TRANSFORM

Argonne NATIONAL LABORATORY

News from Argonne's Transportation Research Program
anl.gov/energy-systems

Volume 15 | Issue 1 | 2015

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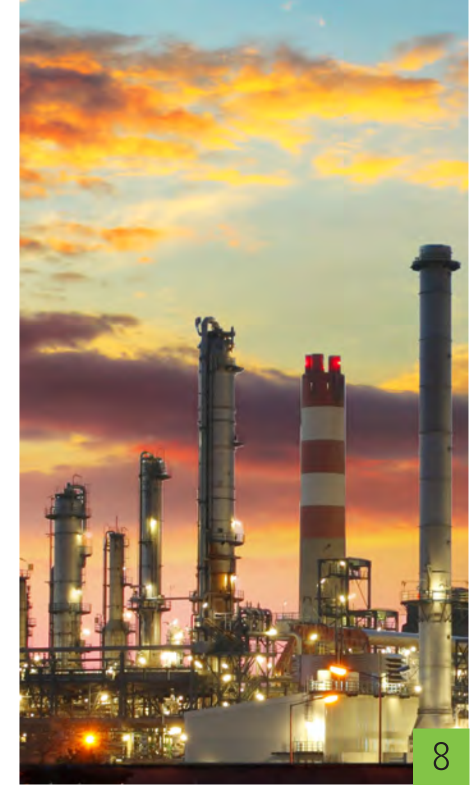
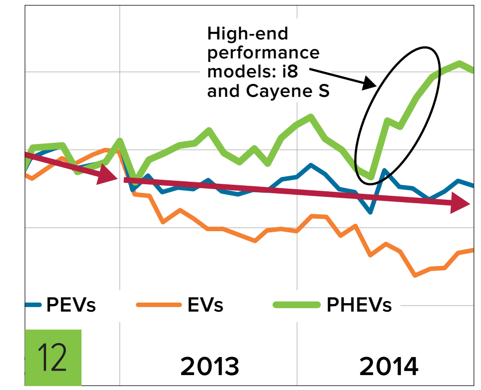
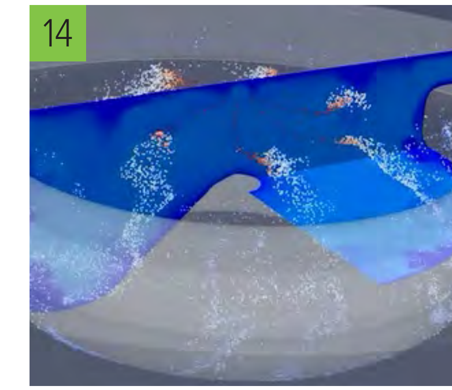




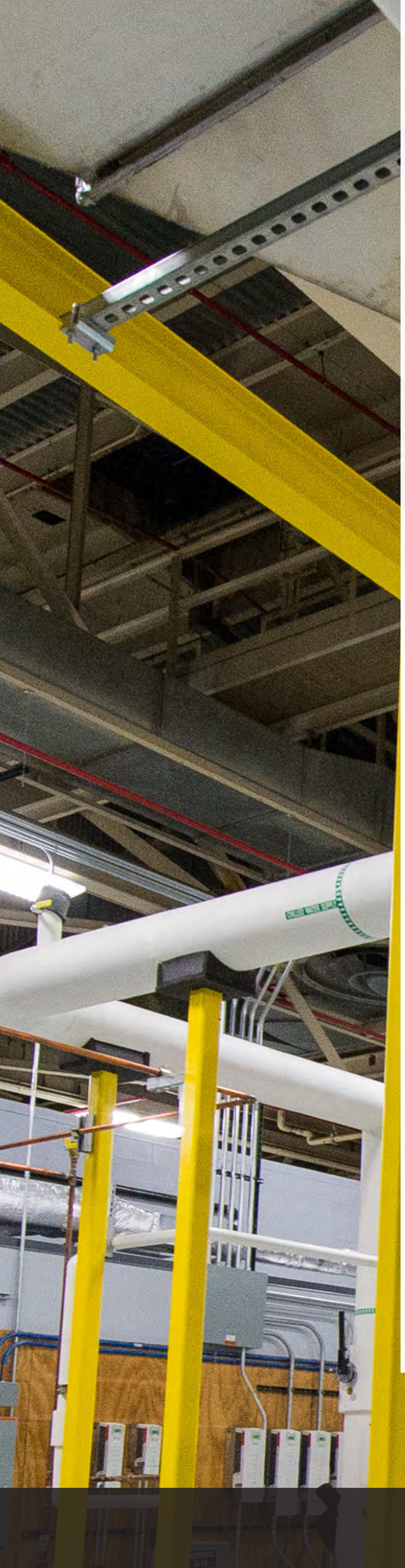


Features

on the cover
Process R&D chemist Trevor Dzwiniel sets up a pilot reactor for multi-kilo chemistry in Argonne's Materials Engineering Research Facility.

shown above
Analytical chemist Gerald Jeka loads a sample of battery materials into a thermogravimetric analysis instrument to help improve process scale-up.

Articles



A Matter of **Scale**

A critical bottleneck in our quest for a cleaner energy future is finding new and promising battery materials with the potential to revolutionize energy storage.

To widen the path to innovation, novel battery materials are being developed with properties that exceed today's top batteries in terms of capacity, power, chargeability and life. Discovering a new material with enhanced storage properties is one thing. But producing sufficient quantities of that material to take it out of the lab and into testing in a cost-effective manner is quite another. Industry typically does not want to take on the financial risk of process scale-up and development of materials that haven't been validated.

Enter Argonne's Materials Engineering Research Facility (MERF), a state-of-the-art laboratory dedicated solely to process research and development (R&D) and scale-up, enabling production of promising energy storage materials in sufficient volume to allow companies and research institutions to effectively and economically pursue next-generation battery technologies.

> MERF has successfully scaled more than 20 materials, distributed close to 30 kilograms of samples, filed half a dozen patents and received an R&D 100 Award.

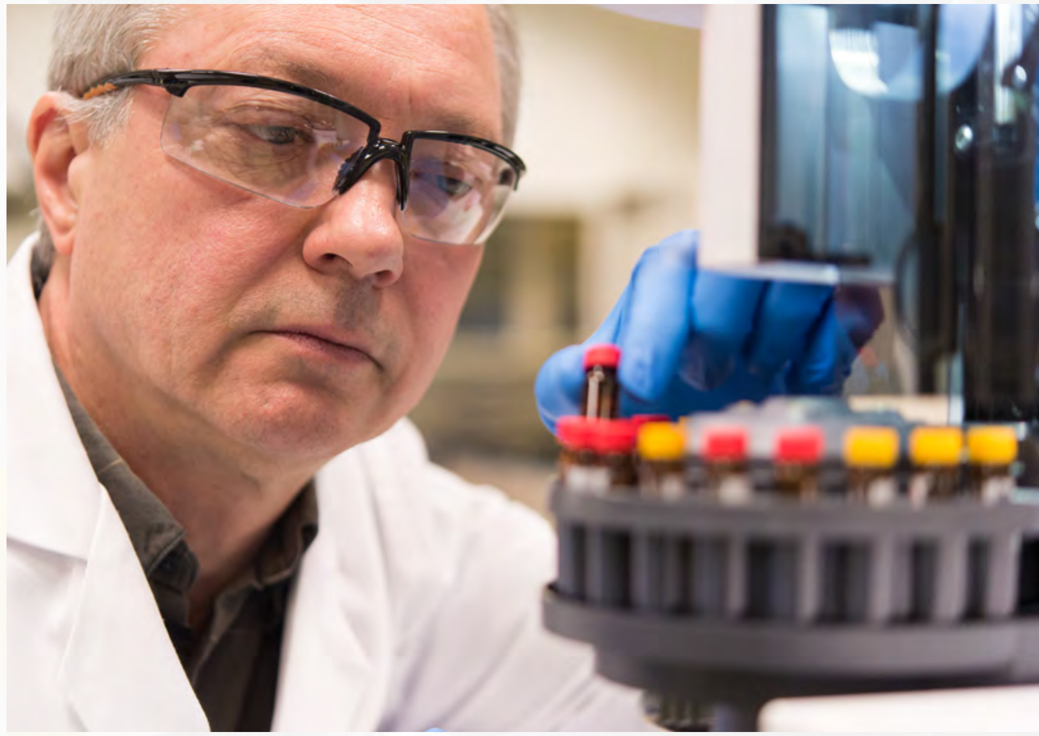
"Production costs are not a priority when new materials are invented. It's all about the performance of the material," said MERF director Greg Krumdick. "But when it comes to scaling the materials up, in our case from just one gram to sometimes more than 10 kilograms, those made at volume must perform as well as the original, minute amounts by using reproducible, manufacturable processes. We need to match the material specifications and performance at a large scale while keeping the cost as low as possible and, as always, as safely as possible."

For technologies to be widely adopted, they must first and foremost be affordable.

So far, so good. The facility has successfully scaled more than 20 materials, distributed samples weighing close to 30 kilograms, filed half a dozen patents and received an R&D 100 Award. All this while assisting other national laboratories, universities, General Motors, Sharp Labs and NASA's Jet Propulsion Laboratory in scaling up materials that may well become the next big thing in batteries.

MERF helps make Argonne the only national laboratory equipped to tackle process development for battery materials. And when combined with Argonne's other energy storage research groups and facilities, such as the Joint Center for Energy Storage Research, the Cell Analysis Modeling and Prototyping facility (CAMP) and the Post-Test facility, MERF makes Argonne a "full service" battery laboratory that runs the energy storage R&D gamut—from the most fundamental research in next-generation materials to the analysis of used and previously tested battery cells in order to identify the exact mechanisms that limit their life.

With its unparalleled expertise and cutting edge facilities such as MERF, Argonne is ground zero in the battle for achieving greater energy storage.



Principal process R&D chemist Kris Pupek loads a sample in a gas chromatograph-mass spectrometer for analysis.

A little history

Krumdick knows all too well the value of scale-up. An Argonne veteran of some 25 years, he has worked on numerous R&D and scale-up projects ranging from the advanced production of aluminum to ultra-fast boride coatings to innovative methods of chemical production at the pilot scale.

It was Krumdick's electrodialysis chemical plant that earlier caught the attention of Jeff Chamberlain, current Director of the Argonne Collaborative Center for Energy Storage Sciences (ACCESS). At the time, Chamberlain managed the laboratory's intellectual property portfolio for its lithium-ion battery programs and knew firsthand that the lab struggled to transfer next-generation materials to interested companies.

Argonne had created a new electrolyte material, and while there was significant interest from the private sector, no one was willing to take the risk and invest without knowing the material's production costs. While the process used to synthesize the material worked well for making bench-scale quantities, it simply was not scalable, particularly in terms of commercial viability.

Enter Krumdick, whose team reduced the 12-step process to four, saving precious time and money. But then, just

Analytical chemist Mike Kras fills a liquid nitrogen transport tank in the service corridor.

as the day seemed to be saved, they ran into a roadblock—they were unable to validate the process because of the hazards involved.

"We ran up against safety regulations that prevented us from having the volume of hazardous materials needed to do the work in our existing labs," said Krumdick. "While the final product may not be hazardous, the feed materials in many cases are, and our labs weren't rated for high hazards work . . . it was around the same time that the Department of Energy (DOE) fortuitously issued a call for proposals for a battery materials scale-up facility."

Essentially, said Krumdick, DOE wanted to decrease the time it took to get next-generation materials into industry.

Both Krumdick, whose expertise lay in scaling things up, and Chamberlain, whose work revolved around batteries, knew exactly what was needed. Together they laid out the idea for what would come to be MERF, an $8 million, high hazard-rated facility containing approximately $3 million in equipment.

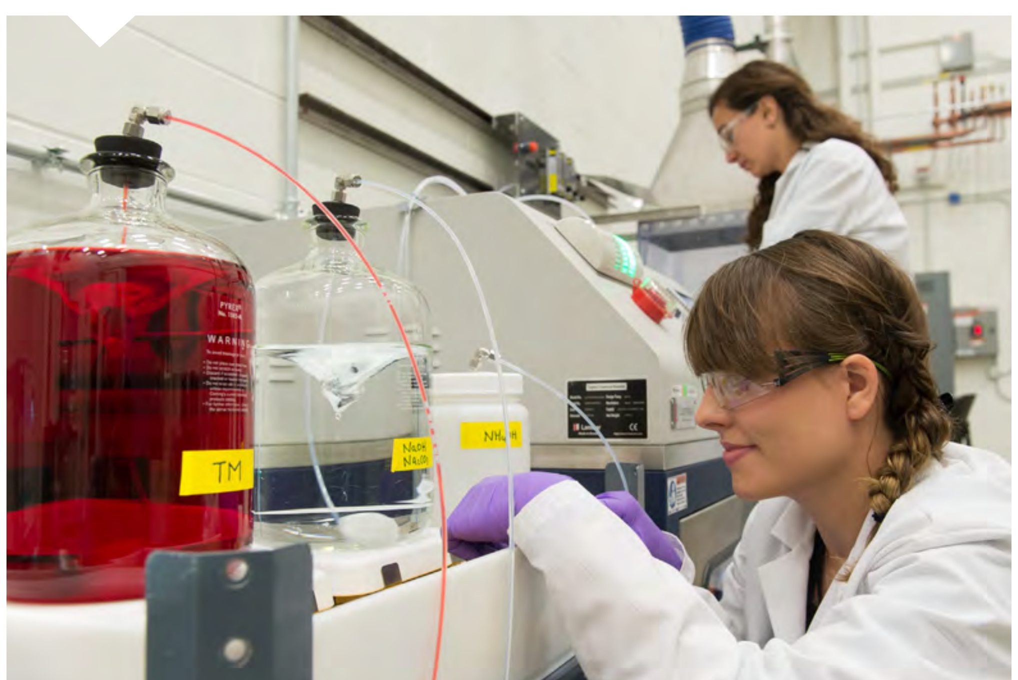
But like every other cutting-edge research facility, the equipment is only as good as the people using it. Staffing MERF would be a unique challenge in itself.

"Process scale-up is typically not taught at a university," said Krumdick. "It's learned on the job." Recent graduates typically lacked the experience for this type of work, so Krumdick hired people from industry such as Young Ho Shin, a materials engineer from a chemical production company in South Korea, and Kris Pupek and Trevor Dzwiniel, organic synthesis chemists who came from the pharmaceutical industry. These experienced researchers brought with them the skills needed to do R&D and materials scale-up. They are able to share their experiences by working with students and postdocs, thus teaching the next generation of MERF engineers how to do process scale-up, and do it safely.

Economies of scale

It all starts in MERF's research and development lab. With five bench-top fume hoods, the process R&D lab is well-suited for plenty of simultaneous research, which in turn helps to expedite the development process. It is here that researchers determine whether the original sample can be scaled up economically while retaining its beneficial properties.

Chemical engineer Ana Kiricova (foreground) and materials engineer Ozgenur Feridun check feed solutions for a cathode precursor synthesis run on a vortex reactor.



"The calorimeter data will tell us if we can control the reaction," said Pupek, a synthesis chemist with more than 20 years of industrial process scale-up experience.

It is also here that researchers attempt to "stress" the reaction by overheating, overdosing and nearly anything else they can do to disrupt it. "We want to see what will happen if something goes awry," said Pupek, "such as a loss of power. Safety is always a top priority."

This "stressing" ensures that the reaction's fundamentals are safe before researchers begin the scale-up process.

When certain properties are validated at the most minute scales, researchers then enter the large walk-in hoods in the scale-up lab to begin the process for which MERF was designed. Here the reactors, some as large as 100 liters, allow researchers to perform a wide range of experiments that will begin to generate the amounts needed for industrial testing and analysis.

But the biggest scale-up is yet to come. The facility's 32-foot-tall high-bays host the largest-scale work and are home to oversize equipment such as large reactors, furnaces and spray dryers. Each high-bay has a five-ton bridge crane to move heavy machinery, and beside each lab is a control room that allows researchers to monitor their experiments.

The facility also features a fully equipped analytical lab that allows for the immediate evaluation of synthesized organic and inorganic materials. Researchers can use the lab's state-of-the-art instruments to determine whether the materials produced at volume have the same properties as their original samples, the key metric when it comes to scaling up.

By having direct access to these tools, scale-up is greatly expedited simply because everything is done in-house, thus avoiding the shipment necessary to obtain outside analysis.

In the end, all of the information required to scale each material up is included in a technology transfer package made available to industry so that they then can do their own cost modeling.

These companies will have everything they need to economically produce the energy storage materials of tomorrow. And they will have MERF to thank.

Research support for the work described is provided by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Vehicle Technologies Office.

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Argonne Teams with **Strem Chemicals, Inc.,** to Provide **Industry** and the **Battery Research** Community with Next-generation **Energy Storage Materials**

Nine chemicals invented at Argonne and initially scaled up at MERF will be produced, marketed and distributed by Strem, a manufacturer and distributor of specialty chemicals founded in 1964.

"We continue to receive requests for samples of materials that we have scaled but have fully distributed," said MERF director Greg Krumdick. "Partnering with Strem made sense to help make these materials available."

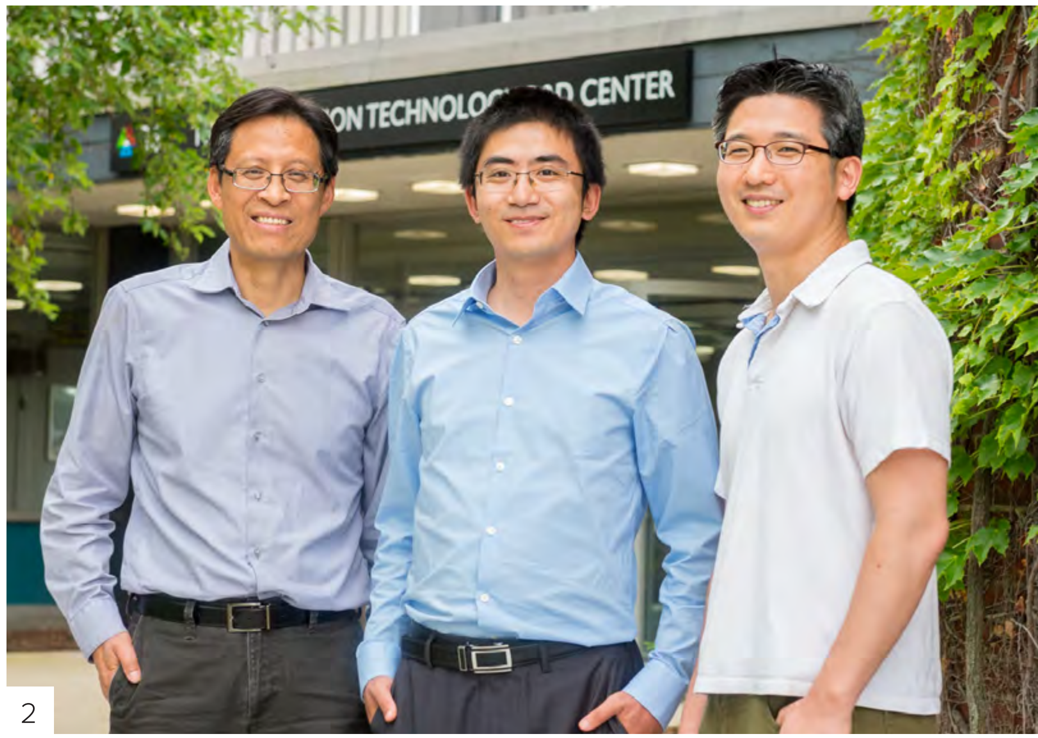
MERF will provide guidance on the synthesis and validation to ensure that the materials produced meet the required chemical purity and electrochemical performance prior to distribution.

"This agreement helps us get these materials out the door and into the hands of industry and researchers," said Krumdick. "It takes us one step closer to our final goal, implementation in commercial batteries."

Analyzing **Carbon Intensity** from Canadian **Oil Sands**

Canadian oil sands production will release approximately 20 percent more carbon into the atmosphere than conventional sources.

1



2

Argonne has shown that gasoline and diesel refined from Canadian oil sands have a higher carbon impact than fuels derived from conventional domestic crude sources.

The research, which was conducted in collaboration with Stanford University and the University of California, Davis, reveals variability in the increase of greenhouse gas impacts, depending on the type of extraction and refining methods. But generally speaking, fuel extracted and refined from Canadian oil sands will release approximately 20 percent more carbon into the atmosphere over its lifetime than fuel from conventional domestic crude sources.

"This is important information about the greenhouse gas impact of this oil source, and this is the first time it has been made available at this level of fidelity," said Hao Cai, the Argonne researcher who led the study.

"Canadian oil sands accounted for about nine percent of the total crude processed in U.S. refineries in 2013, but that percentage is projected to rise to 14 percent in 2020."

Argonne is a recognized global leader in analyzing the environmental impacts of transportation fuels, ranging from conventional gasoline to biofuels to electricity and hydrogen. The laboratory's Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) model is the premier tool for analyzing the environmental footprints of fuels and vehicle technologies. GREET looks at all of the energy inputs for a given fuel pathway, from extraction to transportation, refining and combustion, to determine the full life cycle energy and emissions impacts.

Cai and his fellow researchers used a life cycle approach, gathering publicly available data on 27 large Canadian oil sands production facilities. The study found the additional carbon impacts of Canadian oil sands related primarily to the energy required for extraction and refining, methane emissions from tailing ponds and carbon emissions from land disturbance of oil sands field operations.

The Argonne study is the most in-depth look at the carbon impacts of Canadian oil sands ever conducted. It is part of the laboratory's ongoing effort to characterize the environmental impacts of all types of transportation fuels.

"It was common knowledge that Canadian oil sand extraction was energy intensive, but no study could quantify that intensity with this level of detail and certainty," said Michael Wang, Argonne's leading expert on fuel cycle analysis. "This information will be important for industry and policy makers as they chart a path forward to meet the fuel demands of the United States, while minimizing the environmental impact of that fuel."

The full article, "Well-to-Wheels Greenhouse Gas Emissions of Canadian Oil Sands Products: Implications for U.S. Petroleum Fuels," can be found at http://dx.doi.org/10.1021/acs.est.5b01255.

1 *An Argonne study found that gasoline and diesel refined from Canadian oil sands have a higher carbon impact than fuels derived from conventional domestic crude sources.*

2 *The study was conducted by (from left) senior scientist and group lead Michael Wang, principal investigator Hao Cai, energy systems analyst Jeongwoo Han and life cycle analysis team lead Amgad Elgowainy (not pictured).*

This research was funded by the Bioenergy Technologies Office and Vehicle Technologies Office within DOE's Office of Energy Efficiency and Renewable Energy.

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Biofuel for Boats

Jeff Wasil (front) of Bombardier Recreational Products and John Adey of the American Boat and Yacht Council testing the 16 percent butanol fuel.

The battle for cleaner, greener fuels isn't fought solely on land—America's rivers, lakes and surrounding seas are home to 17 million recreational boats keeping more than 75 million weekend warriors afloat each year.

All that fun in the sun comes with a cost, however, particularly in terms of burnt fuel and emissions.

In an effort to reduce boating's environmental impact, Argonne has teamed with industry to investigate alternative fuels for recreational marine applications.

The laboratory, in collaboration with industrial partner Bombardier Recreational Products (BRP), and with support from the marine industry, including the National Marine Manufacturers Association (NMMA) and the American Boat and Yacht Council, has demonstrated the safety and effectiveness of a blend of fuel that includes 16 percent butanol for use in watercraft.

This demonstration has culminated in the approval of the fuel by the NMMA, a development sure to make waves in the boating arena.

The newly approved fuel has the potential to serve as an alternative to the 15 percent ethanol blend for much of the recreational boating fleet.

The approval is the result of several years of cooperative research between BRP and Argonne, whose research was funded by the Vehicle Technologies Office within DOE's Office of Energy Efficiency and Renewable Energy. The research involved the evaluation of performance, efficiency and emissions, including particulates, as well as durability and lubrication effects over a wide range of recreational boat engine types and sizes from several manufacturers.

Butanol provides the environmental benefits of ethanol without the performance issues.

"Butanol at 16 percent blend level works as well as ethanol at 10 percent under tested conditions," said Argonne's Thomas Wallner, a principal investigator at the laboratory's Center for Transportation Research. "There was a push to increase the amount of ethanol in fuel, from 10 to 15 percent," he said.

Wallner had previous experience researching butanol for cars and trucks, but boats were new territory.

Increasing the percentage of bioenergy in the boating mix would provide environmental benefits; however, the technologies used by a significant percentage of boats, such as carburetors and open-loop controls, are not immediately well suited to the further addition of ethanol in fuel. Furthermore, infrequent usage patterns typical for recreational boats can cause challenges at increased ethanol levels. Because ethanol attracts water, dormancy can allow the surrounding water to enter the fuel tank and form a layer inside, adversely affecting engine performance.

Butanol, on the other hand, lacks the water attraction properties of ethanol, mitigating potential engine performance issues.

Beyond the performance benefits, butanol offers an additional advantage: it can be made from the same feedstock as ethanol. Essentially, butanol provides the environmental benefits without the issues caused by increased ethanol use—a breakthrough made possible through strategic collaboration between Argonne and its industrial partners.

This research was funded by the Vehicle Technologies Office within DOE's Office of Energy Efficiency and Renewable Energy.

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Butanol can be made from switchgrass, one of the same feedstocks used to make ethanol.

The **Good**, The **Bad** and The **Ugly**

When electric vehicles (EVs) first arrived in the United States 15 years ago, there was no shortage of debate as to how they would influence the way in which Americans drive and purchase their cars and trucks.

Now, after a decade and a half, there is plenty to reflect on; we know, more or less, where the missed opportunities and future challenges lie.

Just ask Larry Johnson, Argonne Distinguished Fellow and past director of the laboratory's Transportation Technology R&D Center. Johnson has followed EVs closely since their entry into the marketplace—so closely, in fact, that the Chinese government invited him to discuss their strengths and weaknesses.

The invitation was part of a joint vehicle initiative between the United States and China, both of which have significant interest in EVs as a pathway to reducing fossil fuel consumption and, by extension, harmful emissions.

Johnson's analysis, entitled "Market Trends in Electric-Drive Vehicles in the U.S.: The Good, The Bad and The Ugly," after Clint Eastwood's 1966 spaghetti western, shed a much-needed light on how far EVs in America have come, and how far they have left to go. He worked closely with co-author and Argonne researcher Joann Zhou, who tracks monthly sales data for electric-drive vehicles.

"A presentation on sales data could easily become quite boring, but I found that structuring it around the theme of 'the good, the bad and the ugly' held the audience's attention," said Johnson. "The Chinese audience members may not have seen the movie, but they clearly understood how we organized the data into those three categories."

First, the good: electric vehicles are selling well, and every year more models are available to fit the individual lifestyles of consumers. Incentives at both the state and federal levels have accelerated adoption of these vehicles, particularly in more difficult markets, and a rapidly growing charging infrastructure is taking hold.

> The market for EVs in the United States has come a long way, but obstacles still remain.

But like the Chinese concept of yin and yang, with the good comes the bad. EVs represent fewer than three percent of all light-duty vehicle sales and less than one percent of vehicles on American roads, due in large part to the high price of their batteries and the availability of many fuel-efficient, non-electric alternatives.

Perhaps the most discouraging finding in Johnson and Zhou's research, however, is the correlation between EV sales and the price of gasoline, i.e., "the ugly;" as the price of gasoline declined last year, the sale of hybrid-electric vehicles also dropped. If fuel prices remain low for an extended period, there is a real risk that EV sales will decline in concert.

In order to combat that threat, and the others facing EVs, government action is likely necessary.

While a handful of states currently provide incentives for purchasing EVs, said Johnson's co-author Zhou, economic circumstances require them to monitor their value. As oil prices change, so, too, does the value of providing such incentives.

"To reap the long-term benefits of electric-drive vehicles, incentives, research, regulations, policies and programs will need to continue," said Johnson. "The question is, 'how long can these stimulus programs endure in the face of competing government spending priorities?'"

Funding for this work was provided by the U.S. Department of Energy, Energy Efficiency and Renewable Energy, Vehicle Technologies Office.

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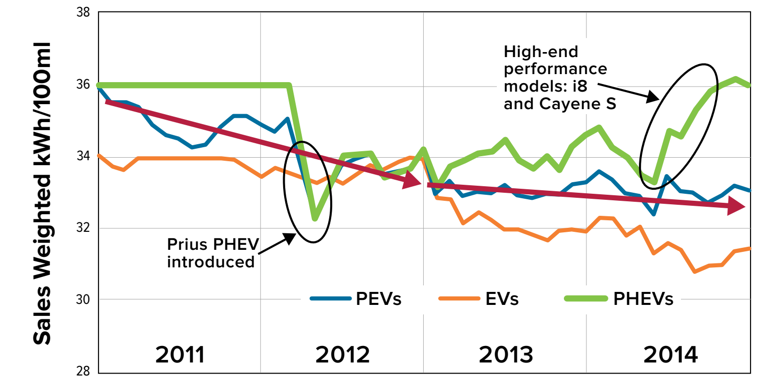
Citation
"Market Trends in Electric-Drive Vehicles in the U.S. (presentation)," L. Johnson and Y. Zhou, *10th Electric Vehicle Initiative Workshop*, Beijing, China (2015).

The Good: Fleet efficiency is improving over time
The Bad: but recently, at a diminishing rate



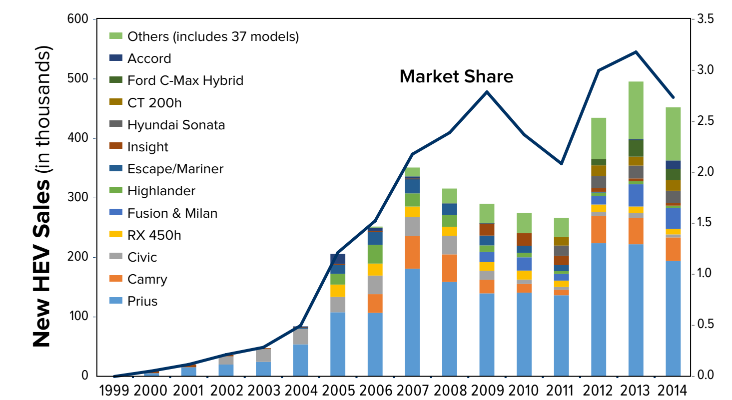
Fleet efficiency = plug-in vehicle sales weighted kWh/100 miles

Improvement is due to higher motor efficiency, better batteries and improved charging efficiency

Decline in efficiency is due to success of larger EVs and high-performance models

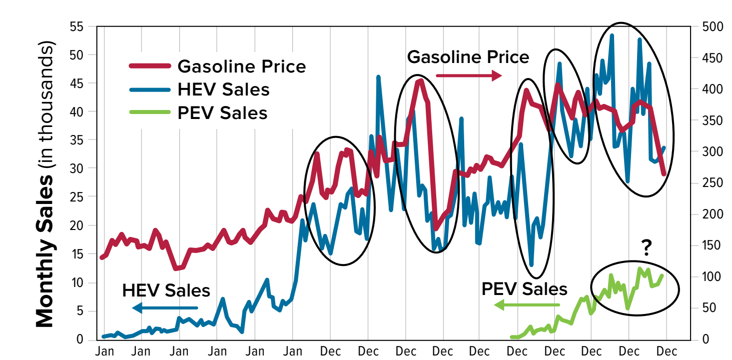
Source: http://tinyurl.com/nvxtarp
Efficiency: www.fueleconomy.gov

The Bad: In 2014 HEVs accounted for less than 3 percent of light duty vehicle (LDV) sales even though over 450,000 were sold.
Toyota accounted for 66 percent of the sales.



Source: http://tinyurl.com/nvxtarp

The Ugly: Declines in the price of gasoline tend to reduce the incentive for people to buy HEVs. PEVs?
The price of gasoline is beyond the control of the automakers. So far it has affected HEVs more than PEVs.



Source: http://tinyurl.com/nvxtarp

VERIFI Code Optimization Yields Three-fold **Increase** in **Engine Simulation Speed**

For engine designers in the digital age, time is money. And that time is measured in computer cycles.

Argonne researchers are partnering with Convergent Science, Inc. (CSI), to speed up a key piece of modeling and simulation software to ensure those cycles are used as effectively as possible, reducing product development time and resulting in better engines and savings for consumers. The scale of the speed gains were recently demonstrated when researchers ran the largest engine simulation to date on more than 4,000 computer cores.

The research is part of Argonne's Virtual Engine Research Institute and Fuels Initiative (VERIFI), which is working with CSI to optimize the company's CONVERGE code, a software program widely used in industry to conduct modeling and simulation for engine design. Although the effort has been ongoing for more than two years, it has recently moved into a code optimization phase that is showing dramatic gains.

"Our latest round of optimization has yielded a three-fold increase in speed, which correlates directly into faster design of better engines," said Janardhan Kodavasal, a postdoctoral appointee who led the optimization work along with with Marta Garcia Martinez, an assistant computational scientist, and Kevin Harms, a senior software developer at the Argonne Leadership Computing Facility. "The unique high-performance computing resources we have available at Argonne allowed us to make great progress in a short amount of time."

Engine designers use modeling and simulation software to test new designs and tweak existing plans in a virtual space, drastically reducing time to market. When the project first started, simulations ran on systems with 50 cores. VERIFI quickly scaled up those numbers to 1,000 cores, and recently conducted an engine simulation on 4,096 cores.

The work is focused on a key aspect of engine design – the extraordinarily complicated fluid dynamics and combustion characteristics that are at the heart of all internal combustion engines. Using high-performance computing and X-ray radiography data from Argonne's Advanced Photon Source, VERIFI was able to gain unprecedented insight into the performance of fuel injectors in engines.

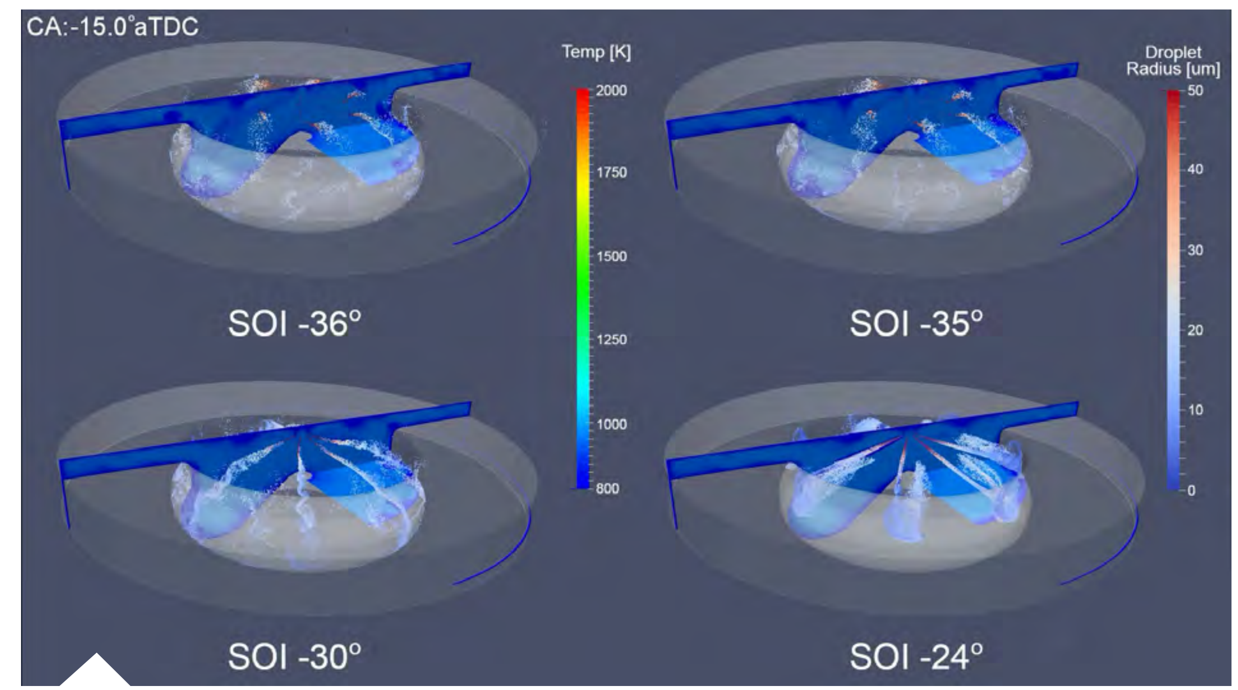
Once that modeling was completed, it was incorporated into CONVERGE and is currently being used by industry partners in engine design.

The latest phase involved optimizing the CONVERGE code for greater efficiency, and one of the key breakthroughs came in the area of load balancing. The varying levels of complexity in the chemistry of ignition meant that some cores weren't actively engaged in computation, while other cores handling more complex parts of the simulation were working overtime. By balancing the computational load evenly over all the cores, great gains in efficiency were achieved.

Another important development came when the team tweaked CONVERGE to use parallel read/write processes, which allow simultaneous file writing by processors, rather than having to wait for one action to complete before taking on another. This resulted in a speed-up of more than 100 times in writing large data files generated by the software.

In the end, the advances mean that engine designers can try out more designs in shorter amounts of time, yielding more efficient, reliable engines with lower cost.

The increase in speed correlates directly to faster design of engines.



Using high-performance computer-generated models, VERIFI researchers demonstrated that in gasoline compression ignition, varying the start of injection (SOI) timing produces significant differences in the reactivity of the fuel mixture, delaying ignition. Such high-resolution modeling was made possible by optimizing the CONVERGE code for parallel read/write processes.

"Working with the people at Argonne allowed us to implement high-performance computing improvements in our software much faster than we could do alone. The Mira computer system at the ALCF is a powerful tool, but it was Argonne's experienced staff that allowed us to really maximize the computing resources available to us and make great progress in a very short amount of time," said Keith Richards, co-founder and vice president of Convergent Science.

VERIFI and CSI will be presenting the findings of the work in a forthcoming paper for the American Society of Mechanical Engineers.

VERIFI research is funded by the Vehicle Technologies Office of DOE's Office of Energy Efficiency and Renewable Energy.

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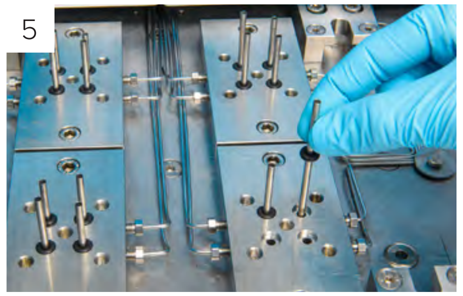
New Labs Enhance Research in Catalysis, Fuel Cells and Materials Research



1 ***When Argonne's new Energy Sciences Building opened, it brought a series of spacious next-generation research laboratories online to support transportation-related work in catalysis, fuel cells and materials. Many of these facilities provide greatly enhanced throughput capacity to speed research and development processes.***

2 *Postdoctoral appointee Jeff Bunquin prepares to test new catalyst formulations using a novel high-throughput system that combines atomic layer deposition for catalyst synthesis with a plug-flow reactor system for catalyst testing.*

3 *Researchers can use a configurable automation system for rapidly preparing complex catalyst formulations covering a wide range of compositions.*

4 *Chemist Xiaoping Wang screens the performance of new electrocatalysts for polymer electrolyte fuel cells using a rotating disk electrode.*

5 *A researcher loads catalyst samples into a high-throughput reactor system capable of evaluating the reactivity of 16 catalysts at one time.*

6 *Materials scientist Vojislav Stamenkovic probes the structure–function relationship of new electrocatalysts being developed for polymer electrolyte fuel cells using an ultra-high vacuum technique.*

7 *The new high-throughput laboratory provides a suite of automated equipment that facilitates rapid synthesis and evaluation of new catalysts and materials.*

Turning **Methane** into Usable **Liquid Fuel**

Shale gas drilling has provided the world with an abundant form of relatively inexpensive energy in the form of natural gas.

Unfortunately, the extraction process also results in plenty of potential energy that simply goes to waste. At least for now.

Researchers from Argonne and the Illinois Institute of Technology have been awarded $2 million over the course of two years to fund studies on hybrid fuel cells—work currently ongoing in the Energy Sciences Building's state-of-the-art labs.

The research seeks to create a fuel cell that would both produce electricity and convert methane gas to ethane or ethylene that could then be converted to a liquid fuel or valuable chemicals. These cells could use natural gas—which is mostly made up of methane—directly.

With the advent of shale gas drilling techniques, methane is fairly abundant and frequently produced as a by-product in drilling operations. Unfortunately, it is often burned off because it is expensive to transport in gas form, and few natural gas pipelines exist. Finding a less expensive way to instead turn that methane into liquid fuel—such as that promised by hybrid fuel cells—could reduce waste and provide energy.

In the fuel cell, researchers plan to add a catalyst that helps make the reaction more efficient, breaking methane up and recombining it into hydrogen—which is then consumed by the fuel cell—and ethylene. The expectation is that combining the steps will make the reaction more efficient.

"The ethylene is just a first step, a placeholder for proof-of-concept," said Argonne chemical engineer Ted Krause, who is heading the project. "The overall goal is to produce liquid fuel from methane."

The funding is provided by ARPA-E, an agency within DOE that was specially created to fund high-risk, high-reward energy research projects and was modeled after the similar defense agency, Defense Advanced Research Projects Agency, or DARPA. Argonne was one of 13 research labs chosen to develop new fuel cell technology as part of ARPA-E's Reliable Electricity Based on Electrochemical Systems (REBELS) program.

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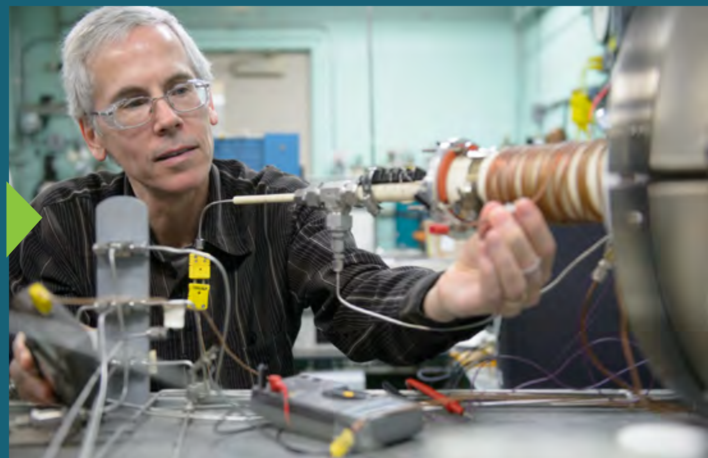

Materials scientist Steve Dorris installs a proton-conducting electrolyte into a furnace to test its chemical stability in shale gas at intermediate temperature (500°C).

ROUNDUP

EcoCAR 3 Year One Winner Announced

The Ohio State University (OSU) has been named winner of Year One in the four-year *EcoCAR 3: An Advanced Vehicle Technology Competition*, continuing their winning streak by following their previous win as the overall champions of the *EcoCAR 2: Plugging In to the Future* challenge.

EcoCAR 3 is a collegiate student competition established by DOE and General Motors and managed by Argonne. The only program of its kind, *EcoCAR 3* challenges 16 North American universities to reengineer a 2016 Chevrolet Camaro to further reduce its environmental impact while maintaining the safety and performance expected from the iconic American car.

Fifteen other teams from North American universities gathered in Seattle for several days of the premier collegiate engineering program that gives students the chance to design, build and demonstrate cutting-edge, eco-friendly automotive technologies.

The Ohio State University bested 15 other teams to take the top prize in Year One of the four-year EcoCAR 3 *competition.*

This first year of *EcoCAR 3* emphasized the use of math-based design tools and simulation techniques for designing a successful vehicle architecture that reduces energy consumption, well-to-wheel greenhouse gas emissions and tailpipe emissions.

"Without having the full picture of the attributes of the new 2016 Camaro, the students from OSU were able to develop a strategy that can turn this high-performance vehicle into a cutting-edge eco-friendly alternative," said Al Oppenheiser, Chevrolet Camaro Vehicle Chief Engineer. "Not only does the 2016 Camaro's leaner, stiffer platform provide an optimal base vehicle for these students to achieve their powertrain goals, the exterior of the vehicle was designed to specifically enhance efficiency."

The Ohio State team is made up of approximately 40 students, ranging from undergraduate freshmen to Ph.D. candidates from a diverse background of majors, including mechanical and electrical engineering, to business and public relations. Throughout the competition the team continuously exceeded expectations during their presentations to industry and government professionals on their mechanical, electrical and control strategies. Judges were also impressed by their efforts in identifying a target market for their vehicle and branding strategy, including a memorable tagline: "Classic.Recharged."

"This year really lays the foundation of vehicle development, which is a critical step in the process for future success," said M.J. Yatsko, OSU engineering manager.

"We have already begun vehicle dynamic analysis for next year and are excited to share some of our innovative features we plan to integrate into our vehicle."

Virginia Tech and University of Waterloo teams came in second and third place, respectively.

Sponsors of EcoCAR 3 include Headline Sponsors—the U.S. Department of Energy and General Motors; Visionary Sponsors—MathWorks, California Air Resources Board, Freescale and Clean Cities; Leadership Sponsors—AVL Powertrain Engineering, BOSCH, ETAS and dSPACE; Sustaining Sponsors—Snap-on Tools, Siemens, GKN Driveline and the Transportation Research Center; Supporters—Enerdel, Proterra and Ricardo; and Contributors—EcoMotors and A123 Systems.

For more information about *EcoCAR 3*, visit
www.ecocar3.org

Improving **Urban Evacuation**

Argonne researchers are using the laboratory's POLARIS traffic flow model to better prepare for mass evacuations in case of emergency.

Getting people into cities has never been a problem. Today's urban populations represent 54 percent of the world, compared with just 34 percent in 1960.

But moving millions out of a city safely and quickly in the case of an emergency is a daunting task. To improve this process, Argonne researchers are studying methods and creating tools for building more resilient mass transit systems to evacuate major cities under a $2.9 million grant announced by the U.S. Department of Transportation's Federal Transit Administration.

The project is bringing together researchers from the laboratory with Chicago's Pace Suburban Bus and Metra Commuter Rail Service to investigate ways to improve the detection, analysis and response to emergencies, and how best to evacuate the city in a major emergency. The research builds on nearly a decade of work at Argonne on transportation resilience, modeling and simulation in the Chicago area.

"In an emergency situation, planning is everything," said U.S. Sen. Dick Durbin, who supported the grant application, along with U.S. Sen. Mark Kirk and a number of U.S. representatives from the Illinois delegation. "A lack of evacuation procedures or a failure of coordination among transit systems can have catastrophic consequences during an emergency. Argonne researchers will use this federal funding to develop tools that can be used by transit agencies across the country for planning and reacting to emergencies."

The project, planned for completion in 2017, is built around Argonne's POLARIS system, which is an open-source, high-speed computing framework tailored for transportation planning needs. Argonne's researchers will create tools within POLARIS to provide complex modeling and simulation of the movement of people via mass transportation during an emergency.

The new system will allow planners to run various simulated emergency events to identify weaknesses in the transportation system, investigate new technologies to integrate resilience into the system and develop new techniques for quickly moving people in a disaster, whether natural or man-made. The tools will also provide real-time assistance during an emergency by enabling officials to see the location of transit assets—such as buses and trains—as well as estimates of population distribution and characteristics, including people who will need extra assistance such as the elderly and those with disabilities.

"Chicago has the second-largest public transportation system in the United States and presents some interesting challenges to transportation planners due to its proximity to Lake Michigan and its system of rivers," said Hubert Ley, principal investigator on the project. "If we can create effective tools for such a challenging environment, they will prove very useful for cities of all sizes."

The project also involves the Urban Transportation Center at the University of Illinois at Chicago, which is evaluating the tools for practicality, and the Department of Civil, Architectural and Environmental Engineering at the Illinois Institute of Technology, which is working on model calibration, validation and case studies.

Funding for this work is provided by the U.S. Department of Transportation's Federal Transit Administration.

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ROUNDUP

Predicting the Economic **Impacts** of **Natural Gas** Stations

Natural gas fueling stations could offer substantial environmental and economic benefits.

A major hurdle to cleaner, greener fuels for cars and trucks is replacing the gasoline infrastructure—there are more than 168,000 retail stations selling fuel, the overwhelming majority of it gasoline, to an energy-hungry American public.

But the benefits of some alternative fuels such as compressed natural gas are simply too obvious to ignore. While the construction of new infrastructure to deliver novel fuels would be costly, it might well be worth it.

To better understand the risks and rewards, Argonne researchers have developed a new tool for analyzing the economic impacts of building new compressed natural gas fueling stations. Called JOBS NG, the tool is freely available to the public and customizable by state or census region.

Mostly made up of methane, compressed natural gas is an alternative fuel for cars and trucks that can offer greenhouse gas benefits over gasoline.

Thanks to new methods, natural gas production has boomed in the United States, raising interest in its use as a vehicle fuel. But there are currently far fewer natural gas stations (concentrated in a areas like California, Oklahoma, Utah and New York) than gasoline stations in the country.

JOBS NG is designed to help states and local governments evaluate the possible economic benefits related to natural gas stations when they are setting new policies. It can also help developers quantify proposals.

"Our model estimates the jobs created and economic output at every stage in the process, beginning with station design and construction and continuing through the operation and maintenance of the station and the sale of natural gas fuel," said Marianne Mintz, an Argonne systems analyst who built the tool.

The analysis even extends to the equipment for the station—accounting for the raw materials that go into components as they are mined, refined, distributed and assembled. Because natural gas generally arrives via pipeline in gaseous form, it has to be compressed at the station to less than 1 percent of its original volume using special equipment.

Development of this tool was supported by the U.S. Department of Energy's Clean Cities program, an initiative of the DOE's Office of Energy Efficiency and Renewable Energy.

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"Clean Cities" University Program **Celebrates** Another **Successful Year**

This summer the Clean Cities University Workforce Development Program (CCUWDP), which pairs college students with a passion for energy and sustainability with local Clean Cities Coalitions, once again provided the next generation of efficiency researchers and engineers with opportunities to reduce the use of petroleum in the transportation industry.

Working with Argonne, DOE's Clean Cities program launched CCUWDP in 2010 to provide the automotive and energy sectors with skilled and knowledgeable talent to help shape the future of on-road transportation. The Clean Cities program advances the nation's economic, environmental and energy security through local actions aimed at slashing the amount of petroleum used in transportation; since its inception in 1993, the program has saved more than five billion gallons.

A national network of nearly 100 Clean Cities Coalitions brings together stakeholders in the public and private sectors to deploy alternative and renewable fuels, idle-reduction measures, fuel economy improvements and emerging transportation technologies.

"A lot of our success and growth has been due to our interns' attention to reaching out to stakeholders," said Carl Lisek, Coordinator for the South Shore Clean Cities Coalition in Illinois.

As an example of the success of the program, CCUWDP alum Mike Terreri gave a webinar to the current group of students on using skills learned through the program to find a position in the field. Terreri, who completed two terms in CCUWDP, now works as a Clean Transportation Specialist at the North Carolina Clean Energy Technology Center. He spoke about how his time in the program gave him valuable knowledge and increased enthusiasm for work in the energy field and how he still works with Clean Cities Coalitions in his area to educate the public about energy use.

Argonne manages CCUWDP via advertising and student selection, as well as by offering educational development programs for career growth. The program began with 25 participants the first year and has resulted in more than 250 students completing the program since then. Nearly 70 of the 86 regional Clean Cities Coalitions have received an intern through the program, and new locations join each semester. Many interns have gone on to work at their coalitions after graduation, or for one of the coalitions' stakeholders.

The summer 2015 term of the program ran from June to August and hosted 38 students at as many coalitions. Students supported the overall Clean Cities mission of reducing petroleum usage in transportation at the local level by organizing outreach events, collecting and analyzing data, developing website and social media content and working on educational campaigns.

Development of this program is supported by the U.S. Department of Energy's Clean Cities program, an initiative of the DOE's Office of Energy Efficiency and Renewable Energy.

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Attending the DOE Clean Cities' event Driving Change at Denver Water *are (from left) Tyler Svitak, Clean Cities Denver Coordinator: Kim Tyrell, Air Quality Program Manager; Alex Lyakhov, CCUWDP intern; and Britt Coyne, Air Quality Program Assistant. Argonne manages CCUWDP via advertising, student selection and educational and career growth offerings.*

FASTRAX

DOE Awards Four Argonne Researchers at Annual Merit Review

Four scientists from Argonne's Energy Systems division have received awards from the Department of Energy's (DOE's) Vehicle Technologies Office (VTO) and Fuel Cell Technologies Office (FCTO). **Raj Sekar**, **Amgad Elgowainy**, **Marianne Mintz** and **Tom Stephens** were each recognized at the DOE's Annual Merit Review meeting in June.

Sekar, a retired senior mechanical engineer and project engineering manager, received the Lifetime Distinguished Achievement Award. The prize honored his 45 years of excellence in research, during which time he published more than 70 papers and received 12 patents.

Sekar sparked an industrial partnership with Electro-Motive Diesel (EMD) that has contributed $1 million annually toward research and development of locomotive diesel engines at Argonne. The EMD contract, signed in February 1996, is perhaps the longest-running Strategic Partnership Project at the laboratory. With Sekar's achievement award, DOE recognizes the growth of Argonne's engine and emissions research from one post doc in 1997 to about 30 researchers today.

Elgowainy, a principal energy systems analyst, was recognized for establishing the Hydrogen Refueling Station Analysis Model (HRSAM), a tool that allows users to accurately evaluate the techno-economic performance of various refueling station configurations and capacities according to the SAE J2601 protocol. HRSAM is a significant step toward optimizing hydrogen infrastructure rollout, and is the main cost analysis mechanism used by the various working groups of the H_2USA partnership.

Mintz, a principal transportation systems analyst, was commended for her part in developing the JOBS model, which estimates the employment impacts of hydrogen infrastructure and fuel cells in terms of earnings, economic output, installation and other variables. This model has investigated the impact of FCTO's deployment activities under the American Recovery and Reinvestment Act, among other initiatives.

Marianne Mintz

Tom Stephens

Stephens, also a principal transportation systems analyst, was recognized for leadership in multi-laboratory, integrated vehicle technology analysis. Though Argonne is his home laboratory, Stephens demonstrated knowledge and insight of work performed at multiple labs and on the priorities of the VTO at DOE headquarters as he directed major analysis projects taking place across multiple collaborating institutions.

VERIFI Researchers Receive FLC Award for Transfer of Engine Simulation Technology

The Federal Laboratory Consortium (FLC) for Technology Transfer has honored a group of Argonne researchers for working with industry to use supercomputers to conduct engine simulations.

The Award for Excellence in Technology Transfer singled out a group of researchers who transferred to private industry a two-part technology for simulating the complex inner workings of internal combustion engines. One part of the technology consisted of a fuel spray model that analyzes the behavior of fuels within an engine. The second part involved load-balancing algorithm software that helps manage the high-performance computing resources necessary for the work.

This type of modeling and simulation forms the core of Argonne's Virtual Engine Research Institute and Fuels Initiative (VERIFI), which continues to cooperate with industry to create tools that will enable development of cleaner, more efficient engines. This work also helped build the bridge between the use of cluster computing in the Laboratory Computing Resource Center and the massively parallel computing resources at Argonne's Leadership Computing Facility.

Principal mechanical engineer **Sibendu Som** and senior computational scientist **Raymond Bair** led the research. Technology manager **Terry Maynard** facilitated the transfer of the technology to industry.

Argonne's Sibendu Som and Ray Bair recently received the FLC Award for Excellence in Technology Transfer. The Argonne team developed a tool to simulate the complex conditions in an internal combustion engine. Pictured (from left to right) are: Paul Zielinski, FLC Chair; Ray Bair (Argonne); Sibendu Som (Argonne); Jetta Wong (DOE); and Dr. Mark Reeves, FLC Vice Chair.

FASTRAX

Building a Benchmark

Elgowainy recognized for analysis of refinery emissions.

Argonne researchers have a reputation for groundbreaking research, and energy systems analyst **Amgad Elgowainy** is no exception.

Elgowainy was lead author of "Energy Efficiency and Greenhouse Gas Emission Intensity of Petroleum Products at U.S. Refineries," an analysis that received *Environmental Science & Technology* magazine's second runner-up in the Environmental Technology category for 2014.

Elgowainy's paper, which sought to determine how alternative fuels stack up environmentally against gasoline, was selected from among the more than 1,500 the journal accepted last year.

The research provided invaluable information for industry and legislators attempting to tackle the question of emissions from U.S. refineries, which are substantial; in 2012 alone they generated 173 million metric tons of greenhouse gases (the average American contributes about 19 tons annually). Reducing this footprint is critical to DOE-relevant missions involving climate change and for meeting newer, stricter regulatory standards likewise aimed at reducing America's carbon footprint.

But in order to get a realistic measurement of a fuel's environmental impact, researchers need to understand its whole lifespan, from extraction to refinement to burning. The refinery process is particularly tricky to quantify because of the many processing units involved and the multiple co-products from each.

Elgowainy and his collaborators understood that by measuring the impact of the refining process on overall emissions, they could develop a reliable benchmark for the most popular alternative fuels.

Working with fuels and chemicals producer Sasol and Jacobs Consultancy, Elgowainy's team derived its data from 43 refineries in four Petroleum Administration for Defense Districts (PADDs) which, taken together, represent 70 percent of the total U.S. refining capacity.

"This research represents the only comprehensive study that covered actual configurations of refineries with real throughput data," said Elgowainy. "We used a representative sample of each PADD, and had good coverage at the refinery level. Refinery CO_2 intensity for each product is key for an accurate estimate of each refinery product's life cycle greenhouse gas emissions."

Amgad Elgowainy

Because each refinery produces different proportions of different fuels, the team looked at the individual units (from distillation to catalytic reformers to cokers) within the refineries to gain a clear picture of the footprint of each fuel. By tracking the burden across a fuel's lifespan, it was possible to calculate energy allocation values for all major refinery fuel products, including diesel, jet fuel, liquefied petroleum gas, petroleum coke and residual fuel oil. Among their findings:

- Jet fuel was the most efficient product overall, with a 93–97 percent efficiency rating.
- Diesel possessed the widest efficiency range of all products (85–95 percent).
- Coke produced by far the largest amount of life cycle greenhouse gas emissions due to its high carbon content.

Quantifying the refinery process allows researchers to better understand the environmental impact of fuels.

"This is important because we need to know how refineries will be affected under various crude mix scenarios," said Elgowainy.

While the research is impressive in its own right, it has paved the way for even more investigation of energy use and emissions regionally and by season, and of impacts of various sources and qualities of crude on the carbon intensity of finished products.

As a bonus, the individual refineries now possess data on how processing a certain type of crude will affect their overall operations and carbon footprints.

Citation
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Tribology Researcher Recognized for Distinguished Career

Argonne researchers take an all-angles approach to getting the most bang for America's energy buck, and one of the key areas of investigation over the past several decades has been reducing friction in an internal combustion engine. The profusion of moving parts present in today's vehicles represents a major opportunity for researchers to not only increase efficiency, but also reduce emissions and extend vehicle life.

Few people are more dedicated to unlocking that efficiency than **Ali Erdemir**. An Argonne staff member since 1987, Erdemir has dedicated nearly his entire career to reducing the friction between moving parts, an effort that recently culminated in his receipt of the American Society of Mechanical Engineers' (ASMEs') Mayo D. Hersey Award "in recognition of distinguished and continued contribution over a substantial period of time to the advancement of lubrication science and engineering."

This latest award is one of many for Erdemir, whose career has garnered five R&D 100 Awards, 16 patents,

Ali Erdemir

290 publications, three edited books and 18 invited book chapters. He is a fellow of ASME, the American Society of Metals, American Vacuum Society, and the Society of Tribologists and Lubrication Engineers (STLE). He is the Vice President of STLE and also serves on its executive committee.

Erdemir is a materials scientist by education, and his tribology research team develops lubricants, materials and coatings, all of which are used in concert to reduce friction and thereby maximize efficiency.

Erdemir's coating research recently culminated in the published "Coating Technology for Vehicle Applications," a book he co-authored with Sung Chul Cha, a senior research engineer at Hyundai Motor Group. Coatings are becoming an increasingly important field in the materials and tribology arenas.

Research **Results**

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For more information, contact Argonne's Technology Development and Commercialization Office at 800.627.2596

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Research **Results**

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"Well-to-Wheels Greenhouse Gas Emissions of Canadian Oil Sands Products: Implications for U.S. Petroleum Fuels," **H. Cai**, A.R. Brandt, S. Yeh, J.G. Englander, **J. Han**, **A. Elgowainy**, and **M.Q. Wang**, *Environmental Science & Technology* **49** (13), 8219–8227 (2015). Available at http://dx.doi.org/10.1021/acs.est.5b01255.

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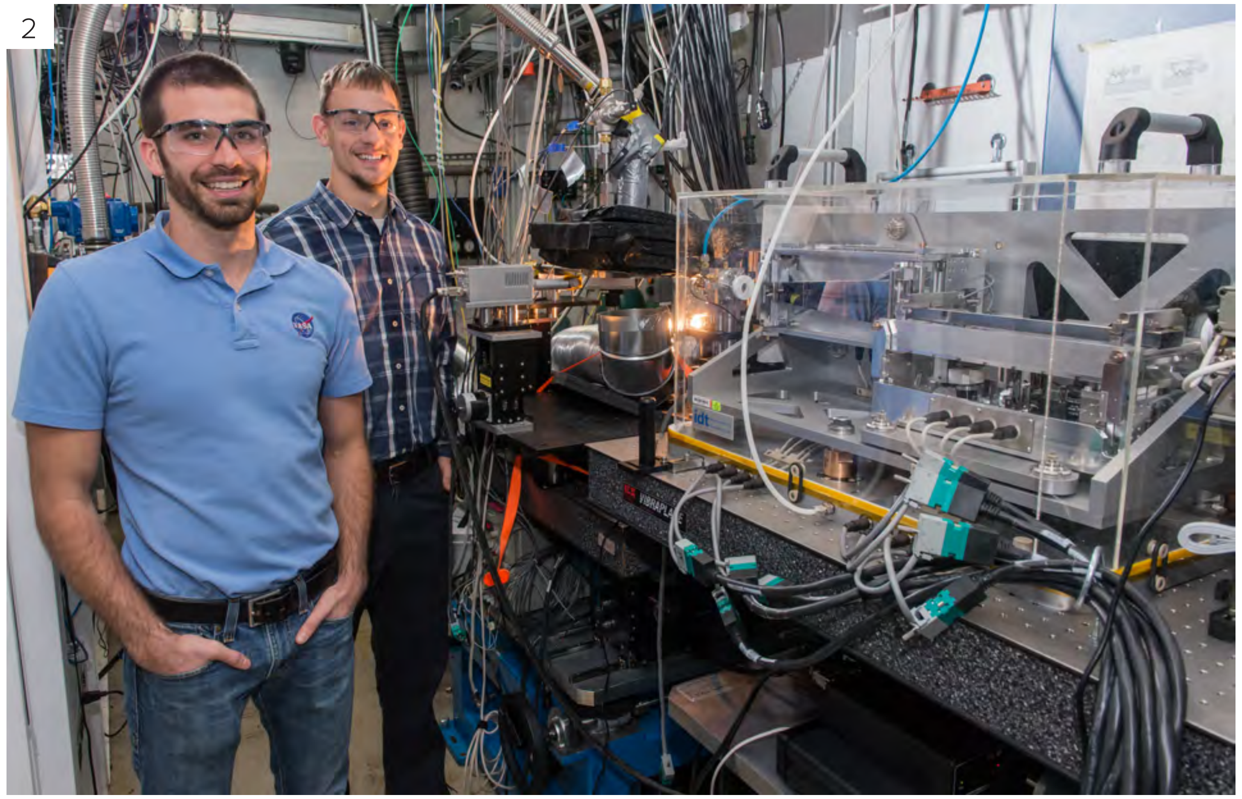
PARTING SHOTS

1 *Argonne researcher Yuelin Li holds a sample containing a single gold nanorod in water. Li and colleagues have revealed previously unobserved behaviors that show how the transfer of heat at the nanoscale causes nanoparticles to change shape in ensembles. Their research may inform the creation of next-generation technologies such as battery materials, water purification systems and cancer research.*

2 *Patrick McManamen (left) and Chris Radke, NASA propulsion system engineers, brought a rocket injector system for the NASA rocket Morpheus to Argonne to test at the world's only X-ray beamline dedicated to fuel injection research at the lab's Advanced Photon Source. It is seen covered in black foam in the center of the picture. The injector is designed for oxygen and methane propellants. NASA staff believe this propellant combination is a critical enabling technology for human exploration to Mars and deep into the Solar System.*

3 *Planting bioenergy crops like willows or switchgrass in rows where commodity crops are having difficulty growing could provide biomass feedstock and also limit the runoff of nitrogen fertilizer into waterways—all without hurting a farmer's profits. As shown below, Argonne researchers are collecting data on nutrient retention and loss in the soil over several years in the Indian Creek Watershed farming community in central Illinois.*

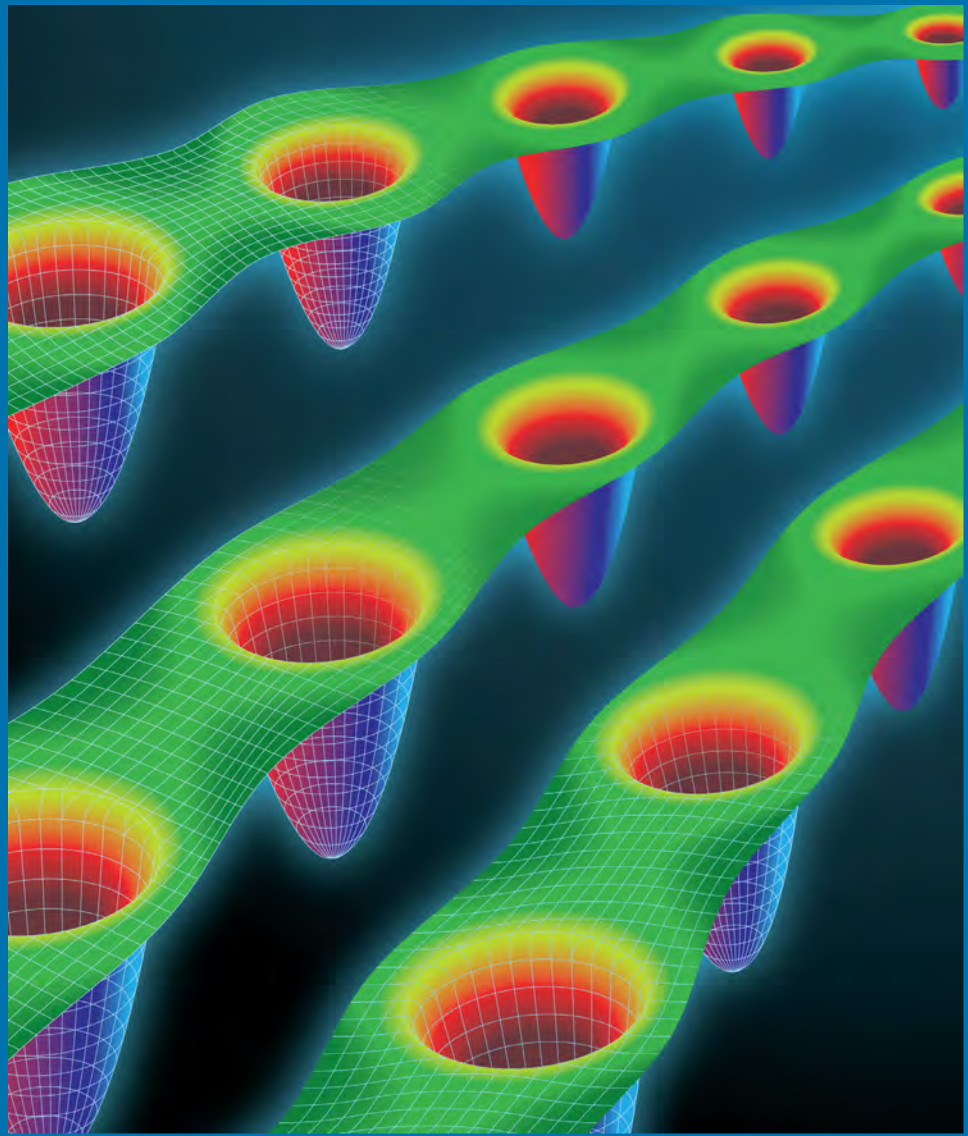
1



2

3

The **Beauty** in **Science** and **Engineering**



Superconductor vortices

Superconductors can conduct electricity perfectly, without ever losing current—but have to be cooled to very low temperatures (at least –280° F) to function.

However, when you apply a magnetic field to a high-temperature superconductor, you get the "vortices" shown above. These stop the superconductor from conducting (the green areas represent superconductivity).

Scientists are very interested in finding a way to "pin" the vortices so they don't move around and inhibit superconductivity. Such a discovery would enable the use of superconductors in applications with magnetic fields, such as engines.

One possible solution is to make ultra-thin strips of superconducting wire, as shown above, so that only one row of vortices can fit (a solution demonstrated by Argonne scientist Valerii Vinokour of the laboratory's Materials Science division).

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Industrial technology development is an important way for the national laboratories to transfer the benefits of publicly funded research to industry to help strengthen the nation's technology base. The stories highlighted in this issue of **TRANS**FORUM represent some of the ways Argonne works with the transportation industry to improve processes, create products and markets, and lead the way to cost-effective transportation solutions, which in turn lead to a healthier economic future.

By working with Argonne through various types of cost-sharing arrangements, companies can jump-start their efforts to develop the next generation of transportation technologies without shouldering the often prohibitive costs of initial R&D alone. Argonne has participated in dozens of these partnerships and has even been involved in helping to launch start-up companies based on the products and technologies developed here.

If working with world-class scientists and engineers, having access to state-of-the-art user facilities and resources, and leveraging your company's own capabilities sound like good business opportunities to you, please contact our Technology Development and Commercialization division and see how we can put our resources to work for you.

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