

Money and Time page 4

Argonne researchers are revolutionizing the world of combustion engine design with their groundbreaking three-dimensional, high-fidelity combustion engine simulations and visualizations.

Advanced Redox Shuttle Additive Prevents Overcharge in Lithium-ion Batteries page 8

Award-winning electrolyte additive prevents overcharging by electrochemically "locking in" a maximum voltage.

Principal engineer Sibendu Som of Argonne's Virtual Engine Research Institute and Fuels Initiative reviews a five-hole injector diesel engine visualization conducted with high-performance computing tools at the Argonne Leadership Computing Facility.

Shown here

Som and senior computational scientist Raymond Bair discuss the details of the largest-ever diesel-engine combustion simulation conducted using Argonne's high-performance computing tools.

Ensuring safe shipment of hazardous materials is easier than ever with Argonne's "Watchful Guardian" RFID tracking technology.

14 DOE Awards Go to Argonne Researchers

Larry Johnson, Ted Bohn, Rajesh Ahluwalia and Vojislav Stamenkovic receive honors from DOE's Vehicle Technologies Office and Fuel Cell Technologies Office.

- **15** Research Results
- **18** Roundup
- **20** Fastrax
- **22** Parting Shots
- **24** Working with Argonne



VERIFI Shrinks Combustion Engine Development Cycles to Save Money and Time

Big challenges loom in the combustion engine development world. Between stringent new fuel efficiency and emissions rules taking effect in the next few years and the reality that future combustion improvements will likely be incremental, most experts agree that the old-school design tools will not take us over the finish line. As a result, engine manufacturers are looking for the edge that will enable them to leapfrog their competition and create engines that can meet the challenges ahead.

Principal mechanical engineer Sibendu Som (left) and senior computational scientist Ray Bair (right) discuss combustion engine simulations conducted by researchers at the Virtual Engine Research Institute and Fuels Initiative (VERIFI).

VERIFI SAVES MONEY AND TIME

Addressing the urgent need to shrink the combustion engine development cycle, Argonne National Laboratory recently announced VERIFI—the Virtual Engine Research Institute and Fuels Initiative—a unique collaborative effort that pairs an unequaled multidisciplinary team of experts in high-performance computing, fuel chemistry, combustion science and engine performance with some of the world's fastest supercomputers, most diverse engine labs and world's brightest X-ray beams.

VERIFI's multidisciplinary approach offers a "dream team" environment in which to answer complex engine questions, narrow uncertainties associated with those answers and shrink development timescales, at a lower cost than designing and building a lab full of prototype engines.

Building on earlier groundbreaking Argonne research, VERIFI researchers consider parameters such as the relationships the resulting influence on engine performance and emission

between the fuel injector and the dynamics of the fuel spray and

A computer-generated visualization shows the multidimensional flow inside the fuel injector sac and the orifice of a multi-hole diesel fuel injector, which accounts for injector needle lift and wobbling. Such visualizations reveal plumeto-plume variations in spray velocity and the two-phase nature of fuel flow.

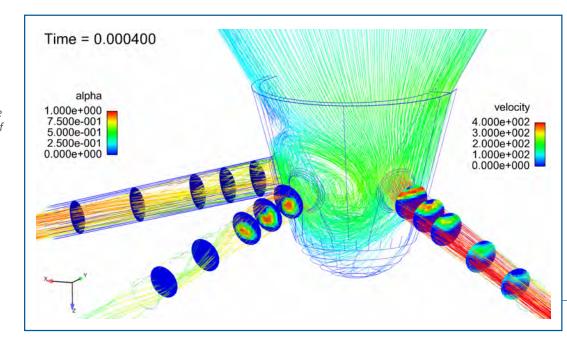
characteristics. "There are lots of parameters and processes that can be optimized to gain better engine performance," said principal mechanical engineer Sibendu Som of Argonne's Energy Systems division. "We are developing advanced simulation techniques to better predict these engine processes."

With a better understanding of how parameters interact, researchers can envision paths to cleaner and more efficient engines. The results will enable combustion engine manufacturers to reduce the expense of prototyping and cut years from their product development cycles.

According to Som, "What's unique about VERIFI is the way we've refined the tools to create engine simulations that are more reliable and then how we've applied high-performance computing resources to run simulations faster and more intensively than ever before." With these advances, VERIFI researchers can identify the most important engine and fuel parameters and develop unique engine simulations and analyses to optimize engine combustion at any operating condition. In the near future, the VERIFI team plans to run diesel engine simulations of unprecedented scale on Mira, Argonne's 10-petaflop IBM Blue Gene/Q supercomputer.

Learn more about VERIFI and see videos of VERIFI simulations at http://verifi.anl.gov.

Funding for this work is provided by DOE's Office of Energy Efficiency and Renewable Energy, Vehicle Technologies Office and the Office of Basic Energy Sciences within DOE's Office of Science.





Sibendu Som (far left) discusses how VERIFI research results will be applied in engine tests with (left to right) postdoctoral appointee Yuanjiang Pei, assistant chemist Raghu Sivaramakrishnan and section manager Doug Longman.



VERIFI Researchers Win **HPC Innovation Excellence Award**

International Data Corporation (IDC) announced in June that VERIFI researchers won a 2014 High Performance Computing (HPC) Innovation Excellence Award. The announcement was made at the 2014 International Supercomputing Conference in Leipzig, Germany.

The award recognized the VERIFI team for its work with a heavy-duty equipment manufacturer and Convergent Science, Inc., to conduct one of the largest internal combustion engine simulations ever. Predictive internal combustion engine simulations necessitate the use of models with very fine spatial and temporal resolutions; high fidelity; and robust two-phase flow, spray,

turbulence, combustion and emissions. The research has allowed the manufacturer to shrink its development timescales, resulting in significant cost savings.

The HPC Innovation Excellence Award recognizes noteworthy achievements by users of HPC technologies. The program's main goals are to showcase return on investment and scientific success stories involving HPC; to help other users better understand the benefits of adopting HPC and justify HPC investments, especially for small and medium-size businesses: to demonstrate the value of HPC to funding bodies and politicians; and to expand public support for increased HPC investments.

For more information, contact Doug Longman, dlongman@anl.gov or Sibendu Som, ssom@anl.gov

Advanced Redox Shuttle Additive Prevents Overcharge in Lithium-ion Batteries

Without adequate protection, overcharging a lithium-ion battery can lead to all kinds of problems, especially in electric vehicles. Perhaps the most significant of these is the risk that a sudden increase in the voltage leads to a rapid increase in temperature in a phenomenon called "thermal runaway," which can start fires.

In order to make sure this doesn't happen, lithium-ion battery manufacturers have built in electronic safeguards designed to shut down overcharging before it begins. But an Argonne research group led by chemist Zhengcheng (John) Zhang has developed a chemical solution to the problem as well.

Winner of a 2014 R&D 100 Award

Known as a redox shuttle additive, the chemical is added to the battery's electrolyte—the material that separates the two electrodes. The redox shuttle additive prevents overcharging by electrochemically "locking in" a maximum voltage that is dependent on the chemical structure of the additive and the nature of the battery material.

"It's an excellent backup system," Zhang said. "Even without the electronic system, the redox shuttle additive on its own is enough to prevent overcharging."

The redox shuttle additive also allows researchers to create an "autobalancing" battery, which refers to the thousands of different battery cells in a pack being electrochemically instructed to charge in concert.

Chemist John Zhang (left) and assistant materials scientist Lu Zhang (no relation) show a flask of Argonne's redox shuttle additive.





Below, starting material for synthesis of the award-winning redox shuttle additive.

Above, John Zhang uses a Rotovap to remove solvent from the extraction solution to produce the award-winning material.

In addition to the overcharge protection, the redox shuttle technology Argonne developed is cost-effective because of the inexpensive starting materials and simple manufacturing process, according to Zhang. "It really addresses our two major issues at the same time: cost and safety," he said.

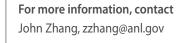
Different batteries charge to different voltages, so Zhang's group created a variety of different redox shuttle additives that are each tailored for a different class of battery cathode materials. Then, Argonne chemist Greg Krumdick and his group scaled up the materials from the gram-level to the kilogram-level, making them attractive candidates for commercialization.

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.



A flask of precursor material awaits processing into the active ingredient for Argonne's redox shuttle additive.





Autonomie-Equipped Low-temperature **Combustion Engine Test Cell** Is **Unique** in the **United States**

Fundamental demonstrations of the potential for low-temperature combustion (LTC) to improve engine performance have been undertaken for many years, starting with experiments conducted by Sandia National Laboratories, Shell (UK), Lund University and the University of Wisconsin during the last decade.

Until now, none have been able to experimentally demonstrate the true potential improvements across a wide range of transient operating conditions in various vehicle applications that will enable the move from theory to practice on a broad scale.

Enter Argonne's Center for Transportation Research, where engineers have enabled the lab's General Motors platform of a four-cylinder LTC test engine to "talk" to Autonomie, Argonne's award-winning modeling and simulation software. This is the only test cell in the United States that offers wide-ranging vehicle emulation coupled with automated drive-cycle testing and control of all key engine-operating parameters, with results publicly available.

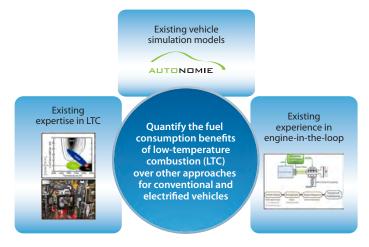
> Principal investigator Steve Ciatti positions an endoscope in one of Argonne's four-cylinder LTC test engines to visualize in-cylinder combustion with high-speed (>10,000 frame/sec) movies.

Demonstrates possibility of

20 to 30 percent improvement in **fuel economy** using low-temperature combustion technology

Argonne principal mechanical engineer Steve Ciatti and his team have focused on low-octane, gasoline-like fuels for compression ignition operation, and explored how factors such as fuel delivery, intake oxygen concentration, fuel chemistry, intake air temperature and boost pressure influence performance. Their research has shown that with the right combination of factors, it is theoretically possible to achieve a dramatic 20 to 30 percent improvement in fuel economy in an engine using LTC technology in a vehicle with a standard powertrain (non-hybrid), as compared to a conventional spark ignition engine using conventional (high-temperature) combustion.1





Argonne's approach leverages existing expertise in vehicle system simulation, component-in-the-loop and low-temperature combustion engine research.

"Connecting the LTC engine test cell with Autonomie allows us to map transient behavior for a complete understanding of how the engine will respond to real-world operating conditions," said Ciatti." This knowledge will enable manufacturers to explore a wide range of operating parameters and modify engines of all kinds to optimize the emissions and fuel consumption benefits of low-temperature combustion—reducing expensive and time-consuming hardware changes each time test scenarios are changed."

One of the biggest remaining challenges in this research involves consistency—specifically, achieving consistent ignition performance within each cylinder under a range of conditions. Once this milestone is achieved, the researchers will then focus on characterizing emissions performance across a full range of emulated vehicles using Autonomie, and reproducing their results using commercially available fuel blends.

¹Ciatti, S., "Use of Low Cetane Fuel to Enable Low-Temperature Combustion," in Advanced Combustion Engine Research and Development, DOE/EE-0872, U.S. Department of Energy, Energy Efficiency and Renewable Energy, Vehicle Technologies Office (2013). Available at http://energy.gov/sites/prod/files/2014/04/f14/ fy13advancedcombustionprogressreport.pdf.

This research is funded by the U.S. Department of Energy, Energy Efficiency and Renewable Energy, Vehicle Technologies

> For more information, contact Steve Ciatti, sciatti@anl.gov

What is **Autonomie?**

Traditional practices in the automotive industry often delay vehicle control system design until late in the process—in some cases requiring several costly hardware iterations. Greater use of computer modeling and simulation during the design process can reduce costs and improve time to market. Argonne's Autonomie is a "plug-and-play" powertrain and vehicle model architecture and development environment that supports the rapid evaluation of new powertrain/propulsion technologies under dynamic/transient testing conditions. Autonomie improves fuel economy through virtual design and analysis in a mathbased simulation environment.

Learn more at autonomie.net.



The Watchful Guardian Advances Transportation Safety for Hazardous Materials

If you have ever wondered about the safety of hazardous materials during transportation and storage, rest assured you aren't alone. While there are plenty of rules and regulations governing how such materials must be packaged and transported, wouldn't it be even better if there were a way to monitor their progress every step of the way?

That's exactly what experts at the U.S. Department of Energy (DOE) thought, too. Considering that in the United States alone, tens of thousands of drums (referred to as packages) containing radioactive and fissile materials are stored or transported annually, this is no small concern. "Modernizing the life-cycle management of these materials requires vision and innovation," explains James Shuler, Manager of DOE's Packaging Certification Program. "We've been seeking a solution, and Argonne National Laboratory delivered with the development of ARG-US, the Watchful Guardian."

ARG-US is a radio frequency identification (RFID) technology that features long-life, customizable sensor tags with an integrated communication platform to perform continuous, real-time tracking and monitoring of nuclear and other hazardous materials in transportation and storage. Major components include wireless RFID tags with sensors, readers, communication networks, computer servers, database software and graphical information displays.



Photo of Mk-III tag showing custom-installed detectors in expansion board, antenna and long-life battery

The system monitors and records the status of tagged containers to assess seal integrity, temperature, humidity, shock, radiation field and battery strength. Deviations from sensor thresholds instantly trigger an alarm that notifies responsible parties so that they can take appropriate action. At all times, system information is accessible via a local area network and secure web links, whether the containers are in processing, storage or transport.

According to the developer of ARG-US, Yung Liu, senior nuclear engineer and section manager in Argonne's Decision and information Sciences division, "Until the development of ARG-US, no one single technology had been available to track, monitor, report, communicate and enable rapid response to potential emergencies related to nuclear and other hazardous wastes in these applications."

Argonne's **RFID advance** will accelerate adoption of

technologies that cut operating costs and improve the safety, security and safeguards of hazardous materials.

The transportation component, ARG-US TransPort, monitors and tracks nuclear or radioactive materials in transport. It incorporates mapping and a satellite global positioning system (GPS) and is integrated with mobile communication equipment in the transport vehicle. It is fully integrated with DOE's unclassified tracking and communication web application, TRANSCOM. ARG-US TransPort is linked to a Geographic Information System (GIS) database to support emergency management tracking capability.

The key innovation in ARG-US—the customizable RFID surveillance tag—consists of a robust plastic/metal enclosure for mounting on multiple types of certified container drums. It has three internal compartments for batteries, tag electronics, sensors, and antenna, as well as an expansion board for incorporating additional sensors.



ARG-US RFID tag shown attached to a 9979 package, designed and certified by DOE for the packaging and shipment of Type A quantities of fissile material

The tags are designed to operate without replacement batteries for up to 10 years, and the results of Cesium (Cs)-137 gamma irradiation tests of tags support an estimated life of 17 years at a field of 200 milliRoentgen per hour (mR/h). The latest Mk-III (Mark III) tag can be tailored to contain a compact

gamma radiation dosimeter, a solid-state neutron detector or both, depending on the areas of application.

"The Watchful Guardian" was first deployed to track the transportation of nuclear materials in early June 2012. "We used ARG-US to track a shipment of material from Oak Ridge National Laboratory (ORNL) to the Nevada National Security Site," said Liu. "The data we collected were transmitted during transport over secure communication channels to the Command Center here at Argonne, where we were able to successfully monitor the packages remotely." Successful deployment and demonstration has led to rapid development of the Watchful Guardian, attracting industry attention and recognition. In a significant milestone, Argonne National Laboratory and Evigia Systems, Inc. (Ann Arbor, Michigan; www.evigia.com), reached a licensing agreement on the ARG-US RFID technology in July 2012.

According to Dr. Navid Yazdi, President of Evigia, the commercialization of ARG-US "enables us to immediately enter new markets with the Evigia EV-3 platform and Argonne's ARG-US technology and deliver a complete, readily deployable wireless sensing solution for these vitally important nuclear and hazardous material transportation and storage operations." Further, Dr. Yazdi believes, "ARG-US will have a significant impact on the RFID industry, resulting in accelerated adoption of automation and sensing technologies that will cut operating costs and improve the safety, security and safeguards of hazardous materials."

After many successful deployments of the ARG-US RFID system across the country, Argonne continues to enhance the capabilities of both the hardware and software of the ARG-US RFID system. Says Liu, "We are working to enhance the ARG-US system by expanding the communication framework to include a wireless mesh network, adding standalone cellular (Global System for Mobile Communications/code division multiple access) communication capability, and adding sensors (such as a hydrogen sensor)."

For example, one recent expansion of ARG-US is Remote Area Modular Monitoring (RAMM)—an expandable, adaptable system for monitoring critical nuclear and radiological facilities. ARG-US RAMM is also well suited to transportation applications. "By incorporating cellular and satellite communication gear," explains Liu, "RAMM can be installed on shipping conveyances (lorries, railcars, airplanes and ships) and can track sensitive shipments as well."

For more details on ARG-US, please visit http://www.dis.anl.gov/projects/argus rfid.html

The development of ARG-US was funded by the U.S. Department of Energy Packaging Certification Program, Office of Packaging and Transportation, Office of Environmental Management.

For more information, contact Yung Liu yyliu@anl.gov

ARG-US Lauded by Industrial RFID Community

In tandem with commercialization, ARG-US has been recognized by the industrial RFID community with the following honors:

- Winner of the 2013 Active Tagging
 Case Study contest conducted by the
 Association for Automatic Identification and Mobility (AIM) Experts Group
- Recipient of RFID Journal's 2011 "Most Innovative Use of RFID" Award
- Finalist at the 2011 World's Best
 Technology Innovation Marketplace



Johnson and Bohn Receive Awards from DOE's Vehicle Technologies Office

The U.S. Department of Energy's (DOE's) Vehicle Technologies Office (VTO) honored two members of Argonne's Energy Systems division, **Larry Johnson** and **Ted Bohn**, during DOE's 2014 Annual Merit Review and Peer Evaluation Meetings held June 16–20, 2014, in Washington, D.C.



Larry Johnson, retired founding director of Argonne's Transportation Technology Research and Development Center (TTRDC) and Argonne National Laboratory Distinguished Fellow, received VTO's Distinguished Achievement Award for "extraordinary dedication to promoting the adoption of advanced vehicles and a lifetime of research to accomplish that goal." Through Johnson's tireless dedication and wide-ranging work with DOE and many major automakers and industrial partners,

Argonne's transportation research program grew to become one of the largest at the laboratory—contributing greatly to the laboratory's future direction and mission and positioning Argonne as the nation's lead laboratory for many areas of transportation.

Principal Electrical Engineer **Ted Bohn** received a VTO Research and Development Award in "recognition of technical leadership in standards development for EV/grid connectivity, interoperability, and wireless charging." VTO recognized Bohn for his work with the Society of Automotive Engineers J2954 wireless charging committee and for his research and development of low-cost sub-meters for application in vehicles and charging infrastructure. Bohn's work has greatly furthered plug-in electric vehicle-grid

connectivity,
interoperability and
wireless charging
throughout the United
States. He is a leading
expert on power
electronics and controls
for pure research as
well as commercial
applied technologies
for business case
product portfolio
development.



Ahluwalia and Stamenkovic Honored by DOE's Fuel Cell Technologies Office

The U.S. Department of Energy's (DOE's) Hydrogen and Fuel Cells Program presented its annual awards at the 2014 DOE Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting on June 17, 2014. Each year, the Hydrogen and Fuel Cells Program presents "Program Area Awards" to recognize exceptional achievements in specific areas. The Hydrogen and Fuel Cells Program also presented "Hydrogen and Fuel Cells Program Awards" that represent accomplishments beyond a single program area. **Rajesh Ahluwalia** of Argonne's Nuclear Engineering division received a Hydrogen and Fuel Cells Program Award and **Vojislav Stamenkovic** of the laboratory's Materials Science division received a DOE Hydrogen and Fuel Cells Program Area Award.

Spanning more than two decades, **Ahluwalia**'s technical insight and guidance regarding fuel cell, hydrogen storage and hydrogen production systems analysis has been outstanding. He is the co-developer of GCTool (General Computational Toolkit), a software package that helps design, analyze and optimize automotive and stationary distributed fuel cell power generation systems and other power-plant configurations. As part of three fuel cell durability projects, he developed models for Electrochemical Catalyst Stability, Durability, and Performance (eCaSt), allowing prediction of the impact of such properties as catalyst particle size and cell operating conditions on fuel cell stack lifetime.

DOE recognized **Stamenkovic** for his outstanding achievements in the area of fuel cell catalysts, specifically in reducing the content of platinum group metals in oxygen reduction catalysts. To reduce the cost of fuel cells, the Hydrogen and Fuel Cells Program is pursuing approaches to lower the amount of precious group metals in oxygen reduction catalysts. For several years, Stamenkovic and his team have employed a materials-by-design approach to design, characterize, understand,



synthesize/fabricate, and test advanced nanosegregated multimetallic nanoparticles and nanostructured thin metal films.

Recently researchers at Lawrence Berkeley (LBNL) and Argonne National Laboratories developed a new class of catalysts that could make fuel cells cost-competitive with other technologies. The research team led by Stamenkovic and LBNL's Professor Peidong Yang created a nanoframe catalyst that uses approximately 85 percent less platinum and has more than 30 times the mass activity than that of conventional catalysts.



Research Results

Recent Patents and Technologies Licensed

Licensed

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

Intertek Testing Services, North America, has signed an agreement to license **Argonne-developed** software and documentation for "EVIDAS (Electric Vehicle [EV] and Supply Equipment SAE 2953 Data Acquisition Software)."

New Patents

"Long Life Lithium Batteries with Stabilized Electrodes," Jaekiik Kim, Khalil Amine and Daniel R. Vissers, United States Patent 8,551,661.

"Electrode Materials for Rechargable Batteries," **Christopher Johnson** and **Kang Su-Ho**, United States Patent 8,557,438.

"Autogenic Pressure Reactions for Battery Materials Manufacture," Vilas Pol, Swati Pol and Michael Thackeray, United States Patent 8,568,914.

"Bioprocess Utilizing Carbon Dioxide and Electrodeionization," Edward St. Martin and YuPo Lin, United States Patent 8,580,096.

"Methods for Preparing Materials for Lithium-ion Batteries," Aymeric Rousseau, Phillip B. Sharer and Sylvain Pagerit, United States Patent 8,591,774.

"Unique Battery with an Active Membrane Separator Having Uniform Physico-chemically Functionalized Ion Channels and a Method Making the Same," **Rex Gerald II, Katarina Ruscic, Devin Sears, Luis Smith, Robert Klingher** and **Jerome Rathke**, United States Patent 8,592,075.

"Polyether-functionalized Redox Shuttle Additives for Lithium-ion Batteries," Zhengcheng Zhang, Lu Zhang and Khalil Amine, United States Patent 8,609,287.

"Materials as Additives for Advanced Lubrication," Vilas Pol, Michael Thackeray, Kuleep Mistry and Ali Erdemir, United States Patent 8,648,019.

"Method of Sealing a Bipolar Plate Supported Solid Oxide Fuel Cell with a Sealed Anode Compartment," **John Carter, Joong-Myeon Bae, Terry Cruse, James Ralph** and **Deborah Meyers**, United States Patent 8,652,709.

"Methane Production Using Resin-wafer Electrodeionization," YuPo Lin, Meltem Urgun Demirtas and Seth Snyder, United States Patent 8,679,314.

"Non-aqueous Electrolyte for Lithium-ion Battery," Lu Zhang, Zhengcheng Zhang and Khalil Amine, United States Patent 8,697,291.

"Production of Battery-grade Materials via an Oxalate Method," Ilias Belharouak and Khalil Amine, United States Patent 8,709,279.

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





Recent Publications

"A Bioinspired Redox Relay that Mimics Radical Interactions of the Tyr-His Pairs of Photosystem II," J.D. Megiatto Jr., D.D. Méndez-Hernández, M.E. Tejeda-Ferrari, A.-L. Teillout, M.J. Llansola-Portolés, G. Kodis, **O.G. Poluektov**, **T. Rajh**, V. Mujica, T.L. Groy, D. Gust, T.A. Moore and A.L. Moore, *Nature Chemistry* **6**, 423—428 (2014). Available at http://dx.doi.org/10.1038/nchem.1862.

"A Spatial Modeling Framework to Evaluate Domestic Biofuel-induced Potential Land-use Changes and Emissions," J. Elliott, B. Sharma, N. Best, M. Glotter, J.B. Dunn, I. Foster, F. Miguez, S. Mueller and M.Q. Wang, Environmental Science and Technology, 48(4): 2488–2496, 2014. Available at http://dx.doi.org/10.1021/es404546r.

"Analysis of Cyclic Variability and the Effect of Dilute Combustion in a Gasoline Direct Injection Engine," **N. Matthias**, **T. Wallner** and **R. Scarcelli**, *SAE International Journal of Engines* **7**(2), 2014. Available at http://dx.doi.org/10.4271/2014-01-1238.

"Examination of Nanoparticles from Gasoline Direct-Injection (GDI) Engines Using Transmission Electron Microscopy (TEM)," **H. Seong, S. Choi** and **K. Lee**, International Journal of Automotive Technology **15**(2): 175—181, 2014. Available at http://dx.doi.org/10.1007/s12239-014-0019-5.

"Geothermal Power Production: Alternative Scenarios and Critical Issues," **J.L. Sullivan**, **T. Stephens** and **M.Q. Wang**, ANL/ESD-14/2, Argonne National Laboratory, Argonne, IL (2014).

"Highly Efficient Non-Precious Metal Electrocatalysts Prepared from One-Pot Synthesized Zeolitic Imidazolate Frameworks (ZIFs)," **D. Zhao, J.-L. Shui**, L.R. Grabstanowicz, **C. Chen, S.M. Commet**, T. Xu, **J. Lu** and **D.-J. Liu**, *Advanced Materials* **26**, 1093—1097 (2014). Available at http://dx.doi.org/10.1002/adma.201304238.

"Impact of Blending Gasoline with Isobutanol Compared to Ethanol on Efficiency, Performance and Emissions of a Recreational Marine 4-Stroke Engine," **T. Wallner**, **A. Ickes**, J. Wasil, J. Sevik and S. Miers, SAE Technical Paper 2014-01-1230, 2014. Available at http://dx.doi.org/10.4271/2014-01-1230.

"Impact of Cetane Number on Combustion of a Gasoline-Diesel Dual-Fuel Heavy-Duty Multi-Cylinder Engine," **A. Ickes, T. Wallner**, Y. Zhang, and W. De Ojeda, *SAE International Journal of Engines*, **9**(2), 2014. Available at http://dx.doi.org/10.4271/2014-01-1309.

"Impact of Updated Material Production Data on the GREET Life Cycle Model," R.D. De Kleine, G.A. Keoleian, S.A. Miller, **A. Burnham** and **J.L. Sullivan**, *Journal of Industrial Ecology* (2014). Available at http://dx.doi.org/10.1111/jiec.12132.

"In Operando Spatiotemporal Study of Li_2O_2 Grain Growth and its Distribution Inside Operating $\text{Li}-\text{O}_2$ Batteries," **J.-L. Shui**, J.S. Okasinski, **C. Chen**, J.D. Almer and **D.-J. Liu**, *ChemSusChem* **7**(2), 543–548 (2014). Available at http://dx.doi.org/10.1002/cssc.201300822.

"Life Cycle Greenhouse Gas Emissions from Geothermal Electricity Production," **J.L. Sullivan** and **M.Q. Wang**, *Journal of Renewable and Sustainable Energy* **5**, 063122 (2013). Available at http://dx.doi.org/10.1063/1.4841235.

"Life-Cycle Energy Use and Greenhouse Gas Emissions of Production of Bioethanol from Sorghum in the United States," **H. Cai**, **J.B. Dunn**, **Z.C. Wang**, **J. Han** and **M.Q. Wang**, *Biotechnology for Biofuels*, **6**:141, 2013. Available at http://dx.doi.org/10.1186/1754-6834-6-141.

"Light-Duty Vehicle Fuel Consumption Displacement Potential up to 2045," **A. Moawad** and **A. Rousseau**, Argonne National Laboratory Report No. ANL/ESD-14/4, 2014. Available at http://www.transportation.anl.gov/pdfs/G/959.PDF.

"Plug-in Hybrid Electric Vehicles," **D.J. Santini,** IA-HEV 2014 Task 15 Report, IEA Hybrid & Electric Vehicle Implementing Agreement, IEA Energy Technology Network (2014). Available at http://www.ieahev.org/assets/1/7/IA-HEVTask15ReportFinalFeb20142.pdf.

"Review on Characterization of Nano-Particle Emissions and PM Morphology from Internal Combustion Engines: Part 2," **S. Choi**, C.L. Myung and S. Park, *International Journal of Automotive Technology*, **15**(2): 219–227, 2014. Available at http://dx.doi.org/10.1007/s12239-014-0023-9.

"Synchrotron X-Ray Techniques for Fluid Dynamics," **A. Kastengren** and **C. Powell**, Experiments in Fluids **55**:1668, 2014. Available at http://dx.doi.org/10.1007/s00348-014-1686-8.

"Thermal Model Development and Validation for 2010 Toyota Prius," **N. Kim**, **A. Rousseau**, **D. Lee** and **H. Lohse-Busch**, SAE Technical Paper 2014-01-1784, 2014. Available at http://dx.doi.org/10.4271/2014-01-1784.

"VISION 2013 User's Guide and Model: Description of Model Used to Estimate the Impacts of Highway Vehicle Technologies and Fuels on Energy Use and Carbon Emissions to 2100," Y. Zhou and A. Vyas, ANL/ESD-14/1, Argonne National Laboratory (2014).

"X-ray Imaging of Cavitation in Diesel Injectors," **D. Duke, A. Swantek, Z. Tilocco, A. Kastengren, K. Fezzaa**, K. Neroorkar, M. Moulai, **C. Powell** and D. Schmidt, *SAE International Journal of Engines* **7**(2), 2014. Available at http://dx.doi.org/10.4271/2014-01-1404.

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

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





EcoCAR 3 Teams Announced, Energy-**Efficient Camaro** is the Goal

The U.S. Department of Energy and General Motors are planning to hand the keys of a Chevrolet Camaro to 16 collegiate teams as part of its EcoCAR 3 competition.

The four-year Advanced Vehicle Technology Competition (AVTC), which was announced to the public on April 24, 2014, is challenging students to rebuild the Chevrolet Camaro to squeeze even more fuel efficiency out of it and reduce the emissions, all while keeping muscle car fanatics satisfied.

Managed by Argonne National Laboratory, EcoCAR 3 challenges 16 North American universities to reduce the environmental impact of vehicles by minimizing the vehicle's fuel consumption and reducing its emissions. In addition, students must consider cost and explore innovation, while retaining the vehicle's performance, safety and consumer appeal.

"EcoCAR is an opportunity for the next generation of automotive engineers to help design and build innovative advanced vehicles that will reduce greenhouse gas emissions, protect the

The EcoCAR 3 Chevrolet



environment and save American families and businesses money at the pump," said U.S. Energy Secretary Ernest Moniz.

The following 16 North American universities will compete in

- ▶ Arizona State University
- ▶ California State University, Los Angeles
- ▶ Colorado State University
- ▶ Embry-Riddle Aeronautical University
- Georgia Institute of Technology
- McMaster University
- Ohio State University
- Mississippi State University

- ▶ Pennsylvania State University
- University of Alabama
- University of Tennessee, Knoxville
- University of Washington
- University of Waterloo
- Virginia Tech
- ▶ Wayne State University
- West Virginia University

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.

To learn more about EcoCAR 3, visit www.ecocar3.org.



Representatives from the 16 university teams and special guests at the EcoCAR 3 Announcement in April in Washington, D.C. Front row, from left to right: Assistant Secretary David Danielson, U.S. Department of Energy; Vice President of Global Vehicle Engineering John Calabrese, General Motors; Associate Laboratory Director for Energy Engineering and Systems Analysis Mark Peters, Argonne National Laboratory; Second row, middle: Secretary of Energy Ernest Moniz, U.S. Department of Energy.

New GREET and **AFLEET Releases** Add Data and **Pathways**

Argonne National Laboratory recently released important updates to its popular Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model and released the newly developed Alternative Fuel Life-Cycle Environmental and Economic Transportation (AFLEET) Tool.

GREET allows researchers and analysts to evaluate various vehicle and fuel combinations on a full fuel-cycle/vehicle-cycle basis. The latest GREET update increases the robustness and flexibility of the model and adds new data for the models and more pathways, such as:

- ▶ New marine fuel pathways and commercial vessel operations
- ▶ New sorghum ethanol pathways
- New tallow pathway
- ▶ Electric power sector technology shares, efficiencies and emission factors by technology and utility regions
- ► CH₄ emissions for natural gas pathways
- ▶ Transmission and distribution (T&D) emission factors, energy intensity, mode shares and distances
- ▶ Biofuels land use change data and new modeling options
- ▶ Cellulosic biomass feedstock updates (e.g., farming, T&D, dry matter losses)
- ▶ Fertilizers and nutrients use for biofuels pathways
- ▶ Petroleum refining efficiency
- ▶ Light duty vehicles (LDVs) tailpipe emission factors
- ▶ Hydrogen production with latest DOE H₂O hydrogen analysis
- Urban share of criteria air pollutant emissions (petroleum, electricity, LDVs)



The AFLEET Tool was released in 2013 to assist DOE's Clean Cities program stakeholders with estimating petroleum use, greenhouse gas emissions, air pollutant emissions and cost of ownership for light-duty and heavy-duty vehicles using simple spreadsheet inputs. AFLEET uses data from GREET's fuel-cycle model to generate necessary well-to-wheels petroleum use and greenhouse gas emissions co-efficients for key fuel production pathways and vehicle types. In addition, AFLEET uses the U.S. Environmental Protection Agency's **MO**tor **V**ehicle **E**mission Simulator and certification data to estimate tailpipe air pollutant emissions. Various sources are used to provide default cost data, including the Clean Cities Alternative Fuel Price Report and American Recovery and Reinvestment Act awards.

> GREET is available for download at https://greet.es.anl.gov/main

The AFLEET Tool is available for download at https://greet.es.anl.gov/afleet

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

For more information, contact:

Amgad Elgowainy at aelgowainy@anl.gov, or Andrew Burnham at aburnham@anl.gov.







Fastrax

Miller and Scarcelli Receive SAE McFarland Award

James Miller and Riccardo Scarcelli received the prestigious McFarland Award from the Society of Automotive Engineers (SAE) for 2014. This award recognizes individuals for their outstanding contributions toward the work of the SAE Engineering Meetings Board (EMB) in the planning, development and dissemination of technical information through technical meetings, conferences and

professional development

programs or outstanding

operations in facilitating or

enhancing the exchange of

technical information. Miller

was cited for "outstanding

in the planning of SAE

technical sessions" and

supporting several

Powertrains, Fuels &

SAE World Congress,

Scarcelli for "outstanding

effort as a session organizer

Lubricants events including

International Powertrains,

Fuels & Lubricants Meeting and the International

Conference on Engines &

is a global association

of more than 138,000

engineers and related

technical experts in the

aerospace, automotive

and commercial vehicle

industries.

Vehicles." SAE International

contribution and leadership

contributions to EMB



James Miller



Riccardo Scarcelli

Elgowainy & Wang Honored by USCAR

Michael Wang and Amgad Elgowainy were among the recipients of the United States Council for Automotive Research (USCAR) 2013 Team Award as members of the U.S. Drive Cradleto-Grave (C2G) Team—an industry cross-cutting team involving members from USCAR, DOE, national labs, utilities and oil companies. The Team Awards recognize those teams and members who leveraged their resources, exceeded expectations, overcame challenges and created outstanding value for the member companies in 2013. The team came together to develop the first C2G assessment and projections of greenhouse gas emissions and energy use for U.S.-relevant light-duty vehicle fuel technology combinations for the years 2025 to 2030. The study was the first of its kind and required building consensus on very sensitive topics among the diverse group of interested organizations.



Eric Rask, principal research engineer in Argonne's Center for Transportation Research, was interviewed by *The Battery Show's* Mindy Emsley. Read the interview at http://tinyurl/id9um4n.







Jehlik Participates in White House's "Extreme STEM" Hangout

Forrest Jehlik was among the participants in a recent "Extreme STEM" Hangout hosted by the White House Office of Science and Technology (OSTP). The event was the latest in OSTP's "We the Geeks" video series. "We the Geeks" aims to inspire students to enter Science, Technology, Engineering and



Mathematics (STEM) fields by shining a light on people who have done particularly exciting or nontraditional work in STEM. Jehlik is a member of the Vehicle Systems section of Argonne's Center for Transportation Research.

Mike Duoba

Duoba Talks to SAE About Advanced Vehicles

Mike Duoba, chief mechanical engineer, spoke with SAE International recently about his work at Argonne. Read the



Argonne Battery Technology Patent Confirmed by U.S. Patent Office

Following a careful reexamination of the relevant prior patents and publications, the U.S. Patent and Trademark Office (USPTO) has confirmed the novelty of U.S. Patent 6,677,082, which claims that the Lithium Nickel Manganese Cobalt Oxide (NMC) cathode technology developed by Argonne improves battery range and reliability, while simultaneously improving safety and reducing manufacturing cost. NMC cathode technology as described in this patent is used in commercial and consumer vehicles' lithium-ion batteries. Argonne's NMC cathode material is designed to the molecular level, enabling batteries to store more energy. It is environmentally safer than the cobalt oxide materials found in most lithium-ion batteries and is more economical to manufacture.

Abraham Interview Featured as UK's *Batteries International* Cover Story

Daniel Abraham of Argonne's Chemical Sciences and Engineering Division was featured in a Spring 2014 cover story by the British journal *Batteries International*. The article, "Beyond Lithium Ion is Part of the Dream" is available at http://tinyurl.com/oc8gtaf.



Daniel Abraham

20 TransForum Previous Article | Contents | Next Page | Next Article

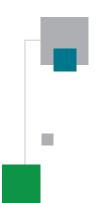


Parting Shots

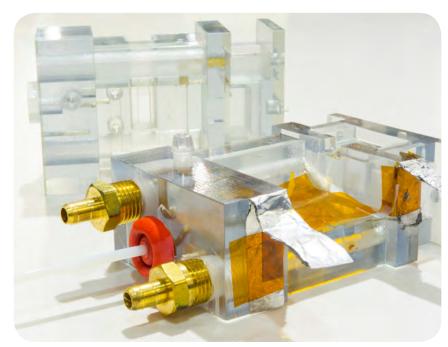
Argonne's New Energy Sciences Building

Argonne's recently completed Energy Sciences Building is set to house some 200 research personnel dedicated to addressing the world's most critical energy challenges. Among the research efforts to be conducted in the new facility include the development of highly reliable, safe and long-lived battery systems; revolutionary, efficient and environmentally friendly chemical transformation processes for creating novel feedstocks and fuels; and transformational systems for solar energy production.





Below, Argonne chief mechanical engineer Mike Duoba (right) discusses the capabilities of the laboratory's Advanced Powertrain Research Facility's Environmental Test Cell with U.S. Department of Energy Secretary Ernest Moniz (left) during his visit to Argonne

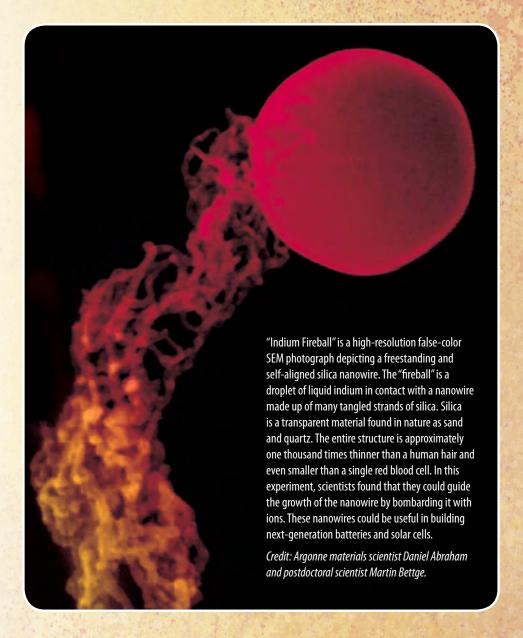


Electrochemical cell made with 3-D printer

An electrochemical cell made with a 3-D printer for studies using high-energy X-rays. This would take five to six months longer to make in aluminum, and would be cost prohibitive and difficult to machine in a mix of metal and nonconductive material. The polymer-based sample holder can maintain a flow of electrodes, temperature and charge in the chamber while the holder is angled in the beam to gather different scattering patterns. Scientists working with the Advanced Photon Source at Argonne National Laboratory can conduct studies remotely by sending in these filled sample holders.



The **Reauty** in **Science** and **Engineering**





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/technology

www.transportation.anl.gov



This publication was prepared as an account of work sponsored

United States Government nor any agency thereof, nor UChicago

responsibility for the accuracy, completeness, or usefulness of any

that its use would not infringe privately owned rights. Reference

by trade name, trademark, manufacturer, or otherwise, does not

thereof. The views and opinions of document authors expressed

herein do not necessarily state or reflect those of the United States

Government or any agency thereof, Argonne National Laboratory,

necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency

herein to any specific commercial product, process, or service

information, apparatus, product, or process disclosed, or represents

Argonne, LLC, nor any of their employees or officers, makes any

warranty, express or implied, or assumes any legal liability or

by an agency of the United States Government. Neither the

Scan with any barcode reader on your smartphone.

TransForum → Volume 14, No. 2, 2014 ISSN 2156-3594 (print) ISSN 2156-373X (online)

Managing Editor: Renée M. Nault

Contributors: Justin Breaux, Kevin Brown, Dana Bubonovich,

Mitch Romanowski and Suzanne Williams

Designer: Cindi Andersen

Photographers: Wes Agresta and Mark Lopez

Copy Editor: Andrea Manning Production: Gary Weidner

Trans Forum is published by the Transportation Research Program, Argonne National Laboratory. Publishing support services are provided by Argonne's Communication, Education and Public Affairs Division.

Information in **Trans** Forum may be reproduced for publication with acknowledgment to **Trans** Forum, Argonne National Laboratory. Address correspondence, subscription requests and address changes to:

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



or UChicago Argonne, LLC.

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

