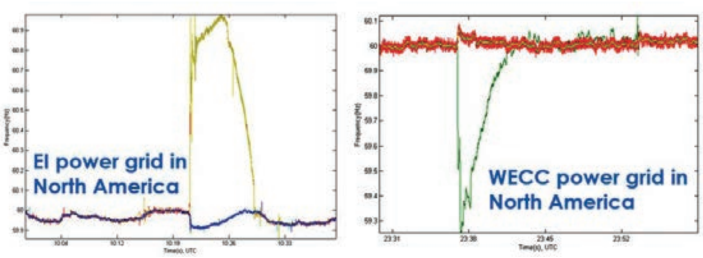

Figure 8. Islanding detection of microgrids by GridEye. (Credit: ORNL, UTK)

Event location. Event location involves estimating the geographic location of a disturbance when a contingency occurs in the power grid, which can help system operators to quickly take appropriate measures. Given that wave propagation speeds are very unevenly distributed in high-renewable power grids, GridEye's event location application incorporates feature selection and machine learning to address the challenge. In all, 3,000 real historical events in the past 15 years were tested, and GridEye accurately located 70% of events. Figure 9 shows an example of our machine learning–based location estimation method; the figure shows that the estimated disturbance location is very close to the true event location, while the traditional method based on time delay of arrival has much higher estimation error.

Figure 9. Output showing GridEye's machine learning–based event location application. Redrawn from You et al. [2]. (Credit: ORNL, UTK)

Power system dynamic model validation. Power grids consist of a huge number of components, so modeling the power grid accurately is not trivial work; it is becoming only more challenging with the increasing penetration of renewables on distribution systems. Using nationwide GridEye measurement data, the power system dynamic model can be fine-tuned to match the dynamic response of a real power system. Figure 10 shows the dynamic response of untuned and tuned models against a real grid measurement. It can be seen that GridEye data can greatly improve the accuracy of a power system dynamic model.

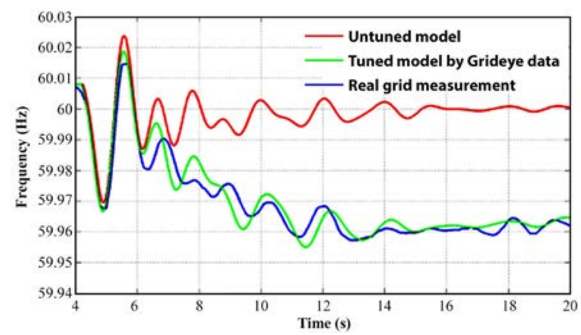

Figure 10. Power system dynamic model tuning and validation. Redrawn from Kou et al. [3]. (Credit: ORNL)

Measurement-adaptive oscillation damping control with GridDamper. In addition to real-time oscillation detection and location, GridEye can also efficiently mitigate and damp oscillation. GridDamper, a field deployment–ready technology developed based on GridEye that won an R&D 100 Award in 2021, can mitigate three major categories of oscillations—natural, forced, and subsynchronous—that will become increasingly important to address as more renewables are integrated into the bulk system. Most existing oscillation damping methods use fixed dynamic models with predetermined control parameters, resulting in poor damping performance due to constantly changing power systems. To address the problem, GridDamper actively updates its parameters to adapt to changes in the power grid, allowing for mitigation of power grid oscillations. GridDamper has been applied to several power grids around the world to validate its performance. Figure 11 shows that the grid frequency in South Italy (Palermo) was successfully stabilized by GridDamper. The top plot shows the frequency without GridDamper, the middle plot shows the frequency with GridDamper, and the bottom plot shows the output of the damping controller.

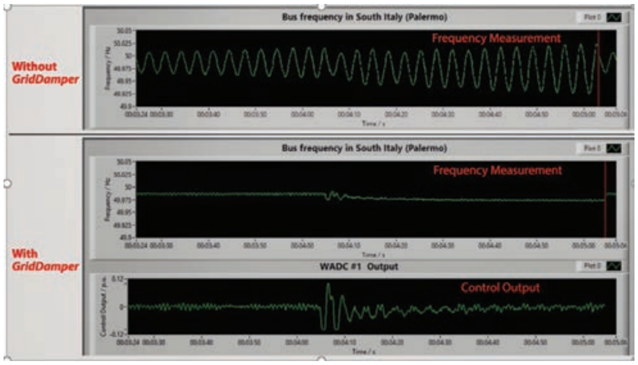

Figure 11. Outputs showing GridDamper's oscillation damping capabilities. (Credit: ORNL, UTK)

LATEST ADVANCEMENTS IN GRIDEYE SENSORS

The GridEye sensor is the key component of the GridEye system, as it provides real-time, high-accuracy grid measurements. The team has been continually enhancing its measurement capabilities by addressing the more urgent measurement problems in the power grids. Table 1 compares the measurement features of our sensor with a transmission phasor measurement unit (T-PMU) and a distribution phasor measurement unit (D-PMU). Advancements to the GridEye sensor are discussed below.

Table 1. Measurement features of ORNL sensor vs. T-PMU and D-PMU.

	ORNL Sensor[1]	T-PMU	D-PMU
Phasor Measurements	✓	✓	✓
Power Quality (PQ) Measurements	✓		
Real-Time GPS Sync POW	✓		
Ultra-high Measurement Rate	✓		
Fault-tolerant	✓		

1. Not all features in one sensor. The sensor can be configured to have one or some of the features.

Extended Universal Grid Analyzer (e-UGA). The e-UGA is a multifunctional measurement instrument that provides traditional synchrophasor measurement functions to the GridEye sensor as well as power quality (e.g., harmonics, sag/swell, signal-to-noise ratio, flickers) and Point on Wave measurement functions. Together, these capabilities enable comprehensive monitoring of renewables in a wide range of frequency and time domains. Figure 12 shows the GridEye e-UGA.

Figure 12. Extended UGA. (Credit: ORNL, UTK)

Ultrahigh-speed grid measurements. Most existing synchrophasor measurement devices take a maximum of 60 measurements per second, resulting in limited system dynamics capture capability. This limitation deters measurement of fast-changing renewable resources, as higher-rate measurements provide better dynamic measurement performance. The team developed a computationally efficient and accurate measurement algorithm that reduces computation time for grid measurements by two orders of magnitude, thus significantly improving measurement resolution. Figure 13 shows that, for a 30 Hz oscillation, the ultrahigh-speed GridEye sensor effectively detects the oscillation while the classic low-rate measurement device (e.g., T-PMU) fails to capture the oscillation.

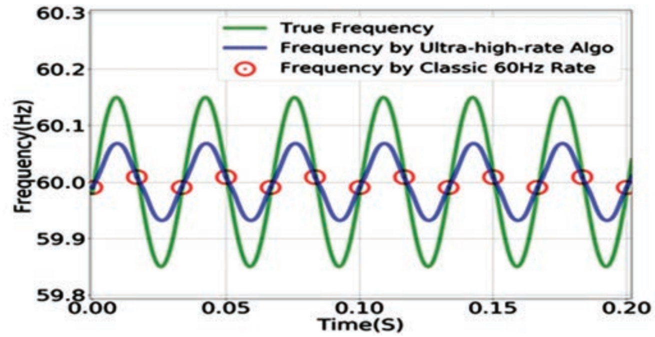

Figure 13. High-frequency oscillation captured by ultrahigh-speed measurement algorithm. (Credit: ORNL)

Fault-tolerant grid measurements. On August 16, 2016, a 700 MW solar photovoltaics (PV) plant in southern California tripped due to erroneous frequency measurements by solar PV inverters during power system transient faults. Our team provided a fundamental solution to the grid measurement uncertainties during grid faults by developing the fault-tolerant frequency measurement technologies embedded in the GridEye sensor. Figure 14 shows the fault-tolerant grid sensor (left panel) and its measurement performance during a system fault (right panel). The figure shows that our measurement is stable during the grid fault while the classic method produces a large error.

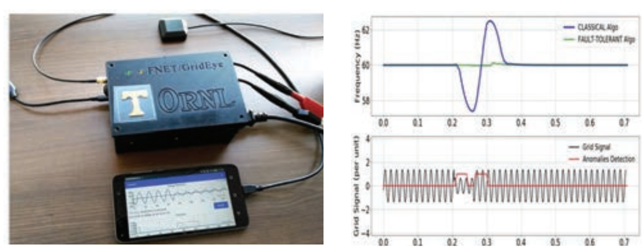

Figure 14. Fault-tolerant grid sensor (left) and measurements (right). (Credit: ORNL)

Mobile Universal Grid Analyzer (m-UGA). To further reduce barriers to obtaining power grid measurements, we have developed m-UGA, which won an R&D 100 Award in 2018. Similar to our traditional GridEye sensor, m-UGA is a time-synchronized, multifunctional, wide-area monitoring and analysis device designed to provide situational awareness capabilities in real time for the power grid at the distribution level. Many power grid monitoring functions can be realized on the m-UGA with novel measurement algorithms. m-UGA can be installed in any location with regular 120V power outlets (e.g., offices, schools, personal residences). Figure 15 shows the m-UGA (left panel) and a snapshot of its measurement output (right panel).

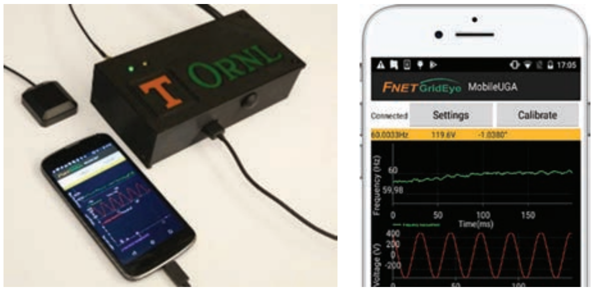

Figure 15. Mobile UGA. (Credit: ORNL, UTK)

CONCLUSIONS

The GridEye system offers wide-ranging capabilities to support the decarbonization of the US power grid with high-renewable resources. Some important applications include real-time visualization, inertia estimation and alert, real-time oscillation detection and location, islanding detection, event location, power system dynamic model validation, and measurement-adaptive oscillation damping control. The latest advancements to the GridEye sensor design, including an e-UGA, ultrahigh-speed and fault-tolerant grid measurements, and a mobile grid analyzer, will further extend GridEye's award-winning capabilities to novel power grid monitoring methodologies.

IMPACT

GridEye is a low-cost, quickly deployable GPS-synchronized wide-area measurement network for power grids. As a unique nationwide power grid monitoring system, over the past 15 years, GridEye and its related applications, GridDamper and m-UGA, have won three R&D 100 Awards. Since its introduction in 2004, the GridEye system has provided nationwide situational awareness to system operators, utilities, industry, and academia. With the hardware and measurement algorithm advancements made in recent years to GridEye sensors, and by applying machine learning and big data techonlogies in GridEye applications, the GridEye system will continue to play a vital role in facilitating the decarbonization of US power grids.

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REFERENCES

1. North American Electricity Reliability Corporation (NERC). *Eastern Interconnection Oscillation Disturbance*. NERC (Dec. 2019). https://www.nerc.com/pa/rrm/ea/Documents/January_11_Oscillation_Event_Report.pdf.
2. S. You…Y. Liu. "FNET/GridEye for Future High Renewable Power Grids—Applications Overview." In *Proceedings of the 2018 IEEE/PES Transmission and Distribution Conference and Exposition–Latin America*, Sept. 18–21, 2018. https://ieeexplore.ieee.org/document/8511657.
3. G. Kou, S. W. Hadley, Y. Liu. *Dynamic Model Validation with Governor Deadband on the Eastern Interconnection*. ORNL Report no. ORNL/TM/2014/40 (2014).

From Signal Processing to Signaling Traffic: Using Digital Twins to Improve Traffic and Reduce Our Carbon Footprint

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INTRODUCTION

Traffic backups and long commutes are an unfortunate reality we all deal with these days. Beyond costing us valuable time, traffic wastes fuel and contributes substantially to our global carbon footprint. If we could design a dynamic, adaptive system to actively coordinate and time lights, choose routes, and even recommend certain lanes, we could greatly alleviate congested traffic and the myriad problems that come with it. Unfortunately, developing such a dynamic system that coordinates traffic across an entire region is easier said than done! Traffic and transit systems are complex, and the testing of new light sequences or traffic patterns in real life can be cost-prohibitive, dangerous, or both. It is for these reasons that the use of digital twins is such an exciting prospect.

BACKGROUND

Chattanooga Digital Twin. Digital twins are virtual reproductions of complex real-world systems. They "offer an effective way to mitigate risks and improve performance without significant loss of time or money" [1].

In 2019, the Chattanooga Digital Twin project, or CTwin, sought to develop a complete transit-level digital twin of the Chattanooga area that could act as a virtual test bed for smart traffic routing. As a low-cost yet accurate-to-real-life traffic environment, the CTwin system allowed researchers to observe virtual traffic patterns and problems and optimize a region-wide virtual controller system that could leverage virtual sensors and cameras to dynamically adapt traffic patterns [2]. A good example of this multimodal sensing-and-control loop can be seen in Figure 1.

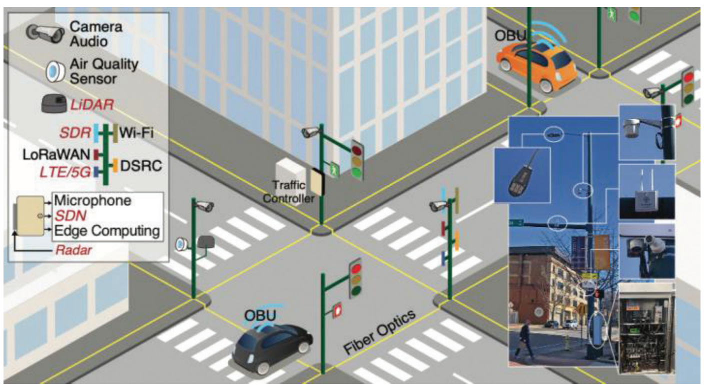

Figure 1. Visualization of how city-level traffic is modeled and controlled in the original CTwin system, which models a virtual version of Chattanooga. (Credit: University of Tennessee–Chattanooga Center for Urban Informatics and Progress)

CTwin2.0 Project. CTwin's successor, CTwin2.0, takes the optimal techniques learned from the virtual CTwin world and applies them to the real Chattanooga, scaling the solution across the entire Chattanooga area. CTWin2.0 brings to life a region-wide, complex traffic controller that coordinates inputs from many sensors as feedback to dynamically change traffic patterns on global and local scales. The idea of adaptive traffic control systems (ATCSs) is not entirely new—there have been versions of ATCSs in use since the 1980s. This is the first controller, however, to both be designed using digital twin technology and specifically optimize for fuel efficiency and emission reduction [3]. The project is a collaborative effort of Oak Ridge National Laboratory's (ORNL's) Computational Sciences and Engineering Division (CSED), Electrification and Energy Infrastructures Division (EEID), and National Transportation Research Center (NTRC); the National Renewable Energy Laboratory (NREL); and the Tennessee Department of Transportation (TDOT). One of the main and most straightforward avenues for realizing this control loop is through the implementation of a next-generation smart fleet routing system for highway freight, helping alleviate traffic congestion on busy highways and city streets.

Fleet Routing Problem. The Fleet Routing Problem (FRP) boils down to optimizing the multistop routes of many vehicles in a fleet to ensure all required stops are made with maximal overall efficiency. FRP has many parameters, both physical and temporal, that must be considered in the optimization process. More concretely, a standard FRP task is planning transport schedules and routes around peak traffic times and locations while still servicing all of the required destinations on a set of customer manifests. When done well, fleet routing can markedly reduce the carbon footprint of freight traffic across entire regions or even the country.

IMPLEMENTATION

Realizing complex sensor systems. While current FRP systems optimize routes and schedules based on historical data in a more static manner, CTwin2.0 aims to go further. Using foundational observations from the CTwin traffic control system in the virtual world, the project aggregates streaming data from a set of distributed multimodal sensors operated and maintained by TDOT. CTwin2.0 utilizes this large set of streaming data to detect incidents and provide a dynamic, situationally aware FRP solution that continuously adapts and updates freight trucking routes and strategies in real time.

Detecting anomalies. CTwin2.0 leverages streaming data from hundreds of Radio Data System (RDS) sensors. These sensors produce lane-level information on vehicle counts, occupancy counts, and average speeds of vehicles aggregated over 20–30 seconds. RDS sensors can be used to quickly detect local anomalies and incidents along TDOT TN SmartWay highways that require immediate attention within the FRP controller. The sensor network is shown in Figure 2.

Figure 2. Map view of the Chattanooga I-75 corridor with RDS sensors utilized by CTwin2.0 shown as green dots. (Credit: A. Berres; J. Brogan, ORNL)

Using cameras as sensors. CTwin2.0 also utilizes cameras from the TDOT TN SmartWay system to supplement the RDS sensor network. CTwin researchers developed lightweight computer vision and machine learning algorithms designed to detect, classify, and track different types of vehicles as they drive by different cameras along major thoroughfares (Figure 3). The output of this algorithm provides traffic counts, relative speed estimates, and throughput metrics that can be utilized as supplemental sensor data for the CTwin controller. To provide real-time data across many incoming video streams, these state-of-the-art computer vision algorithms are deployed using an ORNL-developed computer vision framework called FaRO [4] in NREL's high-performance computing environment, Eagle.

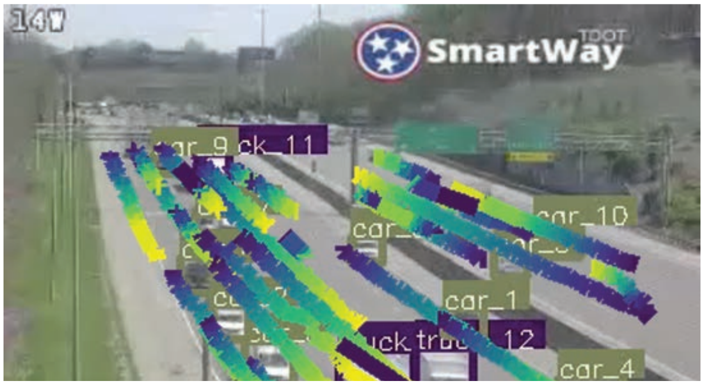

Figure 3. Visualization of what the CTwin2.0 Traffic Vision System sees in an image captured by a TN SmartWay camera. Colored squares represent cars and trucks, while lines represent persistent tracks of each vehicle. (Credit: J. Brogan, ORNL)

Computer vision algorithms summarize real-time traffic flow statistics across hundreds of cameras and coordinate with proprietary roadway sensors to detect traffic incidents and anomalies in real time. Commercial partners will be able to use the system to design daily freight truck routes and update them adaptively throughout the day based on current traffic events and contexts. Research is focused on leveraging this multimodal sensor data to optimize traffic on every level, from traffic light timing to adaptive route avoidance for freight trucks.

Partnering with regional freight. While suggesting route modifications to freight fleets in the CTwin2.0 virtual traffic world is relatively easy, reflecting those modifications in the physical world is much trickier. From a logistics perspective, ORNL and NREL needed to partner with many collaborating entities to realize a physical analog of this dynamic rerouting system. The project focuses on offering integration with industrial and commercial freight fleet operations to provide this unified routing service to as many partners as possible. Currently, two regional fleets are successfully integrated into this work: Chattanooga Public Works Solid Waste and Recycling, whose vehicles visit every city street once a week, and Covenant Transport Group, which runs interstate freighting operations along long-haul lines.

While these initial collaborations provide a good starting point to test the CTwin2.0 controller system, a major portion of the project is focused on building relationships and affiliations with additional public and private institutions to scale up the program to realize its full potential. While there is broad interest across the freighting industry to integrate with CTwin2.0 technology, taking the leap from interest to integration requires a significant amount of technical and logistical coordination. While this effort does take time, we expect to continue expanding CTwin2.0 control system deployment with additional partners over the next project year. In this growing phase, the Technology Readiness Level of CTwin2.0 remains at research levels, meaning ORNL and its collaborating entities will continue to perform maintenance and support for partners integrating with the platform. As the technology matures, further deployment and scaling likely will be handed off to industrial or private partners via technology transfers or cooperative research and development agreements.

RESULTS

The CTwin project has shown breakthroughs in incident detection capabilities, providing early warning of traffic buildups up to 7 min before Waze hazard reports appear and 18 min before official authorities are notified. An example of this capability can be seen in Figure 4, in which RDS sensors and traffic cameras fitted with CTwin2.0 technology show anomalous behavior long before other methods of reporting. This early warning can provide the CTwin FRP controller valuable room to find solutions for rerouting traffic, even before a major traffic jam has formed.

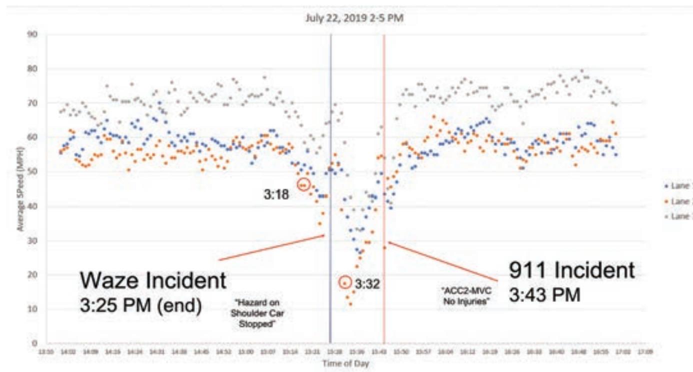

Figure 4. Average speed readings from RDS and camera sensors providing early detection of a traffic jam. Y-axis shows speed readings; x-axis shows time of day. (Credit: A. Berres, ORNL)

Using the CTwin plaftorm to perform fleet routing and dynamically time traffic lights at local levels, a simulated estimate of energy savings shows up to an 18% reduction in energy use and carbon emissions at traffic signals when the dynamic CTwin2.0 FRP controller is utilized. When tested operationally on live traffic signals, a 16% reduction in energy has been realized in real-world controller deployment (Figure 5).

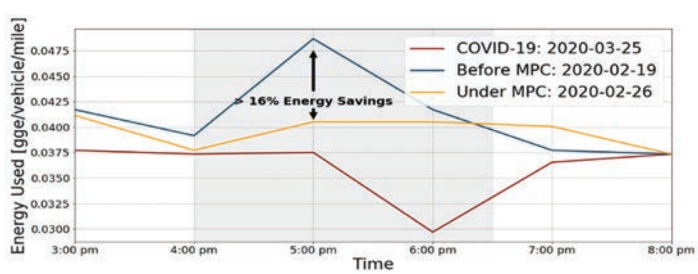

Figure 5. Energy use estimates per vehicle before and after deployment of the CTwin controller, as compared with the 2020 COVID shutdown [5]. (Credit: Wang et al.)

CONCLUSIONS AND IMPACT

Reducing our carbon footprint is one of the highest priorities in today's modern world. Meeting that goal will require a disparate stack of many systems working in tandem, all focused on tackling different problem areas of carbon production. Systems such as CTwin2.0 can help achieve that goal and improve traffic, with the promise of doing so in subtle ways most civilians may not even notice. As our cities continue to grow and become increasingly connected through smart infrastructures, systems like CTwin2.0 will become more instrumental in coordinating the well-oiled transit apparatuses that keep us moving.

To that end, the CTwin2.0 has seen both successes and obstacles while porting digital twin–based traffic solutions to the real-world Chattanooga area. Its deployment will provide measurable benefits to the drivers it serves, yet more work still must be done. As we move forward with further improvements, CTwin2.0 will benefit greatly from wider-reaching freight partnerships that can help implement vehicle-by-vehicle freight control. More sophisticated machine learning algorithms are being explored to better understand the firehose of real-time camera and RDS data streaming in from TDOT TN SmartWay sensors. As self-driving cars inch closer to reality, their sensor and communication networks could greatly benefit the CTwin controller and systems like it, and research in this area is ongoing.

ACKNOWLEDGMENTS

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REFERENCES

1. A. Arabshahi. "Digital Twins," University of Tennessee–Chattanooga, 2020. https://www.utc.edu/research/simcenter/research-thrusts/digital-twins.
2. National Renewable Energy Laboratory. "NREL is Participating in a Project Led by Oak Ridge National Lab to Create a Large-Scale, Real-Time 'Digital Twin' of Traffic Conditions in Chattanooga, Tennessee," February 14, 2019. https://www.nrel.gov/news/program/2019/data-driven-simulations-mirror-a-citys-traffic-patterns-to-reduce-mobility-related-energy-use.html.
3. "Using Artificial Intelligence to Connect Vehicles and Traffic Infrastructure." EurekAlert!, September 23, 2020. https://www.eurekalert.org/news-releases/620145.
4. D. S. Bolme, J. Brogan, et al. "Face Recognition Oak Ridge (FaRO): A Framework for Distributed and Scalable Biometrics Applications." In *Proceedings of IEEE International Joint Conference on Biometrics (IJCB)*, 2020.
5. Q. Wang et al. "Offline Arterial Signal Timing Optimization for Closely Spaced Intersections." In *Proceedings of IEEE Green Technologies Conference (IEEE-Green)*, Virtual, April 7–9, 2021.

ORNL's FuelEconomy.gov delivers consumer savings, reduced vehicle emissions

FuelEconomy.gov, a joint US Department of Energy (DOE) and US Environmental Protection Agency website, provides information that helps consumers make informed fuel economy choices when purchasing a vehicle or achieve the best fuel economy possible from the cars they own—topping $1 billion in savings and reducing transportation sector greenhouse gas emissions (GHGs). The website includes fuel economy tips and information on clean vehicle tax credits and advanced vehicle technologies. The Find a Car tool provides fuel economy, fuel cost, and environmental and safety information for vehicle models back to 1984. Other helpful tools include:

- Fuel savings calculator
- Trip cost calculator
- GHG emissions calculator for plug-in hybrid electric vehicles and all-electric vehicles
- Plug-in hybrid electric vehicle cost calculator
- My MPG, which allows consumers to track and share their fuel economy for conventional and all-electric vehicles
- Web services that provide fuel economy data to other public and private entities

Since its launch in 1999, FuelEconomy.gov has hosted more than 500 million users, saved consumers more than $1 billion in fuel costs, and reduced petroleum use and vehicle-related GHGs.

Image credit: Colby Earles, ORNL

Oak Ridge National Laboratory (ORNL) maintains FuelEconony.gov for DOE and supports the website's collection of fuel-saving tips through fuel economy–related research activities. ORNL staff have conducted numerous studies and published peer-reviewed papers on topics such as aggressive driving, speeding, hauling cargo, idling, air conditioner use, and fuel stability.—*Stacy Davis, Buildings and Transportation Science Division, ORNL*

High-Temperature Alloy Selection for a Future with Hydrogen: Balancing Cost, Mechanical Properties, and Environmental Resistance

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INTRODUCTION

The continuously increasing energy demands in the power generation and transportation sectors need to be met in the future while simultaneously addressing CO_2 reduction targets. A synergistic integration of diverse technologies such as nuclear, hydroelectric, geothermal, wind, and solar is envisioned to accomplish this goal. Hydrogen (''blue'' from traditional sources and ''green'' from renewables) is increasingly being considered integral to the future energy landscape [1]. However, the use of hydrogen as a fuel for power generation or transportation presents new challenges for selection and development of suitable high-temperature materials for hydrogen combustion. The materials of choice, which require high strength and excellent corrosion resistance at temperatures of interest, are expected to be critical to the realization of next-generation energy technologies. The burning of hydrogen is expected to result in higher operating temperatures and higher than typically observed water vapor contents in exhaust gases after burning natural gas (i.e., ~5–10 vol.% H_2O) [2]. Future dry low-emission (DLE) combustion systems operating with pure hydrogen could increase the steam fraction in combustion products to 16 vol.%, while existing wet low-emission (WLE) technologies utilizing steam dilution or water injection may result in exhaust steam contents of up to 85 vol% [3,4]. The impact of hydrogen at precombustion temperatures (i.e., 500°C–600°C) and higher water vapor contents in the combustion products on the long-term high-temperature structural strength and corrosion behavior of existing candidate structural materials has not been studied extensively enough. Significantly advancing contemporary scientific knowledge on long-term material behavior in high-temperature H_2-rich environments is essential to selecting and developing suitable materials for a future hydrogen-driven economy.

The Corrosion Science and Technology (CST) Group in the Materials Science and Technology Division at Oak Ridge National Laboratory (ORNL) is conducting relevant work to investigate the impact of burning hydrogen on the corrosion resistance of candidate structural materials. The ultimate goal is the development of enhanced tools to assist in materials selection and development as well as lifetime predictions while simultaneously advancing our current understanding of underlying material behaviors. Assessing the potential utility of physics-based models as tools to evaluate the combined effects of additional parameters such as alloy composition, temperature, thermal cycling, gas composition, and flow rates to provide a realistic picture of material behavior and enable application-specific material selection while balancing cost, mechanical properties, and environmental resistance is also a key research area.

BACKGROUND

There is no novelty in burning hydrogen for power generation, as several commercial gas turbines using conventional diffusion flame combustion and WLE can already operate with 100% H_2 [2]. However, DLE combustion technologies are required to increase efficiencies and ensure emission-compliant operation with 100% H_2, as first demonstrated by the New Energy and Industrial Technology Development Organization, Kawasaki Heavy Industries Ltd., and Obayashi Corporation [5]. It must be mentioned, however, that this turbine was employed in a co-generation system, meaning it most likely would have operated at lower firing temperatures than typical gas turbines [6]. The exposures to H_2- and O_2-rich environments on opposing surfaces (e.g., gas turbine fuel injector) or co-existence of H_2 with water vapor (e.g., solid oxide fuel cells and electrolyzers) can significantly impact the material's mechanical properties and corrosion resistance [7]. A detailed review discusses the suitability of hydrogen as an alternative fuel for internal combustion engines (ICEs) in terms of improved performance [8]. The article highlighted critical drawbacks of H_2-fueled ICEs, including potentially high-NOx emissions and issues of engine durability and reliability. Addressing the material challenges for a H_2-fueled power generation and transportation industry is an impending task, progress toward which is exacerbated by the continuing battle to balance mechanical properties, environmental resistance, and cost.

The main challenges to realizing a hydrogen-based energy economy continue to be our ability to produce hydrogen in large volumes and to ensure efficient transport and storage of hydrogen. Decades of research on the embrittlement of materials under pressurized hydrogen at room temperature has enabled the safety and reliability of hydrogen pipelines and storage infrastructure [9], leading to the development of a *Technical Reference on Hydrogen Compatibility of Materials* [10]. The same cannot be said about hydrogen–material interactions with high-temperature alloys required in applications for the power generation (e.g., turbines) and transportation sectors (e.g., ICEs). Compared with various types of steels [11], there have been fewer studies examining the impact of hydrogen and hydrogen combustion atmospheres on the mechanical behavior and environmental resistance of high-temperature (i.e., >700°C) structural materials, especially Ni-Cr and Ni-Fe-Cr precipitation-strengthened alloys [6,12,13].

Figures 1 and 2 summarize results from limited literature reviews, which can be used to rapidly screen materials. Results

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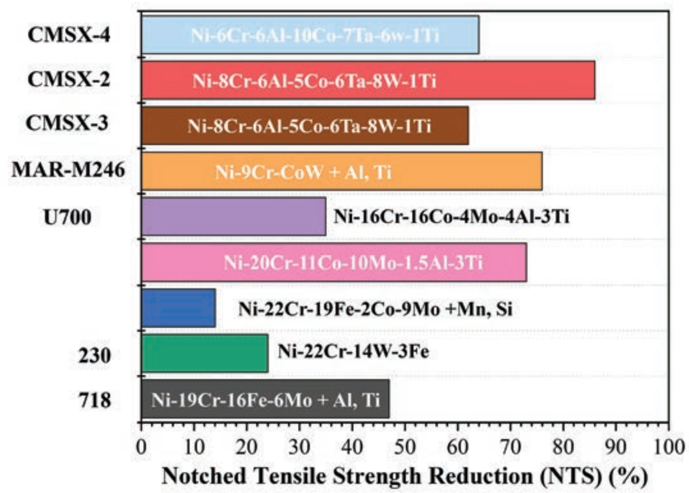

Figure 1. Reduction of notched tensile strength under high hydrogen pressures (i.e., 34 MPa–69 MPa) at 24°C for selected Ni-base superalloys. Data for the figure extracted from Fritzemeier and Chandler, Harris and VanWanderham, Lee, Chandler, Jewett et al. (Credit: Pillai et al.)

demonstrate that differences in materials' microstructural constituents and hydrogen pressures are responsible for large variations in reductions of room-temperature notched tensile strength between studied Ni-base superalloys after exposure to high-pressure hydrogen (i.e., 34 MPa–69 MPa) at 24°C [14–18]. An additional example of the impact of hydrogen on Ni-base alloys can be seen in Figure 2, where as little as 5 wppm hydrogen in the studied alloys led to a significant decrease in elongation at rupture at 23°C after being exposed for 1,000 h to hydrogen at 650°C [14]. Although valuable, these studies did not evaluate hydrogen-induced degradation of high-temperature environmental resistance (e.g., dissolution of strengthening precipitates, loss of key alloying constituents such as Cr and Al needed to maintain protective surface oxide formation), which is an essential performance characteristic to ensure long-term durability of high-temperature Ni-Cr and Ni-Fe-Cr materials.

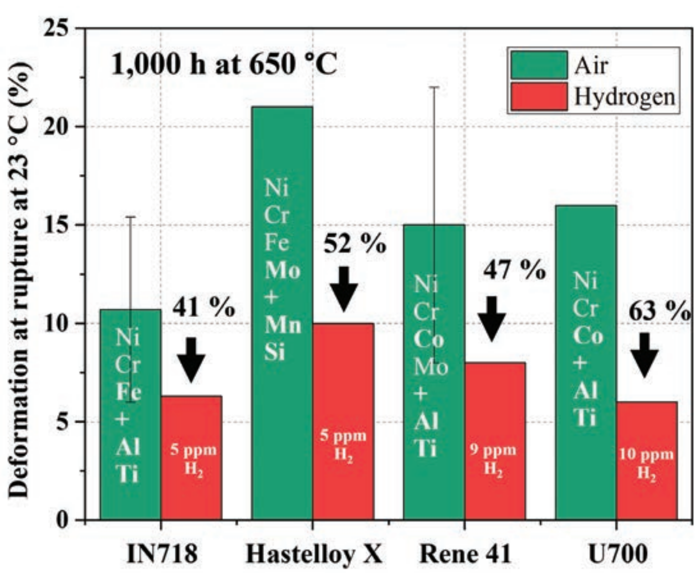

Figure 2. Deformation at rupture of Ni-base alloys at 23°C after 1,000 h in air or hydrogen at 650°C. Data for the figure extracted from Gray [14]. (Credit: Pillai et al.)

Water vapor in exhaust gas is known to significantly deteriorate the oxidation resistance of heat-resistant steels (i.e., 600°C–800°C) [19] and Ni-base alloys (i.e., >800°C) [12] compared to dry air. Increased water vapor content in the combustion products of hydrogen-fueled energy applications is expected to further accelerate the oxidation-induced degradation of these materials by either hindering the formation or inducing evaporation [20] and spallation [21] of protective surface oxides such as chromia and alumina. Interestingly, these thermally grown oxides have been shown to be effective hydrogen-permeation barriers to inhibit hydrogen uptake and subsequent embrittlement [11], emphasizing the strongly coupled interactions between mechanical properties and environmental resistance.

A successful strategy to reduce material costs of high-temperature alloys involves balancing Fe:Ni ratios. Alumina-forming austenitic (AFA) alloys were developed at ORNL [22] to bridge the gap between low-cost ferritic (i.e., Fe-Cr) and austenitic (i.e., Fe-Ni-Cr) steels and more expensive Ni-base alloys. AFA steels provide superior mechanical properties compared with conventional stainless steels while simultaneously ensuring oxidation resistance found in more expensive high-temperature materials. However, the large differences in oxidation rates of Fe and Ni can result in a narrow temperature regime for peak performance of these alloys. Furthermore, in most precipitation-strengthened alloys (e.g., gamma prime phase: γ′), the substitution for Ni must be compensated for by increasing the contents of γ′-stabilizing constituents (e.g., Ti) in the alloy to achieve a similar γ′ fraction (or similar γ′ dissolution temperature) [23]. Detailed understanding of the complex interactions among hydrogen-bearing species, material constituents, microstructure, time, temperature, thermal cycling, gas composition, and flow rates is lacking. It is imperative to understand the properties that govern desired and undesired reactions with high-temperature hydrogen to tailor, control, and design materials at multiple lengths and timescales that will enable the widespread deployment of carbon-neutral hydrogen technologies.

RESULTS

Impact of higher water vapor in exhaust gas on oxidation behavior. Microturbine recuperators are essential to increase the electrical efficiency of co-generation applications (i.e., combined heat and power), but oxidation of thin metal foils (i.e., 100 μm–200 μm) in primary surface recuperators is a major concern [24]. Candidate materials for these applications rely on formation of external chromia scales for oxidation resistance, but water vapor–induced volatilization of chromia scales significantly impacts their lifetimes [20]. The CST Group has evaluated the oxidation behavior of candidate materials for these applications under simulated and actual operating conditions for 25 years. Recent work has developed models to predict material lifetimes as a function of operating conditions and material composition. Preliminary studies have shown a significant impact for higher water vapor contents expected in the exhaust gas of H_2-fired microturbines. Figure 3 shows the back-scattered electron (BSE) images of Alloy 120 after laboratory exposure at 700°C in flowing (i.e., ~1.6 cm/s gas velocity) air + 10 vol.% H_2O (Figure 3a) and in flowing air + 60% H_2O for 5,000 h (Figure 3b). In the low water vapor (10% H_2O) environment, Alloy 120 formed a thin protective external chromia scale. However, under the higher water vapor

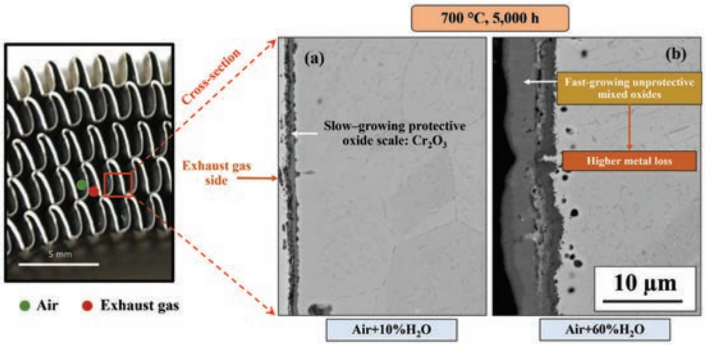

Figure 3. BSE images of Alloy 120 after exposure at 700°C in flowing (i.e., 850 cc/min, ~1.6 cm/s gas velocity) air + 10%H_2O (a) and in flowing air + 60% H_2O for 5,000 h (b). (Credit: R. Pillai, ORNL)

(60% H_2O) environment, much thicker oxides were observed on the Fe-rich Alloy 120 after the same exposure time. These oxides were determined to be Fe-rich and observed to grow much faster (i.e., 3–5 orders of magnitude) than chromia scales, which typically results in accelerated consumption of the underlying metal and consequent loss in structural integrity.

Oxidation-resistant alloys for higher water vapor contents. The growth kinetics of alumina scales are ~100 times slower than chromia scales. Furthermore, alumina scales are known to be more resistant than chromia scales to evaporation-induced losses in water vapor–containing environments [25]. At a temperature of 800°C and under the same environment (i.e., 50% H_2O, 50% O_2, gas velocity of 4.5 cm/s), Al loss from an alumina scale is ~4 orders of magnitude lower than the Cr loss from a chromia scale. Hence, materials with the ability to form an external alumina scale are highly attractive for components operating in high-temperature water vapor–containing environments. These alloys have shown superior performance as materials for recuperator foils compared with materials relying on chromia scales for oxidation protection, thereby enabling us to increase the turbine inlet temperature by 100°C in water vapor–containing environments [26].

Water vapor does, however, have some adverse effects on the protective nature of alumina scales. Decreased adhesion of the alumina scales to the materials during thermal cycling in water vapor has been reported; this can lead to spallation (i.e., detachment from the alloy surface) of the oxide layer and renewed exposure of the alloy to the high-temperature oxidizing environment [21]. The ability of the alloys to form a protective alumina scale during high-temperature exposures may also be hindered with increasing water vapor contents [27].

Initial studies conducted on Ni-base alloys at ORNL have reported similar effects [12]. Figure 4 provides BSE images showing the oxide scale morphology (left panel) and subsurface microstructure (right panel) of Ni-base Superalloy X4, after exposure for 500 h at 800°C (i.e., 100 h cycles) in air + 10% H_2O and air + 60% H_2O. The formation of thinner Ni-Cr–rich oxides on Superalloy X4 in air + 60% H_2O compared with large nodules of mixed oxides in the lower water vapor–containing atmosphere indicates key differences in the mechanisms of early-stage oxidation, which clearly impacts subsurface Al-rich oxide morphologies.

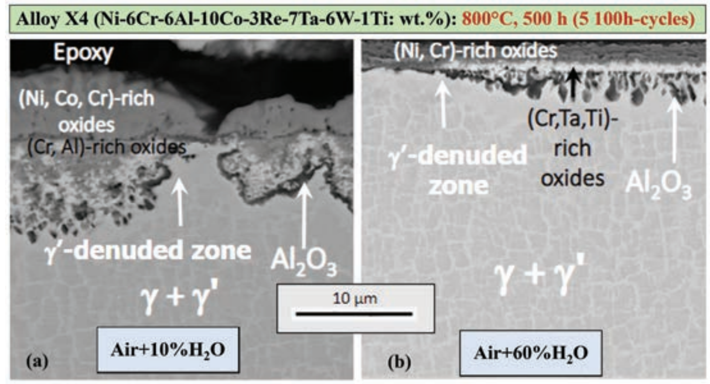

Figure 4. BSE images showing oxide scale morphology and subsurface microstructure of the Ni-based Superalloy X4, after exposure for 500 h at 800°C (100 h cycles) in (a) air + 10% H_2O and (b) air + 60% H_2O (right). (Credit: Pillai and Pint)

Efficacy of oxidation-resistant coatings in high water vapor environments. Inlet temperatures in gas turbines and jet engines are close to the melting points of Ni-base superalloys typically used for manufacturing of the components in the hottest turbine sections. Ceramic thermal barrier coatings (TBCs) provide additional protection to internally cooled components and prevent overheating. The TBCs, mostly consisting of yttria-stabilized zirconia (YSZ), are commonly applied on the structural components of gas turbines and aircraft engines [28]. A metallic bond coating (BC) between the TBC and the Ni-base superalloy provides oxidation resistance for the base material and adherence of the ceramic coating [29]. The BCs are typically of the MCrAlY (M = Ni, Co) or nickel aluminide type and enable the formation of an alumina layer at the BC–TBC interface, which protects the underlying superalloy from accelerated corrosive attack.

The impact of increased water vapor contents in the exhaust gas of H_2-fueled turbines on the performance of oxidation-resistant coatings has been investigated in the literature and extensively at ORNL [30–32]. The formation of faster-growing nonprotective mixed oxides (e.g., spinel-type), instead of alumina, on the BC was reportedly accelerated in the presence of increasing water vapor contents (i.e., 0 vol.%–50 vol.% H_2O) on different thermally sprayed MCrAlY compositions at 1,125°C. This temperature corresponds to a high-boundary temperature felt by the BC in an actively cooled, YSZ-coated turbine blade at inlet turbine temperature [30]. The significant volume increase due to the formation of these mixed oxides and the rapid crack propagation within the brittle spinel in turn could promote early failure of the ceramic TBC [28]. Pint et al. [31] conducted studies on the impact of higher water vapor contents (i.e., up to 90 vol.% H_2O) on the TBC lifetime deposited on Pt-diffusion BCs (γ+ γ′-FCC) and Pt-modified aluminide coatings (β-aluminide) at 1,150°C. They concluded that the TBC lifetimes in furnace cycle testing were not considerably affected for the TBC on Pt-diffusion BCs by the presence of 10% H_2O or 90% H_2O. In contrast, the TBC lifetime on the Pt-modified aluminide coatings was almost halved in the case of 10% H_2O compared with testing in dry O_2. A further increase to 90% H_2O did not significantly influence the lifetime. Thermal cycling in combination with increasing water vapor contents has been shown to be detrimental to TBC lifetimes with MCrAlY BCs [33]. Generally, the reported performance of oxidation-resistant coatings in high water vapor–containing environments suggests the continued efficacy of established oxidation-resistant coatings for H_2-fueled turbines. However, advancing the mechanistic understanding of the impact of varying contents of H_2O, temperature, and thermal cycling is still critical for the development of materials and coatings specifically for H_2-fired power generation and transportation applications.

CONCLUSIONS

Extensive knowledge about the interaction of hydrogen with metals exists for temperatures of <600°C, but we lack an understanding of materials aiming to operate at much higher temperatures (i.e., >800°C). This critical gap further widens in terms of our mechanistic understanding of the combined effects of environmental degradation due to hydrogen and oxidizing species (i.e., oxygen, water vapor). There is a clear need to further investigate the impact of burning hydrogen on the oxidation resistance of candidate structural materials. Key insights are needed to elucidate the role of defects and to reveal key microstructural (e.g., grain size, orientation) and/or compositional features to act as hydrogen-permeation barriers (e.g., thermally grown oxides) and stable hydrogen-trapping sites (e.g., chemical nature and fraction of precipitates) to enhance material lifetimes. Future atomistic and nanoscale investigations of hydrogen–material interactions are essential to enhance our understanding of hydrogen effects under multiple extremes of mechanical and thermal loads, corrosion, and radiation.

IMPACT

ORNL's extensive history in understanding and developing materials for extreme environments provides an excellent foundation to tackle the major gaps in our current understanding of the impact of hydrogen and hydrogen-combustion environments on the mechanical behavior and environmental resistance of high-temperature structural materials. Recent work by the CST Group highlights potential material challenges and proposes mitigating solutions. Ongoing and future work in the group should aim to deliver valuable scientific information to academia and industry with the ultimate goal of accelerating the technical realization of a hydrogen-driven energy infrastructure. The time is opportune for ORNL to be the foremost authority in the development of next-generation materials systems and to enable scientists to overcome a huge barrier in identifying high-temperature structural materials for hydrogen-fueled power generation and transportation technologies.

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REFERENCES

1. M. Noussan et al. *Sustainability* 13, 1–26 (2021).
2. M. H.du Toit et al. *Energ. Fuel*. 32, 6401 (2018).
3. P. Chiesa et al. *J. Eng. Gas Turbines Power* 127, 73 (2005).
4. M. A. Alvin. "Materials and Component Development for Advanced Turbine Systems." In *Proceedings of ASME Turbo Expo 2009*, vol. 4, Orlando, FL, June 8–12, 2009, p. 737 (2009).
5. New Energy and Industrial Technology Development Organization. "World's First Successful Technology Verification of 100% Hydrogen-Fueled Gas Turbine Operation with Dry Low NOx Combustion Technology." July 21, 2020. https://www.nedo.go.jp/english/news/AA5en_100427.html.
6. E. Stefan et al. *Int. Mater. Rev.* 67, 1 (2021).
7. A. Chyrkin et al. *Corros. Sci*. 203, 110338 (2022).
8. Z. Stępień. *Energies* 14, 6504 (2021).
9. US Department of Energy. "DOE Announces $160 Million for Projects to Improve Fossil-Based Hydrogen Production, Transport, Storage, and Utilization." Jan. 15, 2021. https://www.energy.gov/articles/doe-announces-160-million-projects-improve-fossil-based-hydrogen-production-transport.
10. C. San Marchi and B. P. Somerday. *Technical Reference on Hydrogen Compatibility of Materials*. Sandia National Laboratories Report no. SAND2012-7321. Livermore, CA: Sandia National Laboratories (2012). https://www.osti.gov/servlets/purl/1055634.
11. H. K. D. H. Bhadeshia. *ISIJ Int*. 56, 24 (2016).
12. R. Pillai and B. A. Pint. *JOM* 73, 3988–3997 (2021).
13. B. P. Somerday et al. *Technical Reference on Hydrogen Compatibility of Materials High-Alloy Ferritic Steels: Duplex Stainless Steels (Code 1600)*. Sandia National Laboratories Report no. SAND2008-6595P. Livermore, CA: Sandia National Laboratories (2008). https://www.osti.gov/servlets/purl/1706306.
14. H. R. Gray. *Embrittlement of Nickel-, Cobalt-, and Iron-Base Superalloys by Exposure to Hydrogen*. National Aeronautics and Space Administration (NASA) Report no. NASA-TN-D-7805, 1975.
15. L. C. Fritzemeier and W. T. Chandler. "Hydrogen Embrittlement—Rocket Engine Applications." *Superalloys Supercomposites Superceramics*. In J. K. Tien and T. Caulfield, eds. Academic Press, 1989, pp. 491–524.
16. J. J. A. Harris and M. C. VanWanderham. *Am. Soc. Test. Mater., Publ*. 543, 198–220 (1974).
17. J. A. Lee. "*Hydrogen Embrittlement of Nickel, Cobalt and Iron-Based Superalloys*." In R. P. Gangloff and R. P. Somerday, eds. Woodhead Publishing (2012), pp. 624–667.
18. R. P. Jewett et al. *Hydrogen Environment Embrittlement of Metals*. NASA Report no. NASA-CR-2163 (1973).
19. B. A. Pint. *Oxid. Met*. 95, 335 (2021).

20. D. J. Young and B. A. Pint. *Oxid. Met*. 66, 137 (2006).
21. M. C. Maris-Sida et al. *Metall. Trans. A* 34a, 2609 (2003).
22. Y. Yamamoto…B. A. Pint. *Metall. Trans. A* 42a, 922 (2011).
23. R. Pillai, S. Dryepondt, et al. *Surf. Coat. Tech*. 421, 127401 (2021).
24. B. A. Pint et al. "Materials Selection for High Temperature (750°–1000°C) Metallic Recuperators for Improved Efficiency Microturbines." In *Proceedings of ASME Turbo Expo 2001: Power for Land, Sea, and Air*, vol. 1. New Orleans, LA, June 4–7, 2001. https://doi.org/10.1115/2001-GT-0445. (2001).
25. E. J. Opila and D. L. Myers. *J. Am. Cer. Soc*. 87, 1701 (2004).
26. M. Romedenne, R. Pillai, S. Dryepondt, … B. Pint. "High Temperature Oxidation Behavior of Fe- and Ni-Based Alloy Foils in Water Vapor at 850 °C." Paper no. NACE-2021-16594 presented at CORROSION 2021, Virtual, April 19–30, 2021.
27. W. Zhao and B. Gleeson. *Oxid. Met*. 83, 607 (2015).
28. D. Naumenko, R. Pillai, et al. *J. Therm. Spray Technol*. 26, 1743 (2017).
29. B. Gleeson. *J. Propul. Power* 22, 375 (2006).
30. M. H. Sullivan and D. R. Mumm. *Surf. Coat. Tech*. 258, 963 (2014).
31. B. A. Pint et al. *Surf. Coat. Technol*. 206, 1566 (2011).
32. B. A. Pint et al. *Surf. Coat. Technol*. 201, 3852 (2006).
33. M. J. Lance…B. A. Pint. *Surf. Coat. Technol*. 260, 107 (2014).

Making Battery Design Accessible to Everyone

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INTRODUCTION

Lithium ion (Li-ion) batteries are ubiquitous [1]. With applications ranging from handheld communication devices to land rovers running on the surface of Mars, Li-ion batteries have revolutionized human society over the past 30 years. As the world races toward decarbonization, there is an urgent need to sustainably design and produce batteries that can meet rising demands in terms of volume and performance. Designing batteries, however, is a nontrivial task requiring knowledge across multiple domains of materials science, processing science, and engineering.

Solid-state batteries (SSBs) represent a promising group of energy storage technologies that has the potential for widespread application in the electrification of the transportation sector [2]. Due to their mechanical strength, solid-state electrolytes can enable lithium metal chemistries by mitigating lithium dendrite formation. Further, eliminating liquid components in the battery significantly improves the system's overall safety and volumetric capacity. Next-generation SSBs will need to leverage high–voltage cathodes as well as metallic anodes to achieve required performance metrics.

To achieve technoeconomic feasibility, it is imperative to have general design guidelines to predict cell-, module-, and pack-level energy densities based on certain minimum user-defined parameters for the battery system. For conventional battery technology, a spreadsheet-based tool called BatPaC offers these capabilities for integrated battery design, production costs, and thermal management from the cell level to the pack level [3]. Although BatPaC is a robust method for battery design, it is extremely cumbersome to use and requires significant expertise to decouple and leverage the tool for a new material system.

No such design tool existed specifically for SSBs. Likewise, no set guidelines exist for determining system architecture based on performance metrics, so a generally stochastic/iterative process has been applied for research and development. Our research team at Oak Ridge National Laboratory developed the Solid-State Battery Performance Analyzer and Calculator (SolidPAC), a user-friendly, spreadsheet- and graphical user interface (GUI)–based tool that provides specific design rationales for building high energy density SSBs [4] (Figure 1). The GUI tool offers improved user friendliness and accessibility compared with spreadsheet-based models. SolidPAC addresses the lack of SSB-specific battery design tools necessary to account for differences in cathode architectures, transition to the lithium metal anode, stacking modification, and transition to the solid electrolyte. SolidPAC's user-friendly GUI significantly enhances its accessibility for general users. The toolkit is populated with typical material and properties expected to be used for cathode and solid electrolyte materials.

Both the spreadsheet and GUI versions can function with user-entered material systems. User inputs are staggered in the spreadsheet software depending on where they are required, and they are annotated and appropriately color-coded. The user-input tabs in the GUI are the only ones that are accessible; the

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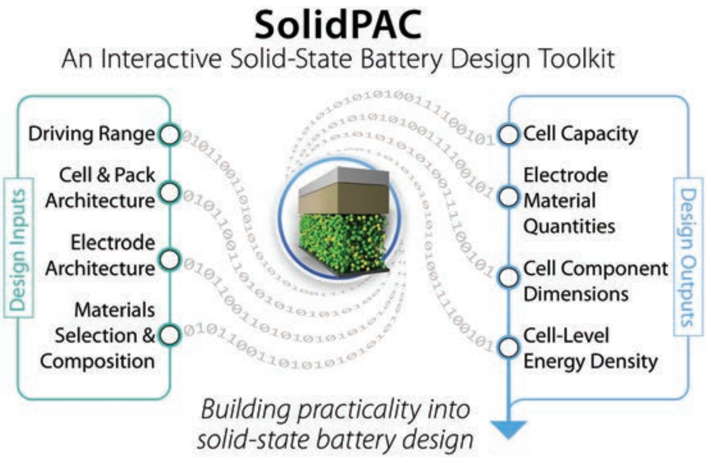

Figure 1. Schematic diagram showing the information flow for SolidPAC, a user-friendly, accessible tool to design and develop SSBs. (Credit: M. Dixit, ORNL)

outputs and calculated metrics cannot be modified by the user. The GUI software is supplied as an installer file that works as a stand-alone application when installed. The first version of this software provides preliminary design criteria for cells, modules, and battery packs using a range of SSB chemistries. Because the data concerning SSB performance under different conditions are limited, the design approach used here is different from those employed for conventional Li-ion batteries with spreadsheet-based modeling tools (see Table 1 for comparison).

The current version of SolidPAC integrates development up to the individual cell level. Future versions will include module and pack design, performance, and technoeconomic models. We will also integrate conventional design approaches based on power, thermal management, and charging as more data become available for SSBs that have different material chemistries.

$$E_g = \frac{C_{cell} \cdot V_{cell}}{\sum m_{components}}, \quad (1)$$

$$E_v = \frac{C_{cell} \cdot V_{cell}}{\sum v_{components}}, \quad (2)$$

where

C_{cell} = the capacity of the cell,
V_{cell} = the average cell voltage,
$m_{components}$ = the mass of the individual components, and
$v_{components}$ = the volume of the individual components.

BACKGROUND

SolidPAC uses the following equations to calculate the gravimetric (E_g) and volumetric (E_v) energy densities of an SSB cell:

SolidPAC borrows its cell configuration and housing specifications from BatPaC. A detailed explanation of the cell housing components can be found in BatPaC's documentation [3]. For SSBs specifically, SolidPAC implements a different calculation to determine the cathode and anode masses to account for the differences in cathode architecutre and use of lithium metal.

The first step in designing a battery with SolidPAC is identifying pack and cell design specifications based on user inputs. Battery design and chemistry selections are also based on user inputs, which are identified in the Cell Design Parameters tab of the included toolkit. Subsequently, the pack parameter calculations and cell design specifications listed below are used to evaluate battery design.

Table 1. Advantages of SolidPAC over BatPaC.

Feature	BatPaC	SolidPAC	The SolidPAC Advantage
Specific for SSBs	No	Yes	Unique. Fills a void in the SSB design process.
Uses spreadsheets	Yes	Yes	
Uses GUIs	No	Yes	The unique GUI makes SolidPAC easy to operate and accessible to more users.
User-friendly	No	Yes	
Open source	Yes	Yes	
Interactive	No	Yes	The SolidPAC GUI facilitates user interaction.

Pack Parameter Calculations

- **Pack energy requirement:** This value is based on a standard energy consumption of a light hybrid electric vehicle per mile of travel as estimated by the Urban Dynamometer Driving Schedule cycle, which is assumed to be 250 Wh/mile.
- **Number of modules per pack:** This is the product of modules per row and rows of module per pack.
- **Total cells per system:** This is the product of cells per module and number of modules per pack.
- **Pack capacity (kWh):** If pack capacity is specified as user input, that value is used. Alternatively, the user can specify pack energy or vehicle range, which is then converted to capacity.
- **Module capacity:** This is the product of pack capacity and number of modules in parallel.
- **Cell capacity:** This is the product of module capacity and number of cells in parallel.
- **Design capacity for 10% capacity loss in first cycle:** Design capacity is assumed to be 10% higher than the identified cell capacity to account for formation losses.

Cell Design Specifications

- **Number of bilayer cells:** This number is calculated differently for conventional and bipolar stacked systems. It represents the number of individual anode–separator–cathode layers present within a single cell.
- **Positive electrode capacity:** This is the product of the nominal capacity of the cathode, mass fraction of the active material in composite cathode, and composite cathode density.
- **Negative electrode capacity:** This is the product of the nominal capacity of the anode and anode density (assuming a 100% dense anode).
- **System energy:** This is the product of the cell capacity and the cell voltage at 50% state of charge (SOC).

- **System voltage:** This is the product of cell voltage and number of parallel packs in the system.
- **Cell voltage:** This value is defined as the open circuit voltage for 50% SOC of the cathode material.

The component weights, dimensions, and resistances are estimated based on these specifications. Although certain spreadsheet-based battery design tools exist, they are difficult to read, interpret, and use on day-to-day basis. SolidPAC's basic operation procedure for using SolidPAC is as follows:

1. When SolidPAC is run, a GUI window opens (Figure 2).
2. Various tabs are controlled by selecting the tabs at the top of the window.
3. User inputs are entered in the first two tabs: Materials Inventory, and Cell Design Parameters.
4. Users work with existing materials or add their own materials to the list by providing all requested data.
5. Battery specifications are input by the user in the Cell Design Parameters tab.
6. When all inputs are entered, the user clicks the Calculate button on the lower right corner of the screen.
7. The Calculate button turns green, and the values for cell design are tabulated in the Cell Calculations and Summary of Results tabs.
8. Users can modify inputs to populate the updated design parameters and click the Calculate button again.

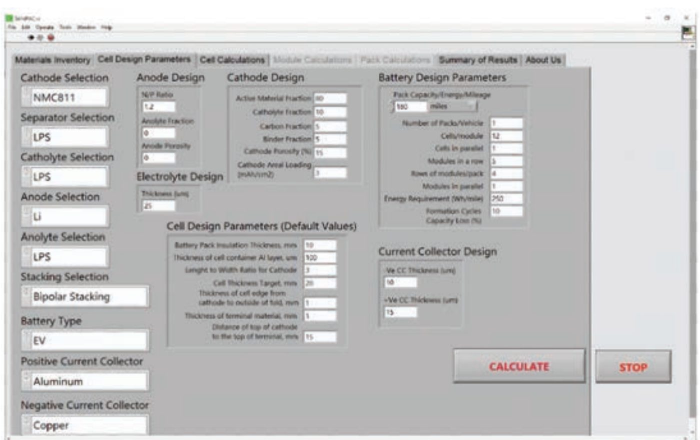

Figure 2. SolidPAC GUI screenshot. (Credit: M. Dixit, ORNL)

RESULTS

To explore the toolkit's capabilities, a few example datasets generated from SolidPAC are discussed below. Results of our investigation are shown in Figure 3. In these cases, Li7P3S11 (LPS) solid electrolyte is used as both separator and catholyte. The cathode active material is chosen to be NMC622, with the cathode composition of NMC622:LPS:PVDF:C as 80:10:5:5, with a negative-to-positive electrode capacity ratio (i.e., negative-to-positive [N/P] ratio) of 1.2. The cathode areal loading used for calculations was 5 mAh cm^{-2}. The impact of the separator thickness on cell-level gravimetric and volumetric energy density with this configuration is visualized in Figures 3a and 3b. When the

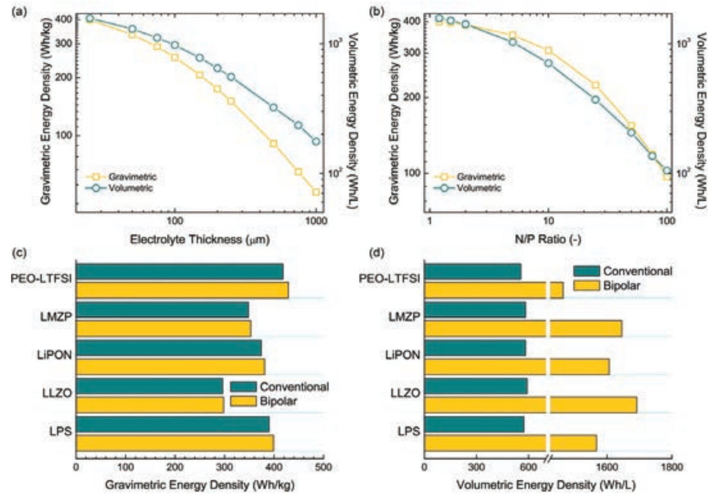

Figure 3. SolidPAC results. (a) Energy density as a function of electrolyte thickness; (b) energy density as a function of N/P ratio; (c) gravimetric and (d) volumetric energy density for SSBs with differing separator materials in conventional and bipolar materials. For the calculations with results shown in (b), LPS solid electrolyte was used as both separator and catholyte. For all the calculations, the cathode active material was assumed to be NMC622, with the cathode composition of NMC622:LPS:PVDF:C as 80:10:5:5, lithium metal anode with an N/P ratio of 1.2 (unless mentioned otherwise) and electrolyte thickness of 25 μm (unless mentioned otherwise). The cathode areal loading used for calculations was 5 mAh cm^{-2}. (Credit: M. Dixit, ORNL)

separator has a 25 μm thickness, this configuration yields an energy density of ~400 Wh kg^{-1} and ~1,550 Wh L^{-1}. This is close to the proposed energy densities for SSBs. However, most reports have separator thicknesses in the range of ~100s of μm, which would result in energy densities in the range of 150 Wh kg^{-1}–250 Wh kg^{-1} and 550 Wh L^{-1}–950 Wh L^{-1}. As a comparison, the energy density of a conventional $LiNiCoAlO_2$–graphite cell is 250 Wh kg^{-1} and 570 Wh L^{-1}. Thus, it is crucial to keep the separator thickness below 100 μm to achieve meaningful cell-level energy densities. Another aspect explored in our work was the impact on the energy density of excess lithium in the cell. At 20% excess, the cell energy densities were estimated as ~400 Wh kg^{-1} and ~1,550 Wh L^{-1}, as determined above, decreasing to 308 Wh kg^{-1} and 707 Wh L^{-1} at the N/P ratio of 10, and further decreasing to 97 Wh kg^{-1} and 105 Wh L^{-1} at the N/P ratio of 100. At the areal cathode capacity of 5 mAh cm^{-2}, the excess anode thickness for N/P = 0.2 is roughly 0.5 μm while, at N/P =10, it is 250 μm. Although they are not typically reported in recent studies, the thicknesses of lithium employed as an anode in SSBs are several 100s of μm. Therefore, keeping a limited amount of excess lithium in the system is a must for achieving high energy density in SSBs. It should be noted that previous works highlighted the importance of limiting electrolyte thickness and lithium excess in SSB research [5,6].

SSBs are a burgeoning technology for next-generation energy storage. Component design and integration need to be tailored to achieve the purported advantages in energy density and power density over conventional Li-ion batteries. Herein, we showcase SolidPAC, an experimental interactive, GUI-based toolkit that can be used for SSB design. The overarching goal of SolidPAC is to enable a battery-on-demand design toolkit, with the current version providing design metrics up to the cell level with associated metrics for energy density. The SolidPAC toolkit will be extremely useful for research organizations and industry engaged in elucidating the potential of SSBs and developing more practical SSBs than are currently available.

CONCLUSIONS

SSBs have the potential to be significant next-generation technologies for high energy density and high power density rechargeable battery applications. It is crucial to identify the metrics that an emerging battery technology should fulfill to achieve parity with conventional Li-ion batteries, primarily in terms of energy density. Limited approaches exist today to assess and extrapolate the impact of battery designs and cell component selection on the cell-level energy density of an SSB. SolidPAC is an interactive experimental toolkit that enables SSB design for user-specified application requirements. The toolkit is flexible, enabling the battery community to quantify the effects on cell energy density and costs of materials chemistry and fractions, electrode thicknesses and loadings, and electron flows and to use reverse-engineering concepts to correlate cell energy density output to materials and cell design inputs.

IMPACT

SolidPAC has seen excellent engagement with the SSB design community since its release in February 2022. The authors have received positive feedback from the global community, with the manuscript [4] listed as one of the most downloaded papers for *Cell Reports Physical Sciences*. It won an R&D100 Award in 2022 in the software category.

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REFERENCES

1. J. B. Goodenough and K. S. Park. *J. Am. Chem. Soc.* 135, 1167–1176 (2013).
2. M. B. Dixit et al. *Energy Environ. Sci.* 14, 4672–4711 (2021).
3. P. A. Nelson et al. Argonne National Laboratory Technical Report no. ANL/CSE-19/2150624 (2011).
4. M. Dixit…I. Belharouak. *Cell Rep. Phys. Sci.* 3(2), 100756 (2022).
5. S. Randau et al. *Nature Energy* 5(3), 259–270 (2020). https://doi.org/10.1038/s41560-020-0565-1.
6. P. Albertus et al. *ACS Energy Letters* 6(4), 1399–1404 (2021). https://doi.org/10.1021/acsenergylett.1c00445.

Taking the Helm: Navigating Net-Zero Futures and Nonproliferation Uncertainty from Floating Nuclear Power Plants

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COMPETING SECURITY CHALLENGES: CLIMATE SECURITY VS. NUCLEAR SECURITY

Critics call them "floating Chernobyls," while embarking countries view them as a net-zero energy delivery system. Regardless of your view, floating nuclear power plants (FNPPs) are unique and pose nonproliferation challenges because of their construction and deployment in the maritime domain, coupled with the novel safety, security, and safeguard issues they raise. FNPPs have remained a dormant technology since first being deployed by the United States in the 1960s with the MH-1A *Sturgis* (Figure 1). FNPPs have re-emerged as a nuclear power option to support a net-zero future [1,2] as the world's energy demand continues to grow. FNPPs offer numerous benefits in the fight against climate change. They can, for example, be deployed to remote or coastal locations, where power options are scarce or nonexistent. As countries explore nuclear power as part of broader decarbonization strategies, FNPPs provide an alternative to land-based nuclear power plants (NPPs) because of the limited infrastructure investment involved and the elimination of the nuclear waste problem, as FNPPs are towed away with the waste returning to the Supplier State.

While FNPPs look appealing for the aforementioned reasons, they pose nonproliferation challenges with regard to safety, security, and safeguards. FNPPs are not addressed by most interna-

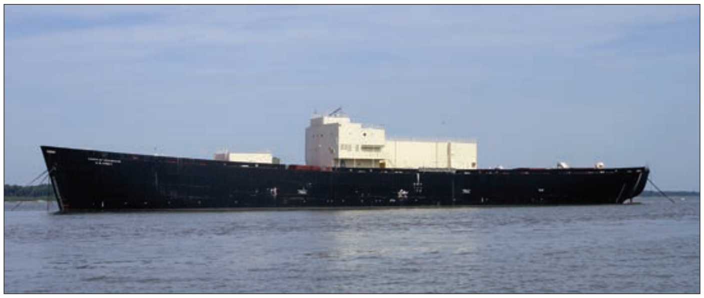

Figure 1. MH-1A *Sturgis*, the first FNPP developed by the United States [1]. Source: US Army Corps of Engineers, Galveston District. (2013). Sturgis [Color photograph]. Public domain. Retrieved from https://www.dvidshub.net/image/1223917/sturgis.

tional instruments in nuclear and maritime law. As a threshold issue, classifying an FNPP within existing international frameworks presents challenges because an FNPP can be categorized as both a facility and in transport, depending on its use at a given time and location. Guidance on physical protection and maritime security measures for FNPPs in international instruments is lacking. Additional issues continue to call the deployment of FNPPs into question. These relate to their deployment and operation and the obligations of host regulatory bodies, which present fundamental questions regarding who is responsible for ensuring the highest standards of safety, security, and safeguards when an FNPP is deployed outside the jurisdiction of the Supplier State.

Over the past few years, researchers in the Transportation Security, Engineering, and Analysis (TSEA) Group within Oak Ridge National Laboratory's (ORNL's) Nuclear Nonproliferation Division have studied the regulatory and technical questions related to FNPPs. Preliminary research has concluded that FNPPs sit at the interesection of nuclear and maritime security, requiring close coordination and collaboration between the International Atomic Energy Agency (IAEA) and the International Maritime Organization (IMO). Recent meetings held by the IAEA highlighted that classifying the FNPP as a vessel, cargo, or platform will require revising international legal instruments. This issue, however, only scratches the surface. Further investigation is needed to outline the required maritime security measures for the FNPP when docked at port. Analysis should include comparing the Maritime Security Zone (MSZ) with the Emergency Planning Zone and determining the impact of both zones on commercial operations at ports. Additional analysis is needed to understand the rights of Transit States as FNPPs transit through a third country's jurisdiction.

These questions and more highlight the interplay between climate change and nuclear security, which raises a fundamental question: how can countries planning to use FNPPs as part of their decarbonization strategies ensure the vessels meet the high standards of nuclear and maritime law? This article presents research and early results, identifying gaps and offering mitigation strategies for FNPP deployment.

FNPPs: SUPPORTING NET-ZERO GOALS OR A NUCLEAR TITANIC?

An FNPP is a nuclear reactor stationed on a barge in the marine environment, providing power to remote or coastal environments. The world's only currently operating FNPP, the *Akademik Lomonosov*, can be towed to and from multiple destinations. It utilizes two KLT-40S reactors that generate ~70 MWe to the deployment area [3]. The KLT-40S is a pressurized water reactor that uses a low-enriched uranium (<20% ^{235}U) core to generate power. The size and general design allows the reactor to operate for longer periods of time before refueling. Figure 2 shows the components of a typical FNPP such as the *Akademik Lomonosov*. At minimum, the refueling cycle for KLT-40S reactors is approximately every 2 years, with the possibility of increasing the length of time between refueling cycles based on operating and design parameters [4]. Additionally, the lower uranium enrichment of the KLT-40S fuel could contribute to enhanced proliferation resistance, according to IAEA guidance [4]. The FNPP's mobility and reactor life cycle make it an attractive energy source alternative for isolated communities or coastal states, as the international community works toward decarbonization.

Although FNPPs sound promising and the technology may appear relatively simple, the nature of the nuclear and maritime domains—and the interface between them—is complex. Careful consideration must be given to an FNPP's deployment

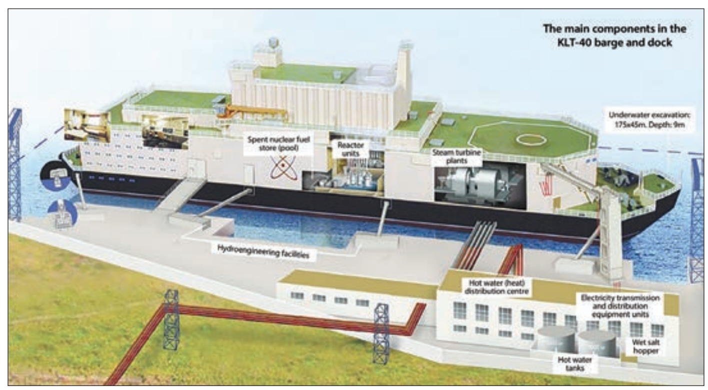

Figure 2. Components of an FNPP [3]. Source: International Atomic Energy Agency. General view of an FNPP with two KLT-40 reactors [Color Graphic]. Retrieved from https://www.iaea.org/publications/10516/legal-and-institutional-issues-of-transportable-nuclear-power-plants-a-preliminary-study.

to ensure it does not become the common cliché, a "nuclear Titanic." FNPPs require integration between maritime and nuclear domains, raising questions about existing obligations; prioritizing one domain over another; and harmonizing practical elements of maritime and nuclear concerns such as safety, security, and policy.

Within nuclear law, the traditional paradigm for nonproliferation is called 3S—Safety, Security, Safeguards—with each pillar having its own international agreement(s) and underlying guidance. The Convention on Nuclear Safety (CNS) addresses nuclear safety, the Convention on the Physical Protection of Nuclear Material (CPPNM) and its Amendment (ACPPNM) address nuclear security, and the Treaty on the Non-Proliferation of Nuclear Weapons addresses nuclear safeguards [5–8]. Under maritime law, maritime safety and security is largely governed by the Safety of Life at Sea (SOLAS) Convention and the International Ship and Port Facility Security (ISPS) Code, an Annex to

SOLAS [9,10]. While these frameworks are sufficient for nuclear material transport in the maritime domain, we must begin to ask ourselves whether they are sufficient to meet nonproliferation uncertainties in view of the maritime requirements needed for FNPPs. For example, given the overlap, could nuclear safety and security be sufficiently covered by the ISPS Code and other relevant IMO instruments? Similarly, in the absence of maritime frameworks governing nuclear material protection, might the CPPNM, the ACPPNM, and other IAEA instruments be sufficient to cover potential legal gaps?

Classification of an FNPP as cargo, a vessel, or a platform will be a major driver in how international frameworks apply and shape safety, security, and safeguards requirements. Once a standard classification is defined for the FNPP and internationally accepted, how might this impact domestic regulations and the decision by a State to use or deploy an FNPP? If a Host State does not have the regulatory or physical infrastructure to sufficiently protect and operate an FNPP within its jurisdiction, extraterritorial considerations may create additional complexities with regard to ensuring the Supplier State complies with international obligations when deploying an FNPP. These scenarios present both regulatory and technical questions that ORNL's TSEA Group is well-positioned to explore, given its interdisciplinary makeup, which includes lawyers, engineers, and physical protection specialists.

IDENTIFICATION OF GAPS AND CHALLENGES TO DEPLOYMENT OF FNPPs

From the perspective of international legal frameworks, preliminary research and analysis indicates that FNPPs fall within a gray zone for much of the existing nuclear and maritime legal instruments. For nuclear safety, the CNS is not applicable because it applies only to land-based nuclear installations. The CPPNM and ACPPNM cover the physical protection of FNPPs; however, the deployment scenarios of an FNPP, either at a port facility or in various locations in the marine environment, highlight the need for additional guidance from the IAEA and IMO on nuclear and maritime security measures. If the FNPP is being built within the jurisdiction of a nuclear-weapon state (NWS), the applicability of safeguards and the extent that the FNPP would be reported under a Comprehensive Safeguards Agreement (CSA) or a Voluntary Offer Agreement (VOA) have yet to be determined. For maritime safety and security, existing maritime requirements specific to the transport of nuclear materials are insufficient with regard to vessel specifications and cargo handling for an FNPP.

Below, we briefly discuss gaps and challenges for FNPPs as they apply to the 3S paradigm. The gaps indicate not just legal and regulatory questions but practical questions regarding guidance on nuclear and maritime safety, security, and safeguards.

Safety. FNPPs are outside the jurisdiction of the CNS because it applies only to land-based NPPs. A cornerstone of nuclear safety, the CNS entered into force a few years after the nuclear accident at Chernobyl, and its articles "represent a commitment by contracting parties to achieve and maintain a high level of safety in [the nuclear field]" [11]. Article 2(i) defines a nuclear installation as:

> … any land-based civil nuclear power plant under its jurisdiction including such storage, handling and treatment facilities for radioactive materials as are on the same site and are directly related to the operation of the nuclear power plant [5].

Because the FNPP by its nature is a marine-based NPP with limited connection to the land, the CNS would be inapplicable. This presents a major gap in how principles of nuclear safety would apply to an FNPP. Alternatively, the IMO, through the SOLAS Convention, provides guidance on the safety of nuclear merchant ships through Chapter VIII of the Convention, though this would imply an FNPP is a vessel and such guidance would be applicable [9]. Additionally, an Annex to SOLAS, the Safe Carriage of Irradiated Nuclear Fuel, Plutonium and High-Level Radioactive Wastes on Board Ships (INF) Code, provides robust safety guidelines for construction of vessels transporting nuclear material [12]. Guidelines address engineered protections for damage stability, fire protection, and redundant systems to ensure protection against marine hazards [13].

As the above illustrates, the overarching problem with applying the current maritime safety framework is that there is no settled taxonomy for whether an FNPP is a vessel or a facility. So, because the CNS is not applicable, existing maritime law is insufficent for this emerging energy alternative. If maritime law could be applied, the FNPP would not need to align with vessel standards particularly specified in the INF Code and Chapter VIII of the SOLAS Convention.

Security. In the TSEA Group's research, the FNPP was analyzed under three scenarios: docked at a port, 8 nautical miles within a State's territorial waters, and in transit. Initial results focused on the response to a nuclear security event during each scenario. The researchers identified appropriate Competent Authorities and their respective security roles and responsibilities during the deployment of an FNPP. These initial results generated questions about nuclear security topics that should be further investigated, including:

- psychological impacts to personnel working on FNPPs and the link to insider threats;
- different threat vectors and whether the threat in each scenario presents more risk of a malicious attack; and
- assessment of how sufficient physical protection measures are based on extraterritorial deployment (e.g., potential changes in the MSZ at the port or in transit, the role of tugboats depending on FNPP classification).

Safeguards. At a high level, it is currently unclear where FNPPs fall, if at all, within existing international safeguards frameworks, as we have not had the opportunity to consider specific needs related to these reactors transiting and operating while moving through multiple jurisdictions. The world's only operating FNPP, the *Akademik Lomonosov*, has not left Russia's jurisdiction, and it is currently unclear whether the FNPP is covered within the country's VOA. Additionally, evaluating how FNPPs are covered by VOAs and CSAs once FNPPs are leased between Host and Supplier States adds complexities to their deployment. For VOAs, this scenario raises questions about NWS obligations to disclose domestic safeguards to the IAEA. The current state of CSAs likewise creates further uncertainties about whether FNPPs are subject to these agreements and how material verification of the reactors on FNPPs will be conducted [14]. Furthermore, different leasing and funding models pose questions about who is fully responsible for safeguarding the material during the life cycle of an FNPP.

NAVIGATING UNCHARTERED WATERS: WHAT'S THE FUTURE FOR FNPPs?

FNPPs illustrate the nexus between climate change and national security and present trade-offs between decarbonization and nonproliferation. While they hold the promise of limited infrastructure investment and eliminated nuclear waste compared with traditional nuclear energy production paradigms, FNPPs introduce novel legal and practical questions that remain to be addressed. As more countries explore net-zero strategies that include FNPP deployments, identifying the nonproliferation risks associated with such technologies will force the international community to develop stronger physical protection regimes, thus guaranteeing these technologies meet the most rigorous international nonproliferation standards.

The research conducted in support of this effort highlights the need for international collaboration. Research on FNPPs spans national laboratories, industry, government, and international organizations. Working with the IAEA and IMO to develop the "rules of the road" for the safe and secure deployment of FNPPs brings together stakeholders from different countries, organizations such as the World Nuclear Transport Institute, and experts from the nuclear and maritime sectors.

The challenges posed by FNPPs require interdisciplinary thinking that accounts for the benefits FNPPs may provide while ensuring that their deployment is safe and secure. The reality is that what looks promising from a climate change policy perspective poses challenges to nonproliferation. Incorporating this emerging alternative to land-based NPPs will require careful balancing of various equities and close cooperation among global partners to ensure nonproliferation and net-zero futures are mutually reinforced universally.

IMPACT

The renewed focus on FNPPs and their governance and on the need to develop guidance to ensure that they meet the highest standards of nuclear safety, security, and safeguards requires not just a review of legal instruments but practical implementation within the 3S paradigm. The TSEA Group's research so far highlights the interdisciplinary nature of this field, touching on nuclear law, maritime law, nuclear engineering, transport security, and physical protection of nuclear material. ORNL staff are supporting international efforts to develop guidance for transport security and safety for the broader class of transportable nuclear power plants, including FNPPs. By helping to develop guidance and offering recommendations for FNPP "rules of the road," ORNL is contributing to the global conversation on transport safety and security of this promising technology.

As global discussions continue related to decarbonization and the role of nuclear energy in achieving net-zero futures, FNPPs will continue to be part of the conversation. Developing guidance and ensuring transport security and safety of this technology are critical tasks for nonproliferation and global security, with experts within ORNL's TSEA Group manning the helm and having both the regulatory and technical expertise to lead these discussions.

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REFERENCES

1. H. B. Honerlah and B. P. Hearty. "Characterization of the Nuclear Barge *Sturgis*." In *Proceedings of the WM'02 Conference*, Tucson, AZ, Feb. 24–28, 2002. https://archivedproceedings.econference.io/wmsym/2002/Proceedings/44/168.pdf.
2. Nuclear Threat Initiative. "Akademik Lomonosov." Oct. 21, 2021. https://www.nti.org/education-center/facilities/akademik-lomonosov/.
3. International Atomic Energy Agency (IAEA). *Legal and Institutional Issues of Transportable Nuclear Power Plants: A Preliminary Study*. Vienna: IAEA (2013).
4. T. Baatar and O. V. Glazkov. *J. Phys. Conf. Ser.* 1689: 012061 (2020).
5. International Atomic Energy Agency (IAEA). Convention on Nuclear Safety (1994), IAEA Doc. INFCIRC/449, entered into force Oct. 24, 1996.
6. IAEA. Convention on the Physical Protection of Nuclear Material (1980), IAEA Doc. INFCIRC/274 Rev. 1 1456 UNTS 125, entered into force Feb. 8, 1987.
7. IAEA. Amendment to the Convention on the Physical Protection of Nuclear Material (2005), IAEA Doc. INFCIRC/274/Rev. 1/Mod. 1, entered into force May 8, 2016.
8. United Nations, Office of Disarmament Affairs. Treaty on the Non-Proliferation of Nuclear Weapons, 729 UNTS 161, entered into force March 5, 1970.
9. International Maritime Organization (IMO), International Convention for the Safety of Life at Sea (1974). 1184 UNTS 2, 284, entered into force May 25, 1980.
10. IMO. International Ship and Port Facility Security Code, Chapter XI-2 of the International Convention for Safety of Life at Sea, entered into force July 1, 2004.
11. W. Tonhauser et al. "International Legal Framework on Nuclear Safety: Developments, Challenges and Opportunities." In K. S. Nick and S. G. Burns, eds. *Principles and Practices of International Nuclear Law* (2002).
12. International Code for the Safe Carriage of Packaged Irradiated Nuclear Fuel, Plutonium and High-Level Radioactive Wastes on Board Ships (INF) Code (1999), entered into force on 1 Jan. 2001; amendments to the INF Code entered into force on July 1, 2009.
13. World Nuclear Transport Institute. *The INF Code and Purpose-Built Vessels*. https://www.wnti.co.uk/wp-content/uploads/2021/01/The-INF-Code-and-purpose-built-vessels.pdf.
14. A. D. Williams et al. *Security Safety and Safeguards (3S) Risk Analysis for Portable Nuclear Reactors*. Sandia National Laboratories Report no. SAND2020-6254C (2020).

A Window and an Opportunity for Advanced Nuclear Fission and Fusion Power Production

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INTRODUCTION

Whether or not the recent hot summers result from climate change, the political, environmental, and scientific message is clear: CO_2 levels in our atmosphere are growing very rapidly (beyond historical levels), and the average global temperature rise since 1970 is monotonically increasing [1]. Figure 1 shows the steep rise in CO_2 levels since the Industrial Revolution, and Figure 2 shows temperature rise between 1880 and 2020. The use of fossil fuels, which powered the Industrial Revolution and enabled today's energy-intensive lifestyles, will have to be phased out if we are to mitigate climate change. Energy sources that do not produce greenhouse gases will be selected for development. Present targets, which are likely to further evolve due to practical realities, point toward the 2050s as a net-zero state, where non-CO_2 energy sources will have largely replaced CO_2-generating ones. This gives us a window of ~30 years to establish new power plants, new energy sources, and a series of new energy paradigms. Nuclear fission, ripe for a resurgence, and nuclear fusion, ripe for start-up initiatives, can strongly contribute to this movement.

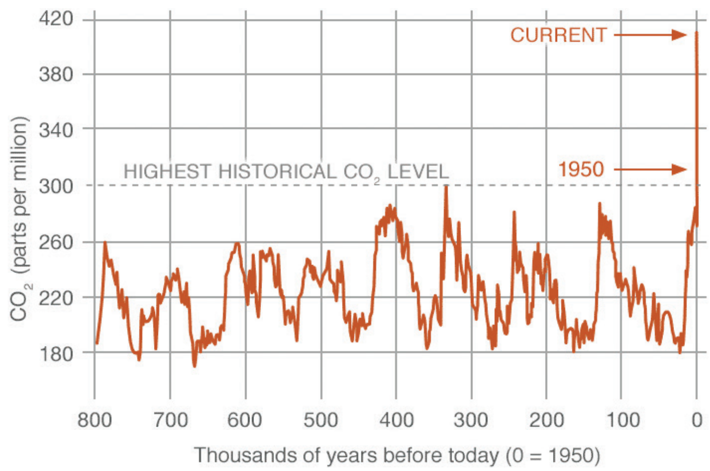

Figure 1. Historical CO_2 levels over nearly 1 million years, highlighting the stark rise in CO_2 levels in the last 100 years (far right). Data sources: Luthi et al., Etheridge et al., Petit et al., National Oceanic and Atmospheric Administration, Scripps CO_2 Program [7–11]. Retrieved from https://climate.nasa.gov/vital-signs/carbon-dioxide/.

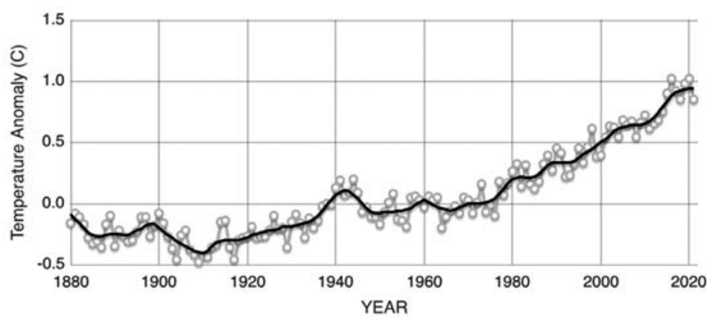

Figure 2. Historical temperature difference from the average between 1880 and 2020. Solid black line is the average historical temperature; gray circles show annual mean temperatures. Since 1970 the rise is more pronounced. Data source: National Aeronautics and Space Administration Goddard Institute for Space Studies [12]. Retrieved from https://climate.nasa.gov/vital-signs/global-temperature/.

BACKGROUND

The Advanced (Fission) Reactor Demonstration Program [2] was recently established by the US Department of Energy (DOE) to rapidly develop significantly improved power plant technologies through partnerships with industry. The partnerships target advanced reactor demonstrations, risk reduction for future demonstrations, and innovative and diverse new designs. The advanced reactors incorporate a wide range of concepts involving passive safety; advanced fluids (e.g., liquid metals, molten salts); new fuel configurations; compact designs; and several other desirable attributes. Initial applications addressed electricity production but now involve a broader scope including desalination plants, hydrogen production plants, chemical/pharmaceutical processing plants, and small (and micro) reactors [3]. The industry-led partnerships rely heavily on the national laboratory complex to provide the infrastructure required to rapidly prototype these advancements in technology.

The technical basis for fusion energy has been rapidly progressing, with an international burning plasma demonstration facility (i.e., ITER) reaching ~75% completion for first plasma in France. The US fusion community, and subsequently the Fusion Energy Sciences Advisory Committee, developed the consensus view that fusion energy must become the focus of the DOE Fusion Energy Sciences program [4]. The target facility, called the Fusion Pilot Plant, is expected to produce an in-service environment prototypical of a fusion power plant (FPP) and a small level of net electric power (i.e., ~10–100 MW_e). In 2021, the National Academy of Sciences, Engineering, and Medicine issued a report calling for an aggressive move to commercialize fusion [5]. In parallel, several private entities have emerged over the past 5 years to pursue a wide range of fusion energy concepts, raising nearly $4.8 billion for R&D. In March 2022, the White House announced a bold decadal vision to accelerate fusion energy development [6], launching an agency-wide DOE initiative. Although the technical aspects of an FPP are at lower Technology Readiness Levels than fission power plants, the DOE initiative calls for moving more deliberately toward viable solutions for energy production.

To move the country forward on fission and fusion R&D, a half-decade ago, the US Congress passed the Nuclear Energy Innovation Capabilities Act of 2017 (P.L.115-248). In 2019, Congress passed the Nuclear Energy Innovation and Modernization Act (P.L.115-439), by which the US Nuclear Regulatory Commission (NRC) is required to begin developing new regulatory frameworks to accommodate these new and innovative designs. The NRC has been developing protocols for assessing advanced fission reactors that entail new fluids and materials and more recently hosted a public forum to hear from stakeholders in fusion. The agency will issue a white paper on licensing approaches.

IMPACT

What is the opportunity for Oak Ridge National Laboratory (ORNL)? Advanced fission and fusion reactors utilize many cutting-edge technologies to vastly improve the safety and performance of power plants, but these require deeper understanding and more complex solutions than we currently have at our disposal.

Research in materials, advanced fluids, material interactions, advanced manufacturing, measurement in nuclear environments, and high-fidelity multiphysics simulations is required to make fission and fusion energy a reality. Groundbreaking scientific investigation into these topics will require both existing and new experimental infrastructure and a cohesive collection of technical disciplines that exist only at ORNL. Large facilities like the High Flux Isotope Reactor, Manufacturing Demonstration Facility (MDF), Spallation Neutron Source, and soon the Material Plasma Exposure eXperiment (MPEX), as well as dedicated smaller experiments, can provide the scaffolding for understanding and advancing the science for a new generation of nuclear power.

Structural materials that can withstand neutron damage and nuclear transmutation are critical to obtaining long-term, reliable reactor component lifetimes. Targeting low-radioactivation materials is central to fusion development. In addition, sustaining high strength at high temperatures will enable us to leverage high thermal conversion (to electricity) efficiencies. The harsh environments present in these reactors modify materials' properties relatively quickly (i.e., in a few years), ultimately resulting in failures if they are not routinely replaced. Understanding material evolution in complex service environments, including temperature, stress, hydrogen, transmutation, and magnetic fields—and large gradients in these parameters—is necessary to design FPPs with confidence. The unique experimental and theoretical materials science capability at ORNL, advanced engineering design and experiments undertaken by ORNL's Fusion and Fission Energy and Science Directorate, and the world-leading simulation resources of the Computing and Computational Sciences Directorate (CCSD), combine to provide the critical mass required to develop the next-generation structural materials fundamental to advanced nuclear systems.

Coupled with these materials are advanced fluids such as liquid metals and molten salts that can operate at higher temperatures than water and simultaneously provide tritium breeding, neutron spectrum control, reactivity control, lower-pressure operation, and more compact cores for higher power density. These fluids are challenging, however, in their thermal and flow behaviors; interactions with solids (e.g., corrosion); neutron and gamma impacts; and their chemistry, requiring sophisticated design and control. In fact, for fusion, the magnetic field can amplify corrosion mass losses by two to three times. Extracting a wide range of impurities from these fluids and maintaining their stoichiometry is critical for their optimal performance and would best include activated corrosion products. Existing flow-loop experiments can be extended to more prototypical and comprehensive experiments, targeting detailed flow behaviors, corrosion/compatibility, and nuclear exposures. Computational advances have allowed, and will continue to allow, high-fidelity simulation of these complex fluid responses under heating, transmutation and gas production, electromagnetic interactions, complex geometries, chemical reactions, and mass transport. Pursuing such fluids without significantly better scientific basis will put these concept proposals at serious risk.

In fusion, plasma-facing materials are exposed to both neutrons and plasma—charged particles, high-energy neutral particles, and photon heating as well as erosion—creating an extreme environment in desperate need of innovative solutions. High heat flux, plasma–materials interactions, and materials science must converge to explore and resolve existing challenges to provide plasma-facing components with long-term lifetimes and robustness to normal, nonsteady, and off-normal loading situations. The surface of these materials can quickly become compromised as they are bombarded by particles and energy, and even potentially melted in off-normal scenarios. Developing material solutions coupled to high-performance cooling approaches is necessary, and again ORNL's existing and developing expertise can be combined to address this need. The MPEX program will allow simultaneous plasma and heat loading, a new helium flow loop has been constructed to explore optimized thermal performance for cooling, and ORNL's deep expertise in fluids simulation enables us to be the scientific leader and innovator for plasma-facing science and technology.

Several special materials are used in fission and fusion reactors to accomplish robust operation; ensure safety; and meet critical operational sustainability related to tritium breeding, neutron multiplication, hydrogen confinement, electrical and thermal insulation, corrosion coatings, neutron shielding, fission fuel and cladding, moderators, reflectors, and neutron absorbers. Their behaviors in the appropriate service environment must be confidently known, or they risk compromising overall reactor core operation. For fusion, breeding tritium fuel to sustain the power plant is a critical function, and the tritium must be recovered and processed before being injected into the plasma chamber. The breeding materials must contain lithium and must be stable and reliable while also allowing the tritium to be released. The harsh reactor environment can significantly change these breeding materials, causing them to reconfigure, and can enhance or inhibit the migration of tritium throughout the reactor core. Neutron shielding is a well-established discipline, but it is challenged in advanced reactor applications by more compact designs, integration and geometry, and severe requirements to protect sensitive components beyond the reactor core. The coupling of neutronics and material simulation is at the forefront of predicting these materials' responses and optimizing materials for their environment (i.e., fluence, temperature, loading, and maintenance).

Making measurements in nuclear systems is extremely difficult because most of the materials and their functionality are severely degraded when exposed, depending on where they are located relative to the neutron and gamma sources. Both permanent damage from accumulated radiation and dynamic radiation effects during direct exposure affect a diagnostic tool's function. A wide range of measurements is needed, including magnetic fields; photon radiation energy; gas pressure; various photon signals; temperatures; and stresses utilizing fibers, bolometers, pressure gauges, electrical wire, strain-gauges, and windows. Virtually all of these need dielectrics to function and/or carry signals. Electronics technology is required to boost signals, cameras are widely used to monitor and inspect, and piezo-motors are needed for motion and rotation. All need to be durable in the harsh neutron and gamma environments of advanced reactors. Advancing measurement and control for advanced fission reactors would enhance their operation and efficiency as well as safety. In fusion, controlling the plasma and monitoring the core engineering systems will be paramount to their reliable operation. Beyond operational monitoring and control, remote inspection and maintenance are complex, relying heavily on diagnostics to function properly. Focusing on radiation-hardening measurement systems and pushing the envelope to allow diagnostics closer to the energy source is vital to advancing fission and fusion reactors. Leveraging advanced manufacturing to embed diagnostics into components may provide a new paradigm for nuclear systems.

Uncovering the science and turning knowledge into solutions is an area in which ORNL has always excelled. ORNL can aggressively support industry and public programs pursuing a climate mitigation strategy that includes fission and fusion energy. Within ORNL, several organizations engage these topics, including the Fusion Energy Division (FED), Nuclear Energy and Fuel Cycle Division (NEFCD), Material Science and Technology Division (MSTD), CCSD, MDF, and US ITER. In addition, ORNL can leverage capabilities such as the Molten Salt Reactor Experiment (MSRE) program to develop novel technologies and knowledge related to material interaction and salt chemistry, advanced modeling and simulation to analyze and model nuclear concepts beyond experimental capabilities, and advanced sensing and instrumentation to fill gaps in development of radiation-tolerant systems within NEFCD. Further, the Blanket and Fuel Cycle program within FED and the Fusion Materials Science program within MSTD, and countless strategic partnerships, firmly position ORNL at the forefront of fission and fusion science. For example, under the MSRE program, several extreme high-temperature thermal fluid loops were built to study material interactions and corrosion, serve as a test bed for technology demonstrations, explore validation examples for modeling and simulations, and provide a tool for purification of thermal materials. A single experiment can support multiple cross-cutting studies.

Eighty years ago, ORNL answered the call to develop nuclear weapons that could change the course of World War II. With the closing of the Manhattan Project, ORNL turned to spearheading peaceful nuclear power, protecting the environment; enhancing energy efficiency; and developing special materials, neutron science, high-performance computing, and many other foundational capabilities when the national need arose. The Earth's climate is this century's challenge, and the United States has begun to search for solutions. How will ORNL respond? If we believe that fission and fusion energy can tackle the challenge of clean energy and climate change, it is imperative that we pursue the most difficult scientific and technological barriers for these energy sources to mitigate the threat posed by climate change.

REFERENCES

1. National Aeronautics and Space Administration (NASA). "Global Climate Change." Sept. 14, 2022. https://climate.nasa.gov.
2. US Department of Energy. "Advanced Reactor Demonstration Program." https://www.energy.gov/ne/advanced-reactor-demonstration-program.
3. Nuclear Energy Institute. "Advanced Nuclear." https://www.nei.org/fundamentals/advanced-nuclear.
4. Fusion Energy Sciences Advisory Committee. *Powering the Future: Fusion and Plasmas.* 2020. https://science.osti.gov/-/media/fes/fesac/pdf/2020/202012/FESAC_Report_2020_Powering_the_Future.pdf.
5. National Academies of Science, Engineering, and Medicine. *Bringing Fusion to the U.S. Grid.* 2021. https://nap.nationalacademies.org/catalog/25991/bringing-fusion-to-the-us-grid.
6. The White House. "Fact Sheet: Developing a Bold Vision for Commercial Fusion Energy." March 15, 2022. https://www.whitehouse.gov/ostp/news-updates/2022/03/15/fact-sheet-developing-a-bold-vision-for-commercial-fusion-energy/.
7. D. Luthi et al. *Nature* 453, 379–382 (2008). https://www.nature.com/articles/nature06949.
8. D. M. Etheridge et al. 2010. *Law Dome Ice Core 2000-Year* CO_2, CH_4, *and* N_2O *Data.* IGBP PAGES/World Data Center for Paleoclimatology Data Contribution Series no. 2010-070. NOAA/NCDC Paleoclimatology Program, Boulder CO.
9. J. R. Petit et al. *Nature* 399, 429–436 (1999). https://www.nature.com/articles/20859.
10. National Oceanic and Atmospheric Administration Global Monitoring Laboratory. "Trends in Atmospheric Carbon Dioxide: Mauna Loa, Hawaii, CO_2 Data." https://gml.noaa.gov/ccgg/trends/data.html.
11. Scripps CO_2 Program. "Keeling Curve Lessons: Lessons for Long-Term Earth Observations." https://scrippsco2.ucsd.edu/history_legacy/keeling_curve_lessons.html.
12. NASA Goddard Institute for Space Studies. "GISS Surface Temperature Analysis (GISTEMP v4)." https://data.giss.nasa.gov/gistemp/.

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