Argonne NATIONAL LABORATORY

TransForum

News from Argonne's Transportation Research Program
www.transportation.anl.gov

Volume 14

Issue 1

Winter 2014

Contents

TransForum

News from Argonne's Transportation Research Program
www.transportation.anl.gov

Rechargeable Nanoelectrofuels for Flow Batteries May Revolutionize EV World *page 4*

Operating at more than 10 times the capacity of a conventional flow battery, the nanoelectrofuel battery promises to revolutionize the practice of energy storage.

Unlocking the Door to Better Diesel Engine Combustion and Emission Performance *page 10*

A revolutionary advance in our understanding of how diesel engines work may unlock new approaches to predicting diesel engine performance and emissions.

On the cover
Chemist Elena Timofeeva sets up an experiment to evaluate nanoelectrofuel performance.

Shown here
John Katsoudas and Dileep Singh review experimental results from a full flow battery test in the fume hood wet lab area.

TransForum | Volume 14 | Issue 1 | Winter 2014

Research Reviews

Rechargeable Nanoelectrofuels for Flow Batteries May Revolutionize EV World

Scientists from the Illinois Institute of Technology (IIT) and Argonne National Laboratory recently won a three-year, $3.44 million grant from the U.S. Department of Energy's Advanced Research Projects Agency-Energy (ARPA-E), a government agency that funds research and development of advanced energy technologies.

Mike Duoba (second from right) explains to the development team how its flow battery would alter the mechanics of electric vehicles, using a contemporary plug-in electric vehicle to illustrate. Also pictured, left to right: Dileep Singh (background), Elena Timofeeva (foreground), Chris Pelliccone (IIT), Carlo Segre (IIT), Douba and John Katsoudas (IIT).

Contents | Next Page | Next Article

Leveraging the properties of nanofluid technology and flow batteries, the team created a groundbreaking concept for storing electrical energy: a rechargeable battery in liquid form. The battery uses nanoelectrofuel—a unique liquid in which tiny battery-active particles are permanently suspended and can be charged and discharged multiple times.

Advantages of Nanoelectrofuels

Operating at more than 10 times the capacity of a conventional flow battery, the nanoelectrofuel battery promises to revolutionize the practice of energy storage, especially for electric vehicles (EVs). High-energy-density nanoelectrofuels offer numerous benefits, including thermal safety, lower cost, higher efficiency, flexibility and adaptability.

Nanoelectrofuel-powered flow batteries offer a key advantage over conventional batteries: the fuels can be separated from the cell. The batteries can be charged at solar plants and transported to market by specially designed trucks or by rail. To recharge, users plug into the grid or replace the spent fuel with charged nanoelectrofuel at special recycling stations.

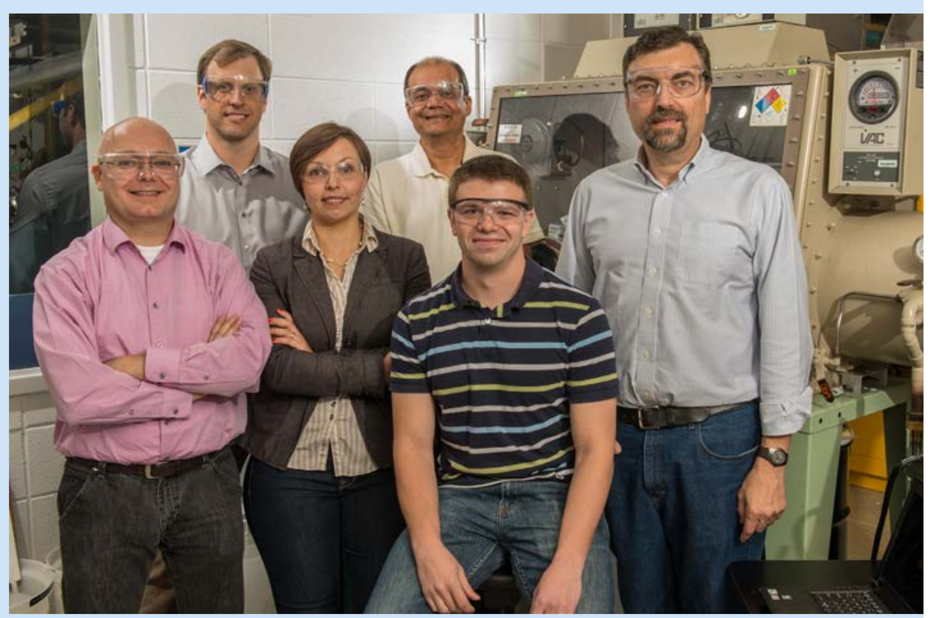
"The ability to directly charge the nanoelectrofuel at the renewable sources themselves, and then transport the fluids to market using the existing U.S. petrochemical infrastructure, precludes the necessity of building a whole new electrical grid system to those locations," said John Katsoudas of IIT.

He continued, "We are not only creating a better battery to allow fast EV refueling, we are fundamentally changing the format by which energy is distributed, into one that is much more amenable to market acceptance. These facts are what I am most enthusiastic about."

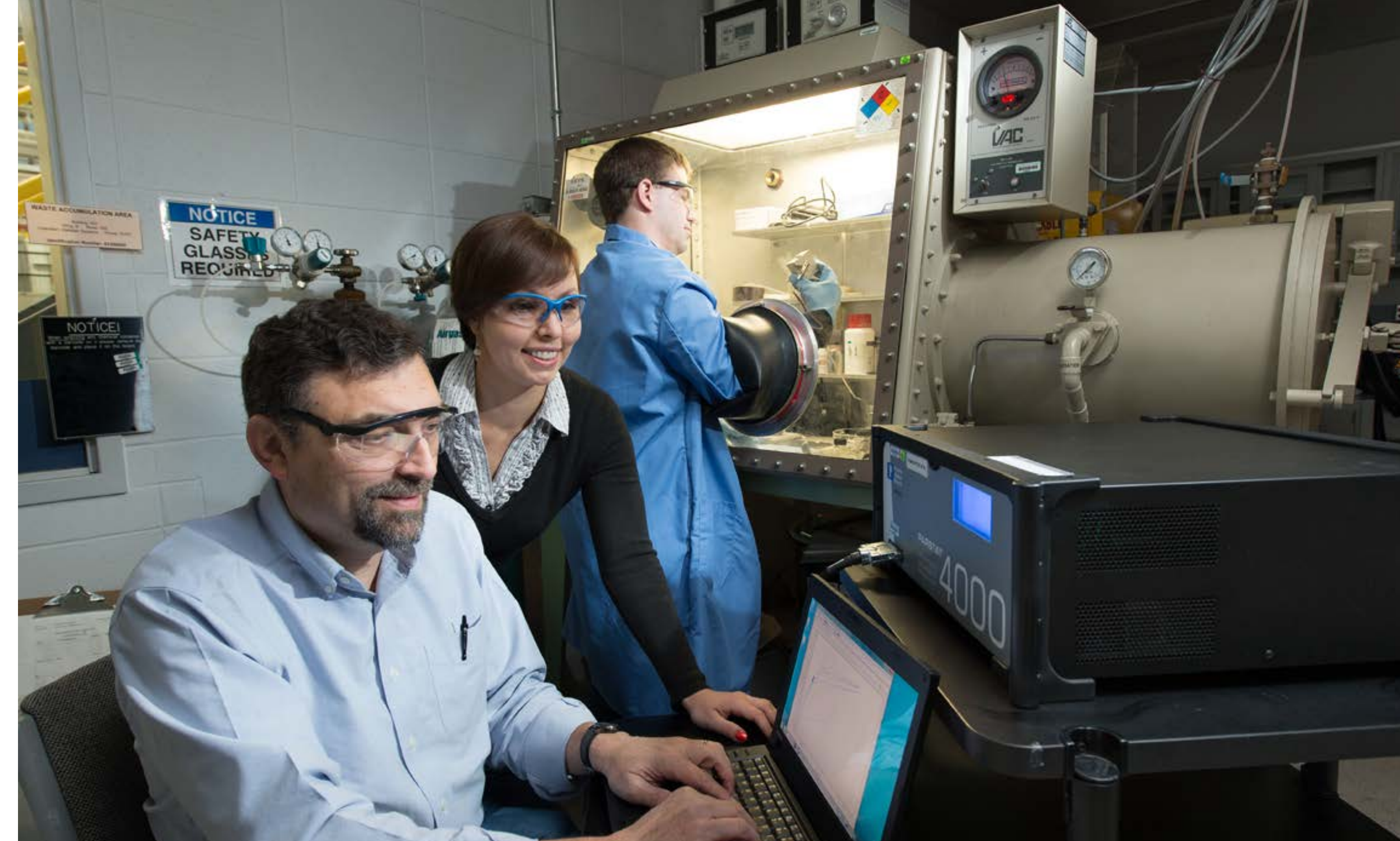
Why Is the Project Important?

The IIT–Argonne team's nanoelectrofuels research was one of 22 projects across 15 states to receive an ARPA-E RANGE (Robust Affordable Next Generation EV-Storage) grant for innovations in transformative EV energy storage. The team will use the funds to build a 1-kWh prototype scalable for electric vehicle needs.

"If the IIT–Argonne team can develop a prototype that can be recharged in the two to three minutes it takes to fill a tank of gas and have the energy density suitable for transportation applications, then the two biggest barriers to widespread vehicle electrification will have been overcome," said Ed Daniels, a deputy associate laboratory director at Argonne. "That's why this funding award is significant and this project so important and exciting."



Members of the development team in their laboratory at the Advanced Photon Source, left to right: John Katsoudas (beamline scientist, IIT), Mike Duoba (mechanical engineer, Argonne), Elena Timofeeva (assistant chemist, Argonne), Dileep Singh (materials scientist, Argonne), Chris Pelliccione (graduate student, IIT) and Carlo Segre (Duchossois Leadership Professor of Physics, IIT).



Carlo Segre and Elena Timofeeva (foreground) conduct electrochemical tests on a flow battery operated by Chris Pelliccione in the glove box behind them.

While the system lends itself to numerous industrial applications, its flexibility is especially important for electric vehicles. Today's EV designs follow their batteries' requirements, which often results in battery placement in the rear of the vehicle, reducing available cargo space in some cases by up to 40 percent. Flow batteries with nanoelectrofuel, on the other hand, can be located virtually anywhere in the vehicle and in any shape—enabling a storage tank to be placed, for example, in the safest place in case of collision.

A nanoelectrofuel-powered flow battery will significantly increase convenience and expand an EV's range—currently only 100 to 200 miles. "That's a major limitation to the widespread adoption of electric vehicles right now," says Argonne principal investigator Elena Timofeeva. "Many people aren't buying electric cars because they can't charge them at home or at a workplace, they don't have an extra few hours to wait at a charging station or their daily commutes are longer than the typical EV's range."

But with nanoelectrofuel, Timofeeva says, an EV will go up to 500 miles on a single charge. "We've demonstrated the battery at the lab scale. With this funding, we'll be able to scale it up and create a multi-cell prototype that can meet an EV's power needs."

While the research is still in its early stages, once the new technology is commercialized, says Timofeeva, "It may improve life for many people. The transportation sector represents about 27 percent of all U.S. greenhouse gas emissions. However, even with our current electric power generation mix of fossil, nuclear and renewable energy sources, it is estimated that on a 'well-to-wheel' basis, an all-electric vehicle will generate 25 percent fewer greenhouse gas emissions than a conventional gas-powered vehicle, with even lower emissions predicted as availability of renewable energy sources increases."

In addition, Timofeeva asserted, nanoelectrofuels offer great potential for stationary energy storage, including local grid leveling and renewable energy generation. "If each household or business equipped with a compact flow battery can capture and store the energy required for its daily operations at off-peak grid hours and then use it during peak hours, it will allow increasing grid efficiency, lower the cost of energy and facilitate the use of intermittent 'green' energy sources."

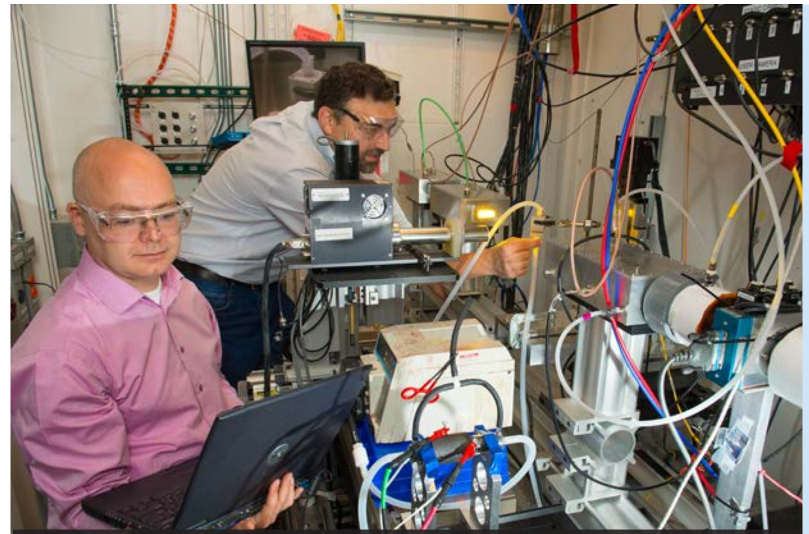
A Multidisciplinary Collaboration

IIT principal investigator Carlo Segre praised the IIT–Argonne partnership. "This project has been a close collaboration between the principal team members for the past four years. It takes advantage of our disparate expertise in electrochemistry, nanotechnology, physics and engineering. We are excited about the opportunity that the ARPA-E funding gives us to develop this potentially revolutionary technology for the market."

Building a prototype that can provide significant power output is a big challenge, involving the work of a multidisciplinary team that addresses all aspects of the technology, from nanoelectrofuel development to cell stack prototype engineering and testing. ARPA-E RANGE funding specifically supports the development of transformational electrochemical energy storage technologies that will accelerate widespread electric vehicle adoption by dramatically improving their driving range, cost, and reliability.

Team members from IIT will lead the development of a flow battery prototype that meets the program requirements and works with the specifics of nanoelectrofuels. Team members from Argonne will develop nanoelectrofuels with sufficient energy density to meet the goal.

The initial developments in nanoelectrofuels were supported by seed funding from the U.S. Department of Energy's Office of Science, a Graduate Assistantship in Areas of National Need (U.S. Department of Education) grant and internal funding from IIT.



John Katsoudas and Carlo Segre set up for an in-situ X-ray absorption spectroscopy experiment in the IIT beamline at the Advanced Photon Source.

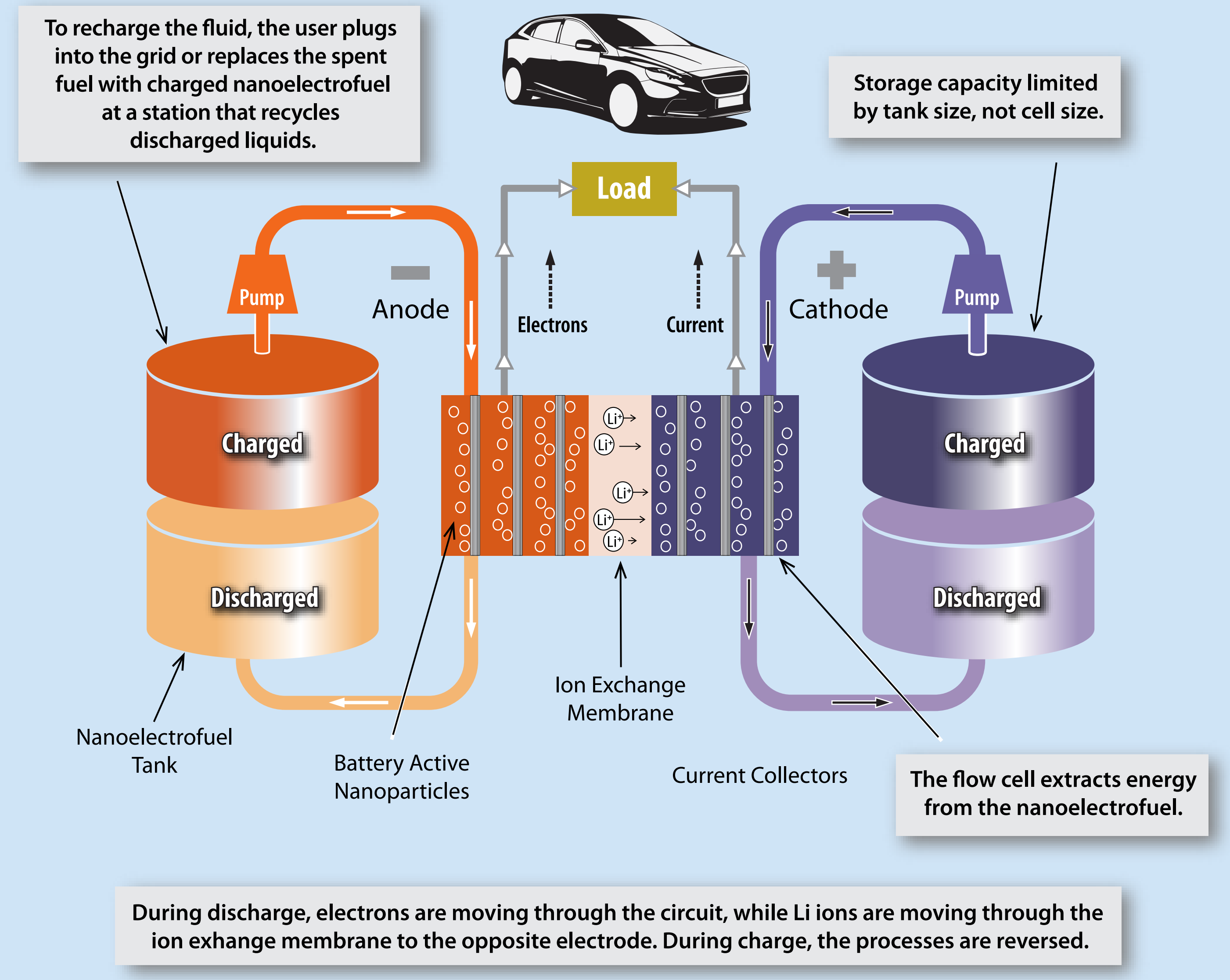
Nanofuels Exceed Critical Performance Factors for Energy Storage

Attribute	Stationary Power	Transportation	Nanoelectrofuel
Cost per kWh	Less than $100 needed	Less than $250 needed	$80
Energy density	25 – 35 Wh/kg	Up to 200 Wh/kg	Up to 600 Wh/kg

For more information, contact
Argonne Technology Development and Commercialization
partners@anl.gov
800.627.2596

Elena V. Timofeeva
etimofeeva@anl.gov

How Does the New Flow Battery Work?



In a redox flow cell, cathode and anode reactions take place in solution on the surface of inert electrodes acting as current collectors. Because the reactants flowing across the electrodes come from the containers outside the electrochemical cell, they are prevented from mixing in the electrochemical cell by the ion-selective membrane or micro-porous separator.

In such a cell, decoupling the electrochemical reactor unit from the storage unit leads to a decoupling between power and capacity, because the available power is determined by the size of the stack (surface area of the electrodes and number of unit cells), while available capacity is determined by the volume of electrolyte in the charged state. Given all the positive characteristics of redox flow batteries, they could be valuable prospects for supplying the energy storage needs of electric vehicles if their energy density can be increased. The novel nanoelectrofuels used in the IIT-Argonne flow battery enable effective charge/discharge and thus, represent a high-density rechargeable, renewable and recyclable advance that addresses the concerns associated with earlier iterations of redox flow batteries.

Contents | Next Page | Next Article

Unlocking the Door to **Better Diesel Engine Combustion** and **Emission Performance**

Argonne researchers demonstrate for the first time ever that quantum tunneling significantly affects compression-ignition engine performance

Traditional diesel engines, also known as compression-ignition engines, are a transportation mainstay. These engines compress the fuel injected into the engine's combustion chamber and auto-ignite it. This differs from spark-ignition gasoline engines, which rely on spark plugs to produce ignition.

Because diesel engines are thermally efficient, they use less fuel and tend to have longer service lives than gasoline engines. One of the bigger challenges involving diesel engines arises from the way they convert the chemical energy in fuel to useful work, which results in unwanted products called emissions. Diesel engines also generate hydrocarbon emissions due to incomplete combustion, because diesel engines typically do not burn off all their injected fuel. With increasingly stringent air quality rules taking effect in the next few years, engine manufacturers need a better understanding of how they can control the ignition process to improve emissions and diesel engine performance.

Sibendu Som and his colleagues used Argonne's MIRA supercomputer to perform the calculations needed to support their research.

Argonne researchers recently reported a revolutionary way to couple quantum effects to real world applications,* potentially unlocking new approaches to predicting diesel engine performance and emissions in the future. Fundamental to the Argonne discovery is a basic quantum mechanics principle known as *quantum tunneling*, which describes how particles overcome

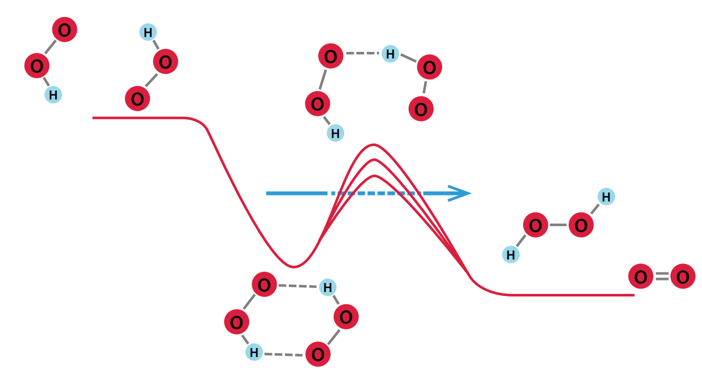
Mechanical engineer Doug Longman (right) explains to (left to right) postdoctoral appointee Yuanjiang Pei, assistant chemist Raghu Sivaramakrishnan and principal mechanical engineer Sibendu Som how the group's chemistry and modeling results will be validated using Argonne's single-cylinder Caterpillar test engine.

barriers they cannot penetrate. Scientists know that as particles attempt to penetrate an impenetrable barrier, the bouncing behavior that results from being repelled by the barrier produces a multi-particle wave that can, under the right conditions, succeed in passing through the barrier that was previously impenetrable to a single particle.

Scientists and engineers have long known that changing the fuel chemistry can influence when compression ignition occurs in a diesel engine, but they were not sure of the mechanisms involved because they did not have the tools to model and visualize what happened inside the compression chamber. Using a unique and sophisticated suite of tools that includes resources at the Advanced Photon Source, high-performance computers for simulation and modeling, and chemical analysis tools, the Argonne team—which includes Sibendu Som, Wei Liu, Gina Magnotti, Raghu Sivaramakrishnan, Douglas Longman and Michael Davis, working together with University of Colorado researchers Dingyu Zhou and Rex Skodje—have demonstrated that the quantum tunneling mechanism greatly affects the chemical reactions that control ignition timing in diesel engines. Because ignition timing greatly influences emissions, the Argonne work can potentially lead to better predictions of diesel engine emissions and performance.

According to principal investigator Sibendu Som, "Scientists and engineers have long understood in principle that quantum-scale effects likely played a role in the fuel chemistry that drives diesel engine ignition, but no one has been able to characterize the influence of that role until now. The uniquely detailed and multidimensional calculations available through the Argonne toolset, combined with the expertise of our multidisciplinary team, are what made our findings possible."

Building on earlier Argonne research into chemical reactions involving hundreds of chemical species and reactions, the team focused initially on reactions involving a blend of methyl butanoate (MB) and n-heptane as a surrogate for biodiesel fuel. They examined how they could influence the ignition process by changing rate coefficients, chemical dynamics and potential energy surface (the impenetrable barrier). Their results led them to study low-temperature chemical reactions by narrowing the temperature range studies to between 800 and 1200 Kelvin (K), the zone in which significant chemistry occurred for ignition. They chose the $HO_2 + HO_2 = H_2O_2 + O_2$ reaction because it plays a significant role in hydrogen abstraction, enabling the researchers to demonstrate how the inclusion or omission of tunneling influences ignition.



The diagram above shows the potential energy surface for the $HO_2 + HO_2 = H_2O_2 + O_2$ reaction. The height of the barrier affects engine performance, as does the quantum tunneling correction the researchers applied (dashed arrow).

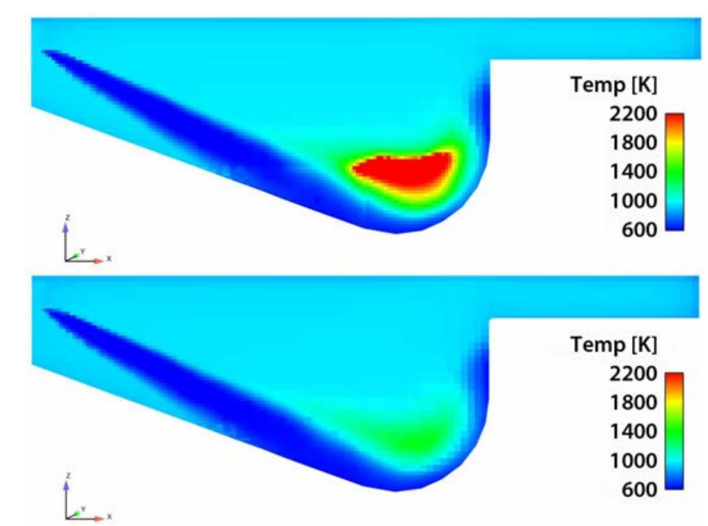
For more information, contact
Sibendu Som
ssom@anl.gov

They found that by including or not including tunneling in their simulation set-up, they were able to vary the ignition timing by up to six percent. While that might not seem like much, it is enough to greatly improve the accuracy of the ignition models used. Said Som, "We demonstrated that the accuracy of several important chemical reactions could alter our modeling of these engines. With a more accurate fuel chemistry model, we were able to see that significant chemistry begins as low as 800 K. This suggests that by accounting for the tunneling effects, we can better predict ignition and emission processes."

Going forward, the Argonne team plans to layer its models together and test hypotheses for a variety of fuels, and then validate the simulation results using the single-cylinder Caterpillar compression-ignition test engine in Argonne's Advanced Powertrain Research Facility.

*S. Som, W. Liu, D.Y. Zhou, G.M. Magnotti, R. Sivaramakrishnan, D.E. Longman, R.T. Skodje and M.J. Davis, "Quantum Tunneling Affects Engine Performance," *Journal of Physical Chemistry Letters* **4**(12): 2021–2025 (2013). Available at http://dx.doi.org/10.1021/jz400874s.

This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, and Office of Energy Efficiency and Renewable Energy.



These two images show the combustion process without (top) and with (bottom) quantum tunneling inside the combustion chamber of a diesel engine. The different colors depict the combustion temperature contours inside the combustion chamber. The red regions are higher temperatures while the bluer regions are lower temperatures.

Previous Article | Contents | Next Page | Next Article

New EV-Smart Grid Interoperability Center Facilitates Global Research Efforts

As part of a unique global research initiative, the U.S. Department of Energy recently dedicated the new Electric Vehicle (EV)-Smart Grid Interoperability Center at Argonne National Laboratory. The center at Argonne will work cooperatively with the European Interoperability Center run by the European Commission's Joint Research Centre (JRC) at facilities in Ispra, Italy, and Petten, the Netherlands. Employing common test procedures, interoperability standards and test comparisons, Argonne and JRC will work together to ensure harmonized technologies and prevent unnecessary regulatory divergence. This collaboration will not only foster and strengthen the development of the transatlantic EV market, but also will create significant employment opportunities and work on initiatives that aim to reduce the amount of energy used by the transportation sector.

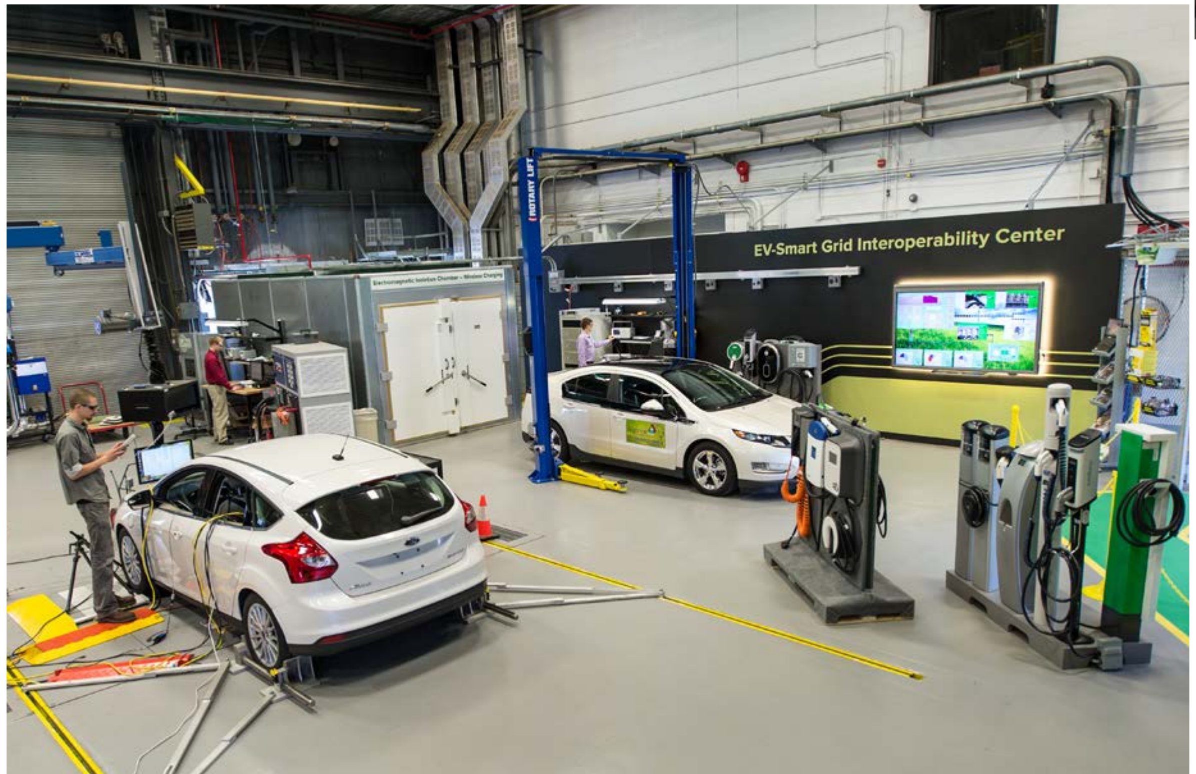
The EV-Smart Grid Interoperability Center supports coordinated initiatives under the U.S.-EU Energy Council and Transatlantic Economic Council.

Representatives from the U.S. Department of Energy (DOE), the European Commission and Argonne National Laboratory celebrated the launch of the EV-Smart Grid Interoperability Center at Argonne on July 18. Left to right: Mr. Giovanni De Santi, Director of the JRC Institute for Energy and Transport; Mr. Dominique Ristori, Director-General of the European Commission's Joint Research Centre; Dr. Phyllis Yoshida, DOE Deputy Assistant Secretary for Europe, Asia and the Americas; and Dr. Eric Isaacs, Director of Argonne National Laboratory.

Electrical engineer Jason Harper demonstrates EV Smart Grid communication concepts during the dedication event.

Left: Electrical engineer Ted Bohn explains some of the features of the wireless plug-in vehicle charging 3-axis positioning fixture and related standards development activities to attendees.

Right: Mechanical engineer Henning Lohse-Busch discusses how the Environmental Test Cell in Argonne's Advanced Powertrain Research Center will complement the work performed in the EV-Smart Grid Interoperability Center.



Below: Argonne engineers will use the capabilities of the EV Smart Grid Interoperability Center to test interoperability between electric vehicles and the grid. The Center's research advances communication technologies and protocols to manage vehicle charging loads, reduce the cost of electric vehicle charging infrastructure, improve the viability of fast/consumer-friendly charging and harmonize global connectivity standards.

For more information, contact
Keith Hardy
khardy@anl.gov

Previous Article | Contents | Next Page | Next Article

Students Gear up for Sustainability Now and in the Future

How do you harness the talents of environmentally minded undergraduate and graduate students and prepare them to tackle energy challenges at the local and regional level? That is the workforce development challenge the U.S. Department of Energy (DOE) faced when it tapped Argonne National Laboratory to develop and manage a workforce development program based on DOE's highly successful EcoCAR program that Argonne developed and manages.

Brennan Bouma, an intern with the Triangle Coalition, speaks to a member of the public at an outreach event showcasing alternative fuel vehicles.

Working with Argonne, DOE's Clean Cities program launched the Clean Cities University Workforce Development Program (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 to reduce petroleum use in transportation; it has reduced petroleum by over 5 billion gallons since it began in 1993. 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.

Argonne manages the ongoing operations of the CCUWDP program—selecting the students and offering educational development programs for career growth. The program began with 25 participants the first year and served more than 100 students in 2013. 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 coalition's stakeholders.

CCUWDP strives not only to educate students, but to provide a resource for Clean Cities coalitions as well. Many CCUWDP students have enabled coordinators to reach new goals by adding fresh skills and perspectives to the team. "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. "They've helped us achieve one of the biggest decreases in petroleum use in a U.S. Clean Cities Coalition region."

Each student works with a specific Clean Cities coalition on a portfolio of projects to reduce petroleum use, such as outreach events; meetings with local stakeholders; and websites, marketing and public relations plans. Students have helped coalitions connect with local campuses, work with local fleet managers and plan local events such as the National Alternative Fuel Vehicle Odyssey Day. Last summer, CCUWDP students helped deploy Argonne's IdleBox to entice fleet managers to adopt idle reduction campaigns in their organizations.

> They've helped us achieve **one of the biggest decreases in petroleum use** in a **U.S. Clean Cities Coalition** region.
>
> *– Carl Lisek, Coordinator for the South Shore Clean Cities Coalition in Illinois*

Interns help coalitions by expanding the number of outreach events they are capable of conducting each year. Here, Alicia Cox, past intern for Yellowstone-Teton Coalition, staffs a booth at an outreach event.

Jaime McKay, an intern for the Greater Washington Region Clean Cities Coalition, says the mix of real-life experience in alternative energy and advanced vehicle technologies, coupled with learning the skills needed to stand out in the growing alternative energy field, have made the internship an incredible experience for her. "After a year in the program, I have strengthened my resume working alongside the leaders of public- and private-sector energy efficiency and petroleum reduction programs," said Jaime. "I learned to handle myself professionally under pressure, and have emerged as an excellent candidate for future employment. All of this was made possible through the great structure and leadership of the CCUWDP."

The CCUWDP is unique in the amount and quality of experience it provides to its students. Because of the grassroots nature of the coalitions, students are involved in their day-to-day operations. For example, Mark Rabinsky, project manager at the Ann Arbor/Detroit Clean Cities Coalition, worked with CCUDWP participant Joshua Rego on a variety of projects during two semesters. "Josh has been an invaluable asset to the Detroit/Ann Arbor Clean Cities Coalition," said Mr. Rabinsky. "The new service models he worked on were valuable for the organization, and his alternative fuel market studies provided stakeholders with compelling arguments for alternative fuel adoption. Developing a sustainable procurement toolkit for fleet managers also provided Josh with an opportunity to design, manage and implement a project."

From Rego's perspective, his work with the Detroit/Ann Arbor Clean Cities Coalition offered him an unparalleled experience. "I had the freedom and support to develop, from scratch, business models that will place both coalitions on a firmer footing financially and increase operational sustainability. CCUWDP allowed me to develop skills I never knew I had, and taught me how to make sustainability a reality," Joshua said.

One unique way CCUWDP participants add value and leverage resources for DOE and the coalitions comes from partnering with EcoCAR teams on mutually beneficial initiatives and goals. CCUWDP students are designated liaisons between EcoCAR 2 teams and Clean Cities coalitions, and the teams and coalitions have partnered to host outreach events, participate in local meetings and connect with important stakeholders.

Kimberlin To (front row, third from right), intern for Dallas Fort Worth Clean Cities Coalition, helped organize a grand opening of a compressed natural gas (CNG) station in the area as part of the CNG Green Across America Road Trip.

For more information, contact

Amanda McAlpin, amcalpin@anl.gov

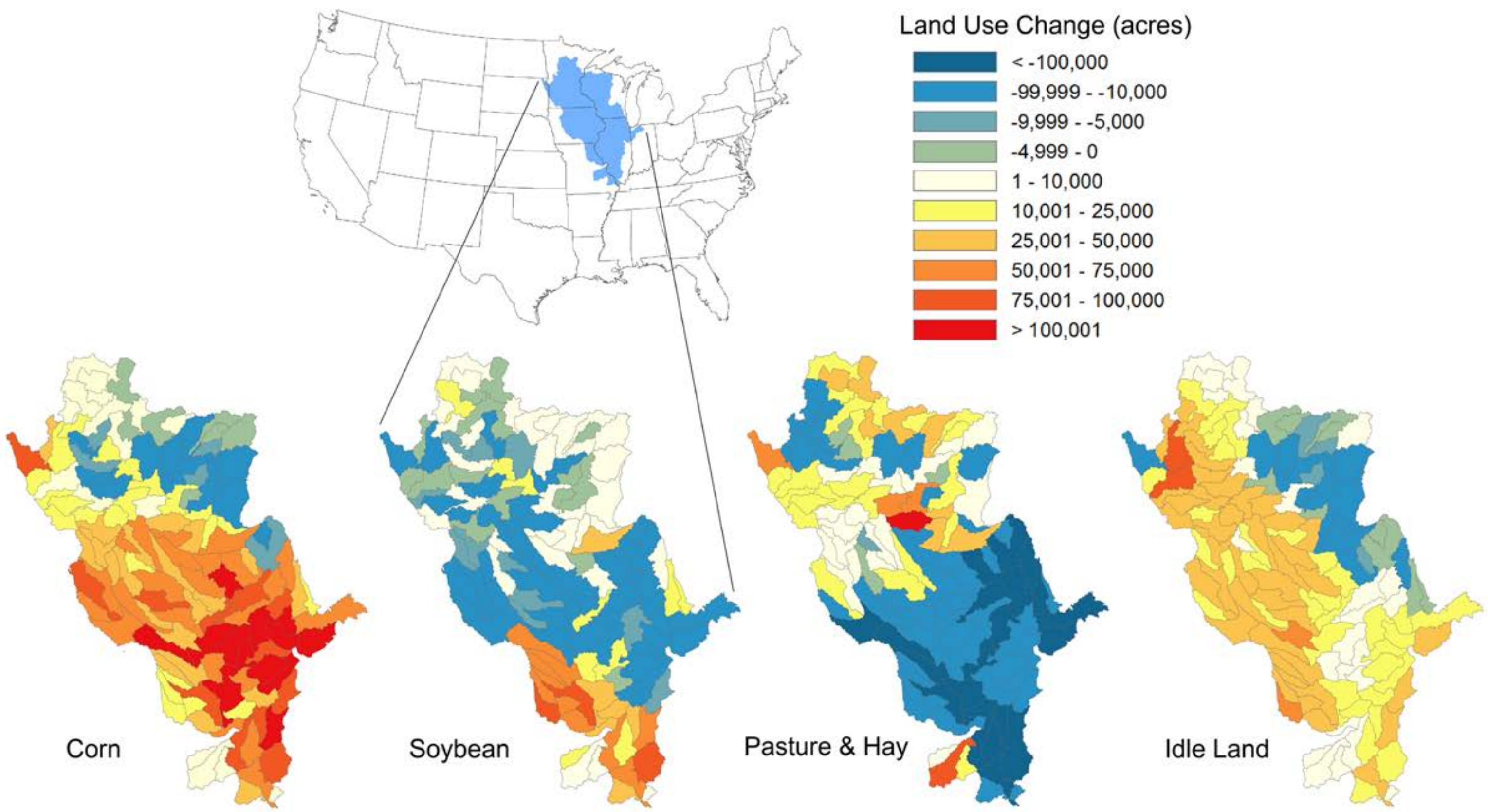
For more information on the Clean Cities University Workforce Development Program, visit the internship section on the Clean Cities website at http://www1.eere.energy.gov/cleancities/. To learn more about EcoCAR 2, visit www.ecocar2.org.

How Might **Increased Biofuel Production Affect Midwest Water Supplies?**

Fresh water is arguably the most valuable natural resource in the world. Yet when talking about the prospect of replacing fossil fuels with plant-based biofuels, discussion often centers on diminishing petroleum supplies, energy security and climate change, and not on the possible effects increased biofuel production may have on the quality and quantity of local and regional freshwater resources in areas where energy crops grow.

Led by principal environmental systems analyst May Wu of Argonne's Energy Systems Division, a team of researchers recently conducted the first investigation into how the changes in land use and agricultural practices projected by a U.S. Department of Energy report for the year 2022 (see sidebar) would affect regional water resources in the Upper Mississippi River Basin (UMRB).

In 2011, the U.S. Department of Energy published an assessment of the ability of the United States to provide energy crops sustainably, in quantities capable of supporting the greatly increased biofuel production goals mandated by the Energy Independence and Security Act of 2007 (EISA). The report concluded that the boost mandated by the EISA could be achieved by increasing crop yields, harvesting agricultural and wood residues and producing dedicated energy crops, all of which would entail land use changes in the eastern, southern and midwestern regions of the United States, including the Upper Mississippi River Basin (UMRB). This area is America's biggest producer of energy crops and will remain so for the foreseeable future. The report is available at www.eere.energy.gov/pdfs/billion_ton_update.pdf.



Meeting mandated biofuel production increases will require land use changes in midwestern counties throughout the Upper Mississippi River Basin.

The researchers used a modified version of the U.S. Department of Agriculture's/Texas A&M AgriLife Research's Soil and Water Assessment Tool (SWAT, available at http://swat.tamu.edu/), a watershed-scale hydrologic model that simulates daily or hourly hydrological and nutritional cycles as well as plant growth under varying soil, climate, land use and land management conditions. The modifications to the model permitted it to simulate practical future biomass production in the UMRB by simultaneously considering changes in land use types, implementing perennial grass (switchgrass), corn stover harvesting, fertilizer applications, tillage practices and increased corn yield for the year 2022. The researchers considered projected land use changes involving pasturelands, idle lands and lands producing corn, soybeans, wheat, hay and switchgrass.

> Whether a parcel of land produces **corn** or **switchgrass** or **is idle** affects the **quality** and **quantity** of the **water stream** in the **watershed**.

For example, whether a parcel of land produces corn or switchgrass or is idle affects the quality and quantity of the water stream in the watershed. In the case of corn, what is left after the corn harvest is corn stover, which consists of the aboveground parts of the corn stalk, except the corncob itself. Farmers usually leave corn stover behind when they harvest, but it can also be an important cellulosic biofuel feedstock. When corn stover is left on the land, it covers the soil and protects against soil erosion, but it is also a source of nitrogen that runs off into water bodies. When stover is removed completely, a portion of the nitrogen contained in the stover is also removed from the field, reducing potential nitrogen loading—but removing the stover also exposes more bare soil to the sun, which results in increased soil runoff. How much stover can be harvested sustainably for biofuel production while maintaining soil productivity and water quality? Understanding these relationships is important to meeting the EISA's goals in a sustainable manner. Said Wu, "Decreased nitrogen loading should benefit the watershed and its aquatic ecosystems, as farming methods change and as farmers adopt best management practices developed by the U.S. Department of Agriculture for improved soil and water conservation."

May Wu

Wu's team compared results of their simulation to corresponding characteristics of a baseline model developed for the UMRB for the year 2006. The study projected that the future feedstock production scenario would have a mixed effect on water quality in the UMRB, resulting in increased nutrient loading in some watersheds and decreased loading in others. Basin-wide, nitrogen loading (primarily caused by fertilizer use) would decrease, though total phosphorus and suspended sediment loadings would increase. The change is partially attributable to a land conversion to grow switchgrass in low-productivity land with poor soil quality. Switchgrass has very deep roots that trap nutrient runoff (nitrogen and phosphorus) from crop fields, and as a result, agricultural soil conservation programs have frequently employed switchgrass crops as part of their soil conservation strategies.

According to Wu, "If no effective nutrient management scheme is applied, the increased phosphorus and sediment loadings might become a major water quality concern in the region, particularly because the increased phosphorus loading may affect aquatic life region-wide: this could lead to an increase in the size of the Gulf of Mexico's low-oxygen (hypoxic) zone." Proper management of fertilizer applications played a critical role in a recent reduction of the hypoxic zone in the Gulf of Mexico, as reported by U.S. Environmental Protection Agency's Gulf Task Force in its recent report, "Reassessment 2013—Assessing Progress Made Since 2008" (available at http://water.epa.gov/type/watersheds/named/msbasin/upload/hypoxia_reassessment_508.pdf).

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

For more information, contact
May Wu
mwu@anl.gov

Previous Article | Contents | Next Page | Next Article

Penn State University Named Winner in Year Two of EcoCAR 2: Plugging In to the Future

Pennsylvania State University was named the overall Year Two winner during the EcoCAR 2 competition held May 13–23, 2013, at the General Motors (GM) Desert Proving Ground and at locations throughout San Diego, Calif. EcoCAR 2 is a collegiate Advanced Vehicle Technology Competition managed for the U.S. Department of Energy (DOE) by Argonne National Laboratory.

EcoCAR 2 teams spent the second year of this three-year competition using cutting-edge automotive engineering processes to redesign their Chevrolet Malibu vehicles. Argonne and GM engineers subjected these vehicles to extensive safety inspections and on-road evaluations, similar to those conducted on new GM vehicles. Each vehicle was evaluated on the basis of how best it achieved reduced fuel consumption and greenhouse gas emissions as well as overall performance, utility and safety.

Penn State's E85 plug-in hybrid electric vehicle impressed inspectors and other judges representing various EcoCAR 2 sponsors with its excellent performance in all the competition's dynamic events. The team's vehicle was also the first to pass safety and technical inspections and on-road safety evaluations.

The second-place team, Cal State-Los Angeles, also demonstrated excellent performance with its ethanol-fueled vehicle and was the first team to complete all the dynamic events. The Ohio State University team took third place with its series-parallel hybrid electric vehicle.

"The students competing in EcoCAR 2 are leading the way in designing and building the next generation of American-made automobiles that will reduce our dependence on oil and save families and businesses money at the pump," said David Danielson, Assistant Secretary for DOE's Office of Energy Efficiency and Renewable Energy.

The 15 university teams will now spend Year Three of the EcoCAR 2 competition perfecting their designs to near-showroom quality before the competition finals in Milford, Mich., and Washington, D.C., in June 2014. For more information on EcoCAR 2, visit www.ecocar2.org.

The Penn State EcoCAR 2 team, which won overall Year Two honors in the competition.

IdleBox Helps Reduce Vehicle Idling

The U.S. Department of Energy's Clean Cities Program is on a mission: to reduce petroleum use in vehicles. On the front lines, grassroots Clean Cities coalitions throughout the United States are accomplishing this by bringing together public and private stakeholders and encouraging them to use alternative and renewable fuels, idling reduction measures, fuel economy improvements and advanced transportation technologies.

To support the coalitions' efforts to reduce vehicle idling and help spread their message to "STOP Idling. START $aving," Argonne developed IdleBox, a suite of tools to engage and educate audiences—from top-level decision makers to fleet/operations managers and their drivers—about the impacts of vehicle idling and the benefits of idling reduction. IdleBox is currently geared to light- and medium-duty fleet vehicles with tools specific to heavy-duty vehicles, coming soon.

Argonne's groundbreaking idling reduction research has helped policymakers and fleet managers understand the drawbacks of idling. Argonne's understanding of the benefits of idling reduction enabled the creation of IdleBox; it incorporates a range of communication products that not only support existing idling reduction outreach efforts, but also help launch new campaigns, including:

- Media releases
- Outreach letters
- Educational presentations
- Idling reduction savings calculators
- Policy pledges to enlist organizational commitment
- Tip sheets, bookmarks and stickers
- Posters

STOP Idling. START $aving.

Idlebox is easy to use and components can be customized with contact information for a local Clean Cities coalition. Idlebox allows Clean Cities coalition members to "hit the ground running" so they can easily recruit members, form alliances and mobilize their coalitions to action.

To date, Clean Cities coalitions across the United States have helped the Clean Cities Program to eliminate use of more than 5 billion gallons of petroleum through alternative fuel use, fuel economy improvements, idle reduction measures and other strategies.

To get IdleBox, go to www.eere.energy.gov/cleancities/toolbox/idlebox.html. To learn more about Clean Cities, visit the Clean Cities website at www.eere.energy.gov/cleancities.

IdleBox poster, available from the Clean Cities website.

Previous Article | Contents | Next Page | Next Article

Argonne Researchers Unlock Critical Keys to Improving Lithium-Air Battery Durability and Performance

As the old saying goes, size matters, and nowhere is that truer than for electric vehicle (EV) batteries. For EVs, the crucial combination of small size and sufficient driving range depends on the energy storage capacity and power density of the battery. While today's EVs rely on lithium-ion (Li-ion) batteries, lithium-air batteries have emerged as promising alternatives for next-generation EVs, because they appear to be capable of packing even more energy into a smaller space.

The rechargeable Li-air battery, which is more accurately referred to as a lithium-oxygen (Li-O_2) battery, is attractive because of its theoretically high capacity. As with all high-capacity batteries, however, one of the biggest challenges for Li-O_2 batteries involves their stability during repeated charge-discharge cycles. Because Li-O_2 batteries depend on an electrochemical reaction with oxygen, they can experience undesirable side reactions and form byproducts that affect their long-term durability, if these side reactions are not managed effectively. Such side reactions can also cause significant deviations of charge and discharge voltages from the theoretical values, known as "overpotentials."

Chemist Di-Jia Liu inserts a "ceramic boat" containing an Fe/N/C composite sample into the tube furnace for thermolysis. The monitor behind Liu displays an image of electrode morphology as captured at the Advanced Photon Source.

For more information, contact
Di-Jia Liu, djliu@anl.gov

Researchers at Argonne National Laboratory, led by chemist Di-Jia (D.-J.) Liu, are exploring new low-cost carbon catalyst materials that could minimize side reactions and reduce undesirable overpotentials in the Li-O_2 battery's cathode. "Porous carbon functionalized by highly dispersed transition metals and nitrogen has been known to promote an oxygen reduction reaction in fuel cell applications. It occurred to us that such material may also promote the similar reactions in Li-O_2 batteries and reduce overpotentials during the discharge-charge cycle, based on the principle of micro-reversibility," theorized Liu.

To test that theory, Liu and his team developed an inexpensive, atomically dispersed iron-nitrogen-carbon (Fe/N/C) composite catalyst that they believed could improve the oxygen evolution reaction during Li-O_2 battery charging. They evaluated the catalyst's performance in a rechargeable Li-O_2 battery for the first time in early 2012, and conducted an extensive catalyst structural characterization using synchrotron X-ray absorption spectroscopy at Argonne's Advanced Photon Source (APS). The researchers successfully demonstrated the role of their composite catalyst in controlling overpotentials, particularly during the Li-O_2 battery-charging step.

Reducing overpotential during charging significantly enhances battery efficiency and lifespan by reducing or eliminating the side reactions that produce byproducts such as carbonate and carbon dioxide (CO_2) as electrolyte decomposes. According to Liu, "We have observed extended battery cycling with no CO_2 formation, suggesting that the catalyst selectively promoted the anticipated electrochemical reaction while preserving the electrolyte, which is a desirable outcome."

Citation

J.-L. Shui, N. K. Karan, M. Balasubramanian, S.-Y. Li and D.-J. Liu, "Fe/N/C Composite in Li-O_2 Battery: Studies of the Catalytic Structure and the Activity towards Oxygen Evolution Reaction," *Journal of the American Chemical Society*, **2012**, 134 (40), 16654–16661. Available at http://dx.doi.org/10.1021/ja3042993.

Research support for the work described is provided by Argonne National Laboratory's Grand Challenge program. This work and the use of the Advanced Photon Source and the Electron Microscopy Center are supported by the U. S. Department of Energy, Office of Science.

Research Results

Recent Patents and Technologies Licensed

Licensed

Broadband TelCom Power, Inc., has signed an agreement to license **Argonne-developed** software and documentation for the "Electric Vehicle and Supply Equipment Communication Controller Linux Kernel."

New Patents

"Lithium Batteries Using Poly(ethylene oxide)-based Non-aqueous Electrolytes," **Zonghai Chen** and **Khalil Amine**, United States Patent 8,475,688.

"Cathode Material for Lithium Batteries," Sang-Ho Park and **Khalil Amine**, United States Patent 8,492,030.

"Fast Cure Gel Polymer Electrolytes," **Khalil Amine** and **Zhengcheng Zhang**, United States Patent 8,492,033.

"Electrochemical Method for Producing a Biodiesel Mixture Comprising Fatty Acid Alkyl Esters and Glycerol," **YuPo J. Lin** and **Edward St. Martin**, United States Patent 8,507,229.

"Flexible Evaluator for Vehicle Propulsion Systems," **Aymeric Rousseau**, **Phillip B. Sharer** and **Sylvain Pagerit**, United States Patent 8,510,088.

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

Recent Presentations

"Development of PLZT Film-on-Foil Capacitors with High Energy Density," **B. Ma**, **M. Narayanan**, **S. Liu**, **Z. Hu** and **U. Balachandran**, Dielectrics 2013, University of Reading, Reading, UK, April 10–12, 2013.

"Can Automotive Battery Recycling Help Meet Lithium Demand?," **L. Gaines**, **J.B. Dunn** and **C. James**, American Chemical Society Annual Meeting, New Orleans, La., April 7–11, 2013.

"Energy and Environmental Impacts of Lithium Production for Automotive Batteries," **L. Gaines** and **J.B. Dunn**, American Chemical Society Annual Meeting, New Orleans, La., April 7–11, 2013.

"Towards Predictive Simulations of the Internal Combustion Engine," **S. Som**, Graduate Student seminar series at University of Connecticut, Storrs, Conn., July 11, 2013.

"A Numerical Investigation on Scalability and Grid Convergence of Internal Combustion Engine Simulations," **S. Som**, **D.E. Longman**, **S.M. Aithal**, **R. Bair**, **M. Garcia**, S.P. Quan, K.J. Richards and P.K. Senecal, SAE Paper No. 2013-01-1095, *SAE 2013 World Congress*, Detroit, Mich., April 2013.

"An Investigation of Grid Convergence for Spray Simulations Using an LES Turbulence Model," P.K. Senecal, E. Pomraning, K.J. Richards and **S. Som**, SAE Paper No. 2013-01-1083, *SAE 2013 World Congress*, Detroit, Mich., April 2013.

"Multi-dimensional Modeling and Validation of Combustion in a High-efficiency Dual-fuel Light-duty Engine," **Z. Wang**, **R. Scarcelli**, **S. Som**, **S.S. McConnell**, N. Salman, Y. Zhu, K. Hardman, K. Freeman, R.A. Reese, P.K. Senecal, M. Raju and S.D. Givler, SAE Paper No. 2013-01-1091, *SAE 2013 World Congress*, Detroit, Mich., April 2013.

"A Study of Grid Resolution and SGS Models for LES under Non-reacting Spray Conditions," **Q. Xue**, **S. Som**, P.K. Senecal and E. Pomraning, *25th Annual Conference on Liquid Atomization and Spray Systems*, Pittsburgh, Penn., May 2013.

Recent Presentations continued

"Three-dimensional Simulations of the Transient Internal Flow in a Diesel Injector: Effects of Needle Movement," **Q. Xue**, M. Battistoni, **S. Som**, **D.E. Longman**, H. Zhao, P.K. Senecal and E. Pomraning, *25th Annual Conference on Liquid Atomization and Spray Systems*, Pittsburgh, Penn., May 2013..

"Towards Accommodating Comprehensive Reaction Mechanisms for Practical Engine Simulations," M. Raju, S. Quan, M. Wang, M. Dai, P.K. Senecal, **S. Som**, M. McHenly and D.L. Flowers, *8th U.S. National Combustion Meeting*, Utah, May 2013.

"The Role of Individual Rate Coefficients in the Performance of Compression Ignition Engine Models," **W. Liu**, **S. Som**, **D.Y. Zhou**, **R. Sivaramakrishnan**, **D.E. Longman**, R.T. Skodje and **M.J. Davis**, *8th U.S. National Combustion Meeting*, Utah, May 2013.

"Comparison of Different Chemical Kinetic Models for Biodiesel Combustion," **Z. Wang, W. Liu**, **S. Som** and **D.E. Longman**, *8th U.S. National Combustion Meeting*, Utah, May 2013.

"Greenhouse Gas Emissions and Natural Gas Vehicles: The Case for Renewable Natural Gas," **M. Mintz**, **J. Han** and **M. Urgun-Demirtas**, *2013 Air & Waste Management Association Meeting*, Chicago, Ill., June 27, 2013.

"Energy Security and Greenhouse Gas Emissions of Natural Gas Heavy-Duty Commercial Trucking," **D.J. Santini**, **M.A. Rood Werpy**, **A.J. Burnham**, **J. Han**, **T. Wallner**, L. Grannis and M.D. Laughlin, *Air and Waste Management Association 106th Annual Conference and Exhibition*, June 18–25, 2013, Chicago, Ill.

Recent Publications

"Configuring a Fuel Cell Based Residential Combined Heat and Power System," **S. Ahmed**, **D.D. Papadias** and **R.K. Ahluwalia**, *Journal of Power Sources* 242, 884-894, 2013. Available at http://dx.doi.org/10.1016/j.jpowsour.2013.01.034.

"Development and Implementation of SAE DC Charging Digital Communication for Plug-in Electric Vehicle DC Charging," **J.D. Harper**, SAE Technical Paper 2013-01-1188, 2013. Available at http://dx.doi.org/10.4271/2013-01-1188.

"Efficiency and Emissions Performance of Multizone Stratified Compression Ignition Using Different Octane Fuels," **S. Ciatti**, **M. Johnson,** B.D. Adhikary, R. Reitz and A. Knock, SAE Technical Paper 2013-01-0263, 2013. Available at http://dx.doi.org/10.4271/2013-01-0263.

"Fe/N/C Composite in Li-O_2 Battery: Studies of the Catalytic Structure and the Activity towards Oxygen Evolution Reaction," **J.-L. Shui**, **N.K. Karan**, **M. Balasubramanian**, S.-Y. Li and **D.-J. Liu**, *Journal of the American Chemical Society*, 2012, 134 (40), 16654–16661. Available at http://dx.doi.org/10.1021/ja3042993.

"Quantum Tunneling Affects Engine Performance," **S. Som**, **W. Liu**, D.Y. Zhou, **G.M. Magnotti**, **R. Sivaramakrishnan**, **D.E. Longman**, R.T. Skodje and **M.J. Davis**, *Journal of Physical Chemistry Letters* 4(12): 2021–2025, 2013. Available at http://dx.doi.org/10.1021/jz400874s.

Vehicle Technologies Program Government Performance and Results Act (GPRA) Report for Fiscal Year 2014, **T.S. Stephens**, A.K. Birky and **J. Ward**, Argonne National Laboratory, ANL/ESD-13/4, Argonne, Ill., May 2013.

Non-Cost Barriers to Consumer Adoption of New Light-Duty Vehicle Technologies, **T. Stephens**, U.S. Department of Energy Transportation Energy Futures Series, 2013. Available at http://www.nrel.gov/docs/fy13osti/55639.pdf.

Vehicle Technology Deployment Pathways: An Examination of Timing and Investment Constraints, **S. Plotkin**, **T. Stephens**, and W. McManus, U.S. Department of Energy Transportation Energy Futures Series, 2013. Available at http://www.nrel.gov/docs/fy13osti/55638.pdf.

"Perfluoroalkyl-Substituted Ethylene Carbonates: Novel Electrolyte Additives for High-Voltage Lithium-ion Batteries," **Y. Zhu**, M.D. Casselman, **Y. Li**, A. Wei and **D.P. Abraham**, *Journal of Power Sources* 246, 184–191, 2013. Available at http://dx.doi.org/10.1016/j.jpowsour.2013.07.070.

"Electrolyte Additive Combinations that Enhance Performance of $Li_{1.2}Ni_{0.15}Mn_{0.55}Co_{0.1}O_2$-Graphite Lithium-ion Cells," **Y. Zhu**, **Y. Li**, **M. Bettge** and **D.P. Abraham**, *Electrochimica Acta*, 2013. Available at http://dx.doi.org/10.1016/j.electacta.2013.03.102.

"Silicon Solid Electrolyte Interphase (SEI) of Lithium Ion Battery Characterized by Microscopy and Spectroscopy," M. Nie, **D.P. Abraham**, Y. Chen, A. Bose and B. Lucht, *Journal of Physical Chemistry* C 117, 13403–13412, 2013. Available at http://dx.doi.org/10.1021/jp404155y.

Recent Publications continued

"Observation of Microstructural Evolution in Li Battery Cathode Oxide Particles by *In situ* Electron Microscopy," **D.J. Miller**, **C. Proff**, **J.G. Wen**, **D.P. Abraham** and **J. Bareño**, *Advanced Energy Materials* 3, 1098–1103, 2013. Available at http://dx.doi.org/10.1002/aenm.201300015.

"Correlating Hysteresis and Voltage Fade in Lithium- and Manganese-Rich Layered Transition-Metal Oxide Electrodes," **K.G. Gallagher**, **J.R. Croy**, **M. Balasubramanian**, **M. Bettge**, **D.P. Abraham**, **A.K. Burrell** and **M.M. Thackeray**, *Electrochemistry Communications* 33, 96–98, 2013. Available at http://dx.doi.org/10.1016/j.elecom.2013.04.022.

"Investigating Phase Transformations in $Li_{1.2}Ni_{0.15}Mn_{0.55}Co_{0.1}O_2$ Lithium-ion Battery Cathodes During High-Voltage Hold (4.5V) via Magnetic, X-Ray Diffraction and Electron Microscopy Studies," D. Mohanty, A.S. Safat, S. Kalnaus, J. Li, R.A. Meisner, E.A. Payzant, **D.P. Abraham**, D.L. Wood and C. Daniel, *Journal of Material Chemistry* A ,1, 6249–6361, 2013. Available at http://dx.doi.org/10.1039/C3TA10304H.

Economic Impact of Fuel Cell Deployment in Forklifts and for Backup Power under the American Recovery and Reinvestment Act, **M. Mintz**, C. Mertes and E. Stewart, Argonne National Laboratory, ANL/13-09, Argonne, Ill., April 2013.

"Cost Effective Annual Use and Charging Frequency for Four Different Plug-in Powertrains," **D. Santini**, **Y. Zhou**, **T. Stephens**, **A. Vyas**, **N. Kim** and **K. Gallagher**, SAE Technical Paper 2013-01-0494, April 2013. Available at http://dx.doi.org/10.4271/2013-01-0494.

"Reducing Light Duty Vehicle Fuel Consumption and Greenhouse Gas Emissions: The Combined Potential of Hybrid Technology and Behavioral Adaptation," **D. Santini** and **A. Burnham**, *SAE International Journal of Alternative Powertrains* 2(2):314–324, 2013. Available at http://dx.doi.org/10.4271/2013-01-1282.

"Analysis of Input Power, Energy Availability, and Efficiency during Deceleration for X-EV Vehicles," **E.M. Rask**, **H. Lohse-Busch** and **D. Santini**, *SAE International Journal of Alternative Powertrains* 2(2):350–361, 2013. Available at http://dx.doi.org/10.4271/2013-01-1473.

"Gasoline Prices, Vehicle Spending and National Employment: Vector Error Correction Estimates Implying a Structurally Adapting, Integrated System, 1949-2011," **D.J. Santini** and **D.A. Poyer**, presented at the 32nd U.S. and International Associations for Energy Economics North American Conference, July 28–31, 2013, Anchorage, Alaska.

"Dialectric Behavior of Lead Lanthanum Zirconate Titanate Thin Films Deposited on Different Electrodes/Substrates," **S. Tong**, **B. Ma**, **M. Narayanan**, **S. Liu**, **U. Balachandran** and D. Shi, *Materials Letters* 106, 405–408, 2013. Available at http://dx.doi.org/10.1016/j.matlet.2013.05.068.

"Development of Film-on-Foil Ceramic Dielectrics for Embedded Capacitors for Power Inverters in Electric Drive Vehicles," **U. Balachandran**, **M. Narayanan**, **S. Liu** and **B. Ma**, *Japanese Journal of Applied Physics* 52, 05DA10, 2013. Available at http://dx.doi.org/10.7567/JJAP.52.05DA10.

"Residual Stress of $(Pb_{0.92}La_{0.08})(Zr_{0.52}Ti_{0.48})O_3$ Films Grown by a Sol–gel Process," **B. Ma**, **S. Liu**, **S. Tong**, **M. Narayanan**, **R.E. Koritala**, **Z. Hu** and **U. Balachandran**, *Smart Materials and Structures* 22(5), 055019, 2013. Available at http://dx.doi.org/10.1088/0964-1726/22/5/055019.

"Temperature-dependent Dielectric Nonlinearity of Relaxor Ferroelectric $Pb_{0.92}La_{0.08}Zr_{0.52}Ti_{0.48}O_3$ Thin Films," **B. Ma**, **Z. Hu**, **S. Liu**, **S. Tong**, **M. Narayanan**, **R.E. Koritala** and **U. Balachandran**, *Applied Physics Letters* 102, 202901, 2013. Available at http://dx.doi.org/10.1063/1.4807665.

"Development of PLZT Film-on-Foil Capacitors with High Energy Density," **B. Ma**, **M. Narayanan**, **S. Liu**, **Z. Hu** and **U. Balachandran**, Institute of Physics (IOP) *Proceedings for Dielectrics 2013*, University of Reading, Reading, UK, April 10–12, 2013.

"Energy Security and Greenhouse Gas Emissions of Natural Gas Heavy-Duty Commercial Trucking," **D.J. Santini**, **M.A. Rood Werpy**, **A.J. Burnham**, **J. Han**, **T. Wallner**, L. Grannis and M.D. Laughlin, Paper #13680, *Air and Waste Management Association 106th Annual Conference and Exhibition*, June 18–25, 2013, Chicago, Ill.

"Case Study–Liquefied Natural Gas," **A. Burnham**, Argonne National Laboratory, fact sheet, 2013.

Visit our website to obtain more information about these papers and presentations:

http://www.transportation.anl.gov/publications/papers_presentations.html

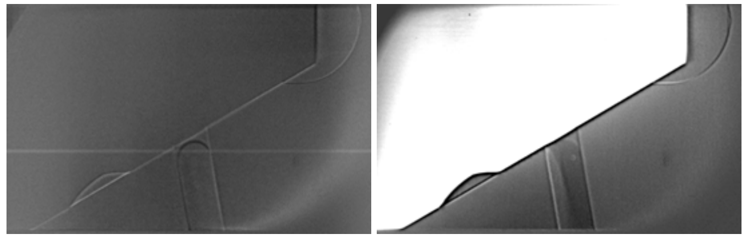
Roundup

First Measurements of Cavitation in Operating Fuel Injectors

Argonne scientists have employed the Advanced Photon Source to make the first-ever measurements of cavitation in operating fuel injectors. This development may enable the design of injectors capable of withstanding higher pressures and suitable for the lifetime of the engine. Using X-rays that can penetrate through the steel injector, high-speed images of cavitation bubbles have been captured inside production diesel injectors. This capability represents a significant advance in cavitation research; until now, simulations of cavitation could only be tested against data acquired in plastic nozzles at lower pressures. These *in situ* data allow cavitation models to be tested at engine-relevant conditions, and will lead to a better understanding of cavitation in fuel injectors.

This work is funded by the U.S. Department of Energy, Energy Efficiency and Renewable Energy, Vehicle Technologies Office under the sponsorship of Gupreet Singh.

For more information, contact Chris Powell, powell@anl.gov.



The image on the left shows the injector geometry without fuel flow. The image on the right shows cavitation as a lighter grey region in the lower middle of the image.

In-depth Testing Provides Comprehensive Data on Vehicles and Components

On any given day in Argonne's Advanced Powertrain Research Facility, advanced vehicles and their components undergo what is known as "Level 2," or in-depth testing and benchmarking. For this type of testing, researchers and technicians install significant, and often invasive instrumentation on the vehicles—including torque sensors, power analyzers and thermocouples—to collect a very comprehensive set of data that will enable a more complete understanding of powertrain system operation. Testing is being performed on advanced gasoline engine vehicles with standard transmissions, as well as on alternative-fueled vehicles and vehicles with electric powertrains.

Compared to the standard "Level 1" vehicle-level benchmark research, this in-depth approach provides an extensive vehicle performance assessment, including detailed component-level efficiencies and operating behavior across a range of conditions and driving profiles. These data will be used to validate vehicle performance estimates, inform the creation of vehicle standards in the United States and help benchmark new transportation technologies. An independent evaluation of the state-of-the-art technologies generates data to support performance and cost target development and hardware/model validation.

Argonne's unbiased testing is carried out in collaboration with companies and organizations representing the various phases of advanced vehicle development, including the U.S. Department of Energy (DOE), SAE International, the United States Council for Automotive Research, DOE's Advanced Vehicle Testing and Evaluation project, Chrysler Group LLC, General Motors Company, Ford Motor Company and many other automotive manufacturers and component suppliers.

Argonne disseminates these data to its collaborators, academia, other national laboratories and universities. Selected data and analyses are also provided on Argonne's Downloadable Dynamometer Database (D3) website at http://www.transportation.anl.gov/D3/index.html.

Vehicles tested recently include the 2010 Toyota Prius, 2012 Hyundai Sonata, 2012 Chevrolet Volt, 2012 Ford Focus BEV (battery electric vehicle) and 2013 Peugot 3008 Hybrid 4; the Honda Accord plug-in hybrid electric vehicle will be tested in the near future.

Argonne will continue its in-depth benchmarking of state-of-the-art vehicles for integration into DOE planning, target-setting, modeling/simulation development and standards development activities.

DOE's Energy Efficiency and Renewable Energy, Office of Vehicle Technologies, funds this work under the sponsorship of Lee Slezak.

For more information, contact Eric Rask, erask@anl.gov.

In addition to a dynamometer, the equipment required to perform Level 2 testing is costly and requires unique expertise to configure and use. In this case, the testing equipment takes up almost all of the back seat area as well as a cart outside the car. Because it's portable, though, it can be moved from vehicle to vehicle.

VISION estimates the potential energy use, oil use, and carbon emission impacts of advanced light- and heavy-duty highway vehicle technologies and alternative fuels to the year 2100.

New VISION Model Brings Powerful Impacts Analysis to the Desktop

Argonne National Laboratory recently released the 2013 update to the U.S. Department of Energy's VISION model, which estimates the potential energy use, oil use and carbon emission impacts of advanced light- and heavy-duty highway vehicle technologies and alternative fuels to the year 2100.

A Microsoft Excel spreadsheet-based model, VISION applies vehicle survival and age-dependent usage characteristics to project total light and heavy vehicle stock, total vehicle miles of travel (VMT), and total energy use by technology and fuel type by year, given market penetration and vehicle energy efficiency assumptions developed exogenously. VISION also estimates total carbon emissions for on-highway vehicles by year. Updates in this newest release include:

- The VISION 2013 Annual Energy Outlook (AEO) Base Case incorporates greenhouse gas (GHG) and upstream energy rates from GREET1_2012_rev2.
- The historical stock and VMT of light-, medium- and heavy-duty trucks now reflect the changes in the Federal Highway Administration Highway Statistics Table VM-1.

Government agencies, research institutes, universities and consulting companies all use the VISION model; for example, the National Petroleum Council and National Academies have used the VISION model in recent scenario studies.

VISION is available for download at http://www.transportation.anl.gov/modeling_simulation/VISION/index.html.

Previous Article | Contents | Next Page | Next Article

Fastrax

GM Recognizes and Supports Additional Development of Argonne's Autonomie Software

In a letter to the U.S. Department of Energy (DOE), General Motors expressed its appreciation for the development of **Argonne's Autonomie** and supported further development of the software to expand the tool capabilities for Model-Based System Engineering. In its letter, GM said Autonomie "…has enabled GM to quickly and efficiently create system simulation models." This includes GM's compiled production-embedded controller code (SIL), which allows the company to build a virtual hardware-in-the-loop (HIL) capability that is being used for control algorithm development; and performance studies and robustness analysis, which encompasses the effects of parameter variation due to manufacturing tolerances, environmental conditions and aging. Autonomie is now part of GM's formal vehicle development process and is deployed to hundreds of engineers in this area. GM said of Autonomie's benefits, "While is it very difficult to properly estimate the true cost savings generated by Autonomie, we are seeing significant time saving on numerous projects. For example, costly hardware testing is now being replaced by virtual processes. Before using Autonomie, the process to manually integrate the controls software with the hardware models took two or more weeks. Now, it takes seconds to minutes to accomplish. Considering that these processes are repeated on a regular basis throughout GM, the gain of time and consequently money is certainly considerable."

Department of Energy Recognizes Argonne Research Trio

Argonne Distinguished Fellow **Khalil Amine**, Senior Scientist **Michael Wang** and Principal Energy Systems Analyst **Amgad Elgowainy** were recently recognized by the U.S. Department of Energy's Vehicle Technologies Office (VTO) and Fuel Cell Technology Office (FCTO) with 2013 DOE VTO/FCTO R&D Awards for their extraordinary contributions toward the advancement of energy-efficient vehicles.

Amine, of the Chemical Sciences and Engineering Division, was recognized for his "discovery of new materials for next-generation, breakthrough battery technologies for automotive applications," while Wang and Elgowainy of the Energy Systems Division were jointly honored for their "outstanding contributions to life cycle assessment of alternative fuel vehicles." The awards were announced at the Annual Merit Review of the VTO and FCTO programs in Arlington, Virginia.


Khalil Amine


Michael Wang

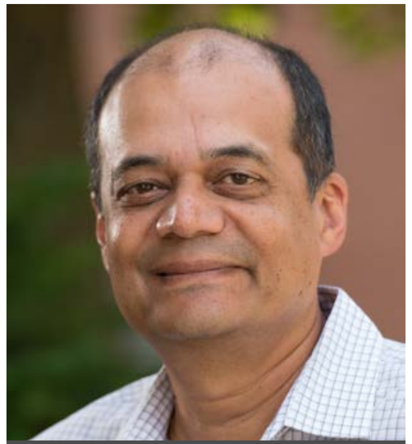

Amgad Elgowainy

Singh Receives Prestigious Lee Hsun Award

Dr. Dileep Singh, Materials Scientist in Argonne's Nuclear Engineering Division, received the 2013 Lee Hsun Award from the Chinese Academy of Sciences-Institute of Metals Research in Shenyang, China. The award honors individuals who have made outstanding contributions to the field of materials science and engineering. Dr. Singh was recognized for his sustained innovative work in the field of materials science that has resulted in technologies with commercial impact.

Dr. Singh is a Fellow of the ACerS and an Academician of the World Academy of Ceramics, Italy. He has authored/co-authored more than 150 papers, holds 17 U.S. and international patents, and has edited several conference proceedings. He is a recipient of two R&D 100 awards, an American Society of Materials Visiting Lecturer Award and a Federal Laboratory Consortium Award for Technology Transfer. He is a past chair of the Engineering Ceramics Division and serves as an associate editor of the International Journal of Applied Ceramic Technology.

Singh leads the Thermal Management efforts at Argonne's Center for Transportation Research. He and his group investigate innovative technologies for improving the cooling in heavy-duty truck engines and power electronics used in hybrid electric vehicles. Using multifunctional nanoparticles, he is working on the development of heat transfer fluids with enhanced thermo-physical properties for concentrated solar power (CSP), power plant cooling and power electronics applications. In addition, he is involved in the development of high-efficiency thermal energy storage systems for CSP and vehicle systems. Singh's nanofluids research contributed to the new flow battery starting on on page 4 of this issue of *TransForum*.


Dileep Singh

Abraham Receives Outstanding Postdoctoral Supervisor Award

Battery researcher **Daniel Abraham** of the Chemical Sciences and Engineering Division was named one of two 2013 Outstanding Postdoctoral Supervisors by the Argonne's Postdoctoral Programs Office. The award recognizes exceptional work in the supervision of postdoctoral employees and in developing the next generation of scientists and engineers.

Recipients of the Outstanding Postdoctoral Supervisor Award promote and create work environments that encourage and boost scientific curiosity, continuously fuel individual passions toward scientific ideas, hold high standards for scientific performance, advocate and provide additional opportunities for postdocs inside and outside of the lab and encourage and provide opportunities for the development of both technical and professional skills that support the advancement of early career scientists and engineers.

Abraham joined Argonne in 1994. He has served as a materials scientist and team leader for the Advanced Battery Research for Transportation program since 2001.


Daniel Abraham

Media Highlights

***BBC Future:* Research Highlights from Argonne's Advanced Powertrain Research Facility.** Reporter Jon Stewart of the BBC visited Argonne in August and reported on several stories from the Advanced Powertrain Research Center, "How X-ray Vision Will Fuel Better Car Engines," "The Lab Pushing Petrol Car Engines to New Extremes" and "Electric Vehicles: A Universal Plug for All Models?" **Chris Powell**, **Steve Ciatti**, **Jason Harper** and **Keith Hardy** were among those interviewed (photos at right). The in-depth video features are available at http://tinyurl.com/oqlgxys.

Chris Powell

Steve Ciatti

***Google+:* Argonne Virtual Field Trip on Vehicle Electrification.** Argonne researchers **Henning Lohse-Busch**, **Lynn Trahey** and **Kris Pupek** recently presented a "virtual video field trip" on Google+ for students from Carl Schurz and Niles North High Schools in Illinois (photos at left). The interactive tour and question-and-answer session demonstrated how the Internet can bring students and scientists together to advance science education. Watch the video at http://tinyurl.com/p8thze5.

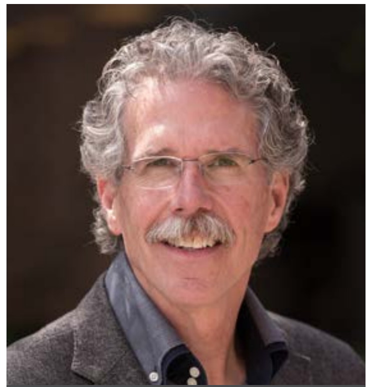
Henning Lohse-Busch

Lynn Trahey

Kris Pupek

Top left: Henning Lohse-Bush, and left to right: Lynn Trahey and Kris Pupek were presenters during Argonne's recent Google+ virtual field trip on Vehicle Electrification.

Jason Harper



Keith Hardy

***CBS News:* Powering the Future.** Argonne battery researchers **Jeffrey Chamberlain**, **Christopher Johnson** and **Michael Thackeray** were featured in recent CBS News videos about "Powering the Future" (photos at right). Chamberlain spoke about "Liquid Battery Possibilities," Johnson's topic was the "Future of Batteries is in Air, Liquids or Both" and Thackeray discussed "Batteries after Lithium ion." Watch the videos at http://tinyurl.com/lemem5z.

Jeff Chamberlain

***Crain's Chicago Business:* Chupas Named One of 2013's "40 under 40."** Chemist and battery researcher **Pete Chupas** of Argonne's X-ray Science Division was named as one of Crain's Chicago Business' "40 under 40" for 2013 (photo at left). Chupas became Argonne's youngest group leader four years ago after finding a faster way to study noncrystalline materials at the molecular level. Crystalline materials are relatively easy to examine because their molecules line up and repeat themselves, but the vast majority of materials are noncrystalline, requiring higher resolution to be viewed at the molecular level using techniques he developed. Watch an interview with Chupas at http://tinyurl.com/k8dhggq.

Pete Chupas

Christopher Johnson

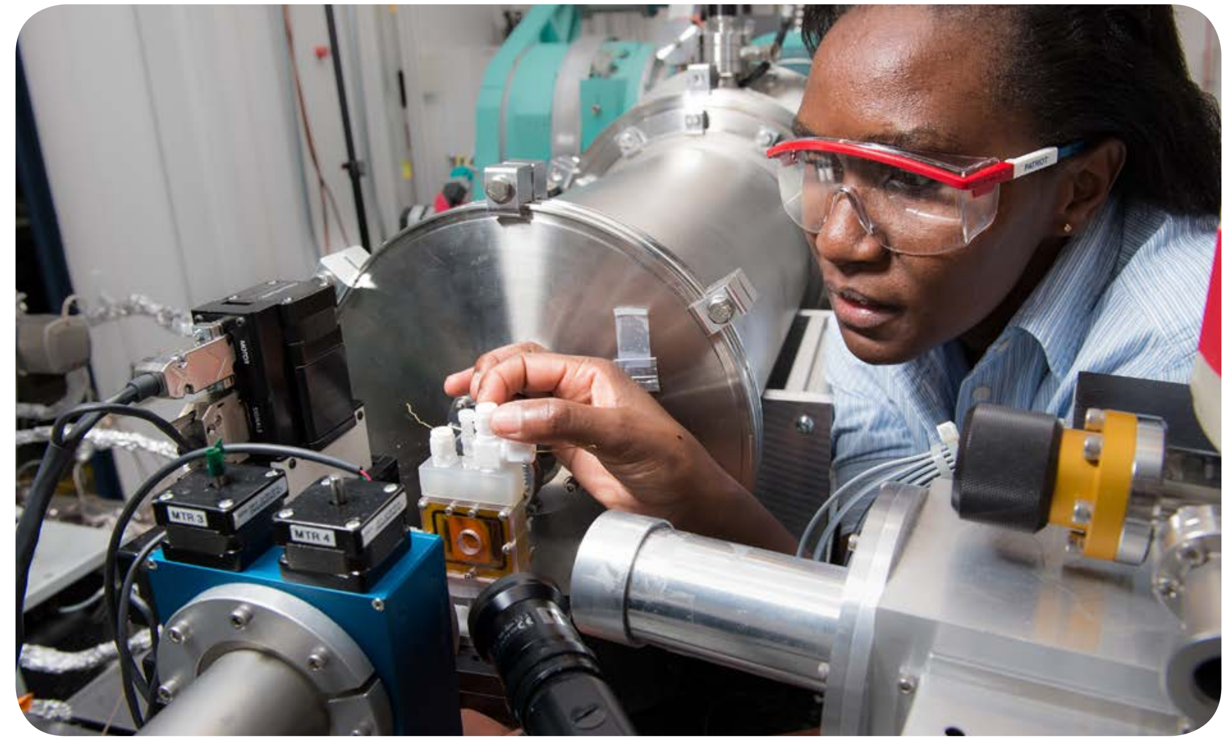
Michael Thackeray

For complete Argonne transportation research press coverage, visit http://www.transportation.anl.gov/media_center/press_coverage.html.

Parting Shots

By day, Mike Kern is an engineer in Argonne's Advanced Powertrain Research Facility, working to conserve energy use in advanced vehicles by configuring them to burn less fuel. During his time away from the lab, Kern is also crew chief for a top fuel dragster team in the National Hot Rod Association, the premier drag racing organization in North America. There, he says, his job is to burn as much fuel as you can to make as much power as you can. Kern says that there are benefits to working both of these jobs: what he learns running cars at the track, he brings back to Argonne and uses in his work there, and some ideas he learns at Argonne he applies to the race cars for which he's responsible.

U.S. Senator Dick Durbin (D-Ill.) joined Argonne staff to celebrate the dedication of MIRA, the lab's newest supercomputer. Along with other computing resources in Argonne's Leadership Computing Facility, MIRA is used for a wide range of transportation-related modeling and simulation research. MIRA is an IBM Blue Gene/Q system consisting of 48 racks of computers and 786,432 processors. It has 768 terabytes of memory and is capable of 10 quadrillion calculations per second.

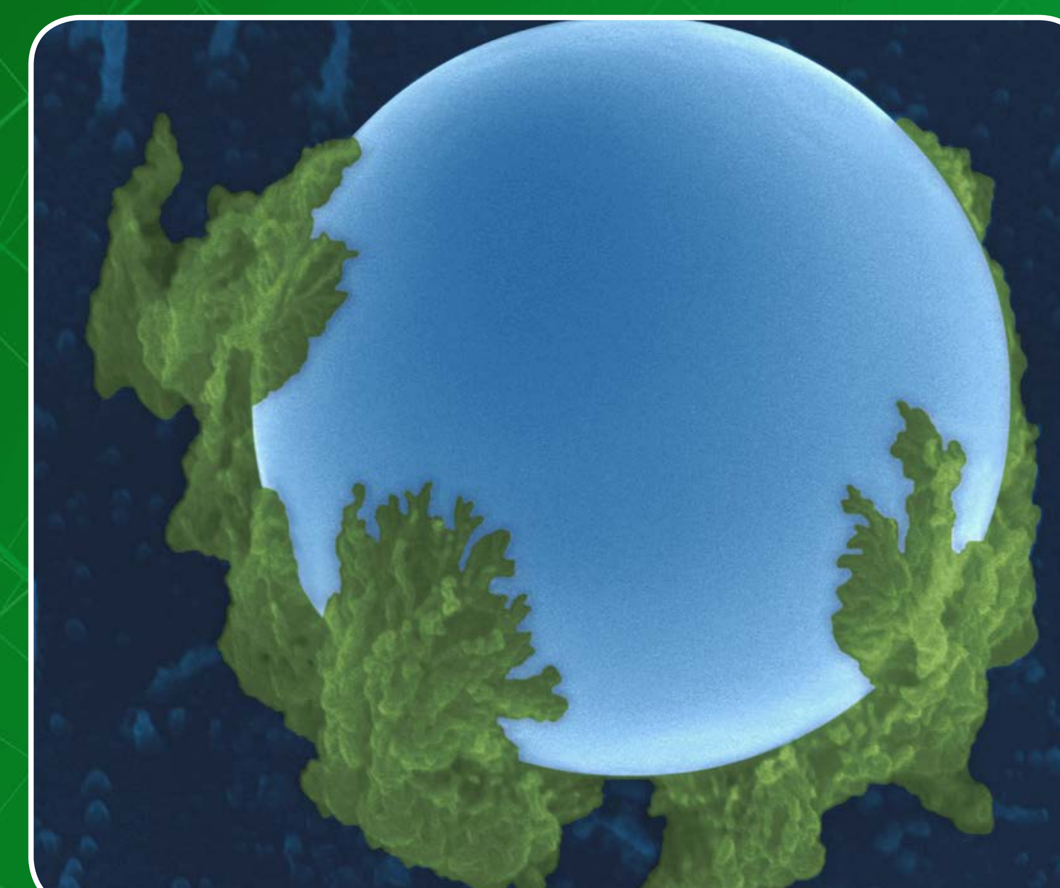


Chemist Nancy Kariuki prepares an x-ray experiment involving a nanoparticle catalyst electrode at the Advanced Photon Source, as part of ongoing research into degradation mechanisms affecting electrocatalysts for fuel cell applications.

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

Titled "Genesis" or "Element Planet," this electron microscope photograph recently won 2nd place in Argonne's 2013 Art of Science contest. It depicts the emergence of silicon nano strands (green) from an indium droplet (blue) during a plasma-assisted physical vapor deposition growth process. In the process, a thin indium film is deposited on a silicon surface. At 190°C, the indium film self-organizes into a seed layer of molten droplets, each receiving atomic silicon from a magnetron sputtering source. Silicon nano strands, with diameters as small as 5 nm, rapidly emerge from each droplet. These strands form a single loose bundle, eventually consolidating to form aligned nanowires. The aligned arrays of silicon nanowires can be used as electrodes in high-power lithium–ion batteries for transportation applications.

Credit: Argonne materials scientist Daniel Abraham and postdoctoral scientist Martin Bettge.



Previous Article | Contents | Next Page | Next Article

Argonne NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, IL 60439

Non-Profit Organization
U.S. Postage Paid
Lemont, IL
Permit No. 87

WORKING WITH ARGONNE

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.

Technology Development and Commercialization
Argonne National Laboratory, Bldg. 201
9700 South Cass Avenue, Argonne, IL 60439
800.627.2596
partners@anl.gov
www.anl.gov/techtransfer

www.transportation.anl.gov

Scan with any barcode reader on your smartphone.

TransForum ▸▸ Volume 14, No. 1, Winter 2014
ISSN 2156-3594 (print)
ISSN 2156-373X (online)

Managing Editor: Renée M. Nault
Primary Contributor: Suzanne Williams
Contributors: Dana Bubonovich, Vic Comello, Imelda Francis, Kathryn Jandeska, Louise Lerner, Amanda McAlpin and Mitch Romanowski
Designer: Cindi Andersen
Photographers: Wes Agresta and Mark Lopez
Copy Editor: Andrea Manning
Production: Gary Weidner

TransForum is published by the Transportation Technology R&D Center, Argonne National Laboratory. Publishing support services are provided by Argonne's Communication, Education and Public Affairs Division.

Renée M. Nault
TransForum
Argonne National Laboratory
9700 South Cass Avenue, Bldg. 208
Argonne, IL 60439-4815
630.252.6064
rmnault@anl.gov

U.S. DEPARTMENT OF ENERGY

Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

Previous Article | Contents | Cover