Sustainable Transportation Program

2016 Annual Report

OAK RIDGE National Laboratory | NATIONAL TRANSPORTATION RESEARCH CENTER

ORNL/SR-2017/271

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16-G01647/cae

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Table of Contents

From the Director 6

Integrating Technology 8
- High-power wireless charging surges forward with 20-kW system
- ORNL partners with Delphi on inverter for 2016 Chevy Volt
- Novel motor achieves 75% higher power without rare earth materials

Accelerating Solutions 10
- Microscopy captures real-time view of evolving fuel cell catalysts
- Facility provides capabilities to examine materials at their core
- Hydrogen storage vessel solves embrittlement problem

Running Smoothly 12
- New perspective on ignition modes opens opportunities
- Advanced catalyst technology excels at low temperatures
- Discovery will inform future design of fuels and engines

Analyzing Possibilities 14
- Data help officials keep the nation's freight moving
- Compare vehicles, mileage, and more at fueleconomy.gov
- Market acceptance modeling tool available online
- ORNL data support strategic decisions, public outreach

Building Biomass 16
- US holds potential to produce a thriving bioeconomy by 2040
- Energy-efficient reaction drives ORNL biofuel conversion technology
- Developing international codes and standards for the bioenergy industry
- World's experts tour region's biomass resources

Sustainable Transportation Program by the Numbers 18
- Transferring technology to market

Propelling Innovations 20
- Atoms to engines: Accelerating alloy development using high-performance computing
- Turbocharging R&D with high-performance computing

Connecting to the Future 22
- Algorithms rev up fuel efficiency for connected and automated vehicles
- Coming soon to a road near you: safer, more secure vehicles
- Improving cybersecurity for connected and automated vehicle technologies

Driving Results 24
- Cross-laboratory capabilities speed development of new Ce-Al alloy
- ORNL contributes to standards development for heavy-duty trucks
- Real-time tracking system monitors fuel shipments

Improving Costs 26
- Laser treatment creates strong, multimaterial joints for vehicle lightweighting
- Lower cost alloys for higher temperature exhaust valves improve vehicle efficiency
- Predictive engineering tools for injection-molded carbon fiber composites

Rolling Along 28
- Building better batteries with neutrons and computational modeling
- Electron beam technology cures cathode coatings instantly
- Fast formation protocol speeds production, improves battery capacity

Leadership Science 30

Honors and Awards 32

Publications 34

Dr. Claus Daniel, Director

Delivering innovations in sustainable, secure mobility

The efficiency and security of the transportation system affect us all—from the time and energy spent on our daily commutes to the availability of goods in our local stores. Also impacted are our pocketbooks, both as individuals and as a nation.

Transportation accounts for about 70% of national petroleum use, with Americans spending more than $177 billion to import oil in 2015. That same year, oil dependence cost the US $29 billion in lost potential GDP. Creating transportation technologies that reduce dependence on foreign oil; boost America's economy; improve national energy security; and deliver to consumers affordable, environmentally friendly choices is of critical importance.

ORNL's Sustainable Transportation Program (STP) works with government and industry to develop scientific knowledge and new technologies that accelerate the deployment of energy-efficient vehicles and intelligent, secure, and accessible transportation systems.

Scientists are tackling complex challenges in transportation using comprehensive capabilities at ORNL's National Transportation Research Center and the laboratory's signature strengths in high-performance computing, neutron sciences, materials science, and advanced manufacturing. Research focuses on electrification, efficiency of combustion and emissions, data science and automated vehicles, and materials for future systems. Highlights from 2016 include:

Electrification

Researchers developed and demonstrated the world's first high-power (20-kW) wireless charging system for passenger cars. The system achieved 90% efficiency at three times the rate of the plug-in systems commonly used for electric vehicles today. ORNL and partners Toyota, Cisco Systems, Evatran, and the Clemson University International Center for Automotive Research received an R&D 100 Special Recognition Award for the technology.

Efficiency of combustion and emission controls

Scientists at ORNL took a leadership role in the DOE Co-Optimization of Fuels and Engines initiative, which aims to accelerate the introduction of innovative combustion strategies and fuels designed together to maximize performance and fuel efficiency. Researchers also developed new catalyst technologies that operate effectively in the low-temperature exhaust from high-efficiency engines.

Data science and automated vehicles

Through the development of vehicle-based algorithms, ORNL data scientists simulated optimized traffic flow for connected and automated vehicles (CAVs) merging at highway on-ramps, demonstrating the potential to reduce fuel consumption by 50% and travel time by 7%. Further analysis showed that 40% fuel savings could be achieved even if only 30% of the vehicles on the road are CAVs.

Materials for future systems

Leveraging ORNL's high-performance computing and materials characterization capabilities, researchers partnered with FCA USA and Nemak to develop a new class of affordable, 300°C-capable cast aluminum alloys for use in next-generation engines.

This annual report is a short summary and snapshot featuring several other accomplishments from the STP team. From motors that achieve higher power density without rare earth materials to thought leadership on combustion as a continuum to new technologies in multimaterial joining and vehicle cybersecurity, ORNL researchers are shaping the future of transportation.

I would like to thank our major sponsors for supporting this research and development, including the DOE Office of Energy Efficiency and Renewable Energy's Sustainable Transportation Offices, consisting of the Vehicle Technologies Office, Bioenergy Technologies Office, and Fuel Cell Technologies Office, as well as the US Department of Transportation, our 88 active industry partners, and other key sponsors and partners.

Many thanks as well to the team of researchers from across the laboratory who devote their energy and expertise to delivering innovations in transportation. Together, we are driving toward a sustainable, secure, and accessible mobility future.

Dr. Claus Daniel, Director
Sustainable Transportation Program

ORNL's 20-kW wireless charging system achieved 90% efficiency at three times the rate of the plug-in systems commonly used for electric vehicles.

High-power wireless charging surges forward with 20-kW system

They're zooming across American roadways, spreading from the cities to the heartland. Since 2011, more than half a million plug-in electric vehicles have been sold in the United States.

For the electric vehicle trend to continue, however, vehicles must adapt to consumer needs—providing more convenience, charge, efficiency, and affordability. New advancements at ORNL are addressing these challenges.

Researchers in ORNL's Power Electronics and Electric Machinery Research Center developed and demonstrated the world's first high-power (20-kW) wireless charging system for passenger cars. The ORNL system achieved 90% efficiency at three times the rate of the plug-in systems commonly used for electric vehicles.

Industry partners from Toyota, Cisco Systems, Evatran, and Clemson University International Center for Automotive Research contributed to the technology development.

> "We have made tremendous progress from the lab proof-of-concept experiments a few years ago," said research team lead Madhu Chinthavali. "We have set a path forward that started with solid engineering, design, scale-up and integration into several Toyota vehicles. We now have a technology that is moving closer to being ready for the market."

The 20-kW system features a unique architecture with an ORNL-built inverter, isolation transformer, vehicle-side electronics, and coupling technologies. For the demonstration, researchers integrated the single-converter system into an electric Toyota RAV4 equipped with an additional 10-kWh battery.

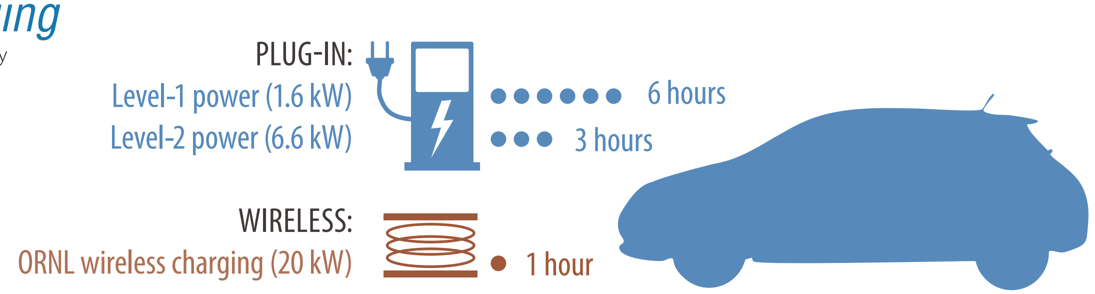
The research team is not stopping at 20 kW. On the horizon is a 50-kW charging system that would match the power levels of commercially available plug-in quick chargers. Providing the same speed with the convenience of wireless charging could increase consumer acceptance of electric vehicles and is considered a key enabler for hands-free, autonomous vehicles. Higher power levels are also essential for powering larger vehicles such as trucks and buses.

"Wireless power transfer is a paradigm shift in electric vehicle charging that offers the consumer an autonomous, safe, efficient, and convenient option to plug-in charging," said Dr. David Smith, vehicle systems program manager. "This technology is a stepping stone toward electrified roadways where vehicles could charge on the go."

The DOE Vehicle Technologies Office provided funding for this competitively selected project. Other members of the ORNL project team were Steven Campbell, Paul Chambon, Dr. Omer Onar, Dr. Burak Ozpineci, Larry Seiber, Dr. Lixin Tang, Cliff White, and Randy Wiles, as well as retired staff members Curt Ayers, Chester Coomer, and Dr. John Miller.

Electric vehicle charging

Calculated charging times for a 20-kWh battery



ORNL partners with Delphi on inverter for 2016 Chevy Volt

Technology innovations developed as part of a DOE and U.S. DRIVE co-funded project contributed to the inverter design of the 2016 Chevrolet Volt.

The Volt uses a second-generation "Voltec" extended-range electric powertrain with a traction power inverter module (TPIM) designed to increase efficiency, performance, and durability. The module includes a novel dual-sided cooled package, which is used as the power device for the Volt's TPIM.

ORNL conducted electrical characterization, modeling, and drive system simulation to assist Delphi with technology development. Researchers evaluated the Delphi-developed 600-V package over a range of temperatures (25°C to 150°C), currents (10 A to 300 A), and voltages (250 V to 325 V). ORNL data were used to develop behavioral loss models that were incorporated in the system-level model.

The silicon dual-sided cooled power device package enabled the inverter module to deliver more uniform current density than traditional single-sided power modules. The improved packaging delivered a 30% reduction in thermal resistance and a 17% reduction in conduction losses, contributing to a 10% increase in vehicle fuel economy.

Research for the project was supported by the DOE Vehicle Technologies Office and conducted in collaboration with the National Renewable Energy Laboratory.

2016 Chevy Volt

Novel motor achieves 75% higher power without rare earth materials

Most motors in electric and hybrid electric vehicles rely on permanent magnets to make the rotors spin and produce torque. These permanent magnets are commonly made with imported rare earth materials that account for about 40% of the total motor cost.

Researcher Tim Burress works with a prototype motor that uses ferrite permanent magnets.

ORNL researchers Tim Burress, Jason Pries, Dr. Lixin Tang, and Randy Wiles designed and demonstrated a prototype motor that achieved 75% higher power than commercial motors without the use of expensive rare earth materials. Instead, the novel motor uses permanent magnets made of ferrite, a common iron oxide that is both highly electrically resistive and magnetic.

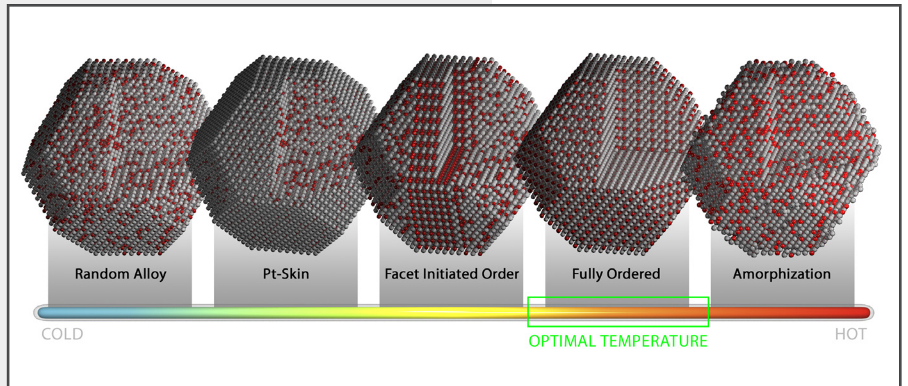
"We are focused on increasing energy security for the nation by designing efficient high-performance motors built with materials that are both economical and abundantly available here in the United States," said research lead Tim Burress.

In dynamometer evaluations, the motor achieved a peak power of 103 kW and exceeded DOE targets for specific power, efficiency, and cost. It is comparable in size to the 60-kW motor found in the Toyota Prius.

The design is a promising solution to eliminate costly rare earth materials in motors while packing more power into a smaller package.

This research was supported by the DOE Vehicle Technologies Office.

Microscopy captures real-time view of evolving fuel cell catalysts



Models of platinum-cobalt nanoparticle catalysts illustrate how specific atomic configurations originate and evolve as the particles are heated.

Atomic-level imaging of catalysts by scientists at ORNL could help manufacturers lower the cost and improve the performance of emission-free fuel cell technologies.

Fuel cells rely on costly platinum catalysts to enable the necessary reactions that convert chemical energy into electricity. Alloying platinum, for example, with transition metals such as cobalt reduces the overall cost, but these alloyed catalysts vary in performance based on their atomic structure and processing history.

ORNL scientists used scanning transmission electron microscopy to track atomic reconfigurations in individual platinum-cobalt nanoparticle catalysts as the particles were heated inside the microscope. The in situ measurements allowed researchers to collect atomic-level data that could not be obtained with conventional microscopy techniques.

Very small changes in the positions of platinum and cobalt atoms affect the catalyst's overall activity and selectivity, so annealing—a gradual heating, holding, and cooling process—is often used to modify the alloy's surface structure. The ORNL in situ microscopy experiments documented exactly what, when, and how specific atomic configurations originate and evolve during the annealing process.

"You can anneal something from room temperature to 800°C, but you don't know at which point you should stop the process to ensure the best catalytic performance," ORNL researcher Dr. Miaofang Chi said. "Because you don't know how the particle evolves, you might be missing the optimum surface configuration."

The atomic-level detail in the ORNL study will guide researchers and manufacturers who want to fine-tune their catalysts' atomic structure to meet the demands of a specific application.

"This work paves the way toward designing catalysts through post-synthesis annealing for optimized performance," Chi said.

The research was sponsored by the Fuel Cell Technologies Office in DOE's Office of Energy Efficiency and Renewable Energy, and microscopy was performed at ORNL's Center for Nanophase Materials Sciences, a DOE Office of Science user facility. Other research team members include ORNL's Dr. Karren More, Dr. Andrew Lupini, and Dr. Lawrence Allard, as well as partners from Johns Hopkins University, University of Pittsburgh, and Argonne National Laboratory.

Facility provides capabilities to examine materials at their core

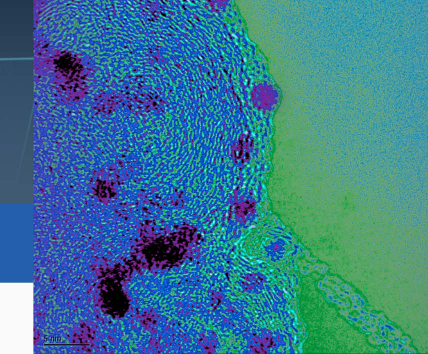
Unraveling the mysteries of the materials that shape and support the world involves characterization, taking a deeper dive into chemical processes. From catalysis and corrosion to fluid transport, characterization allows scientists to better understand what makes materials react and change.

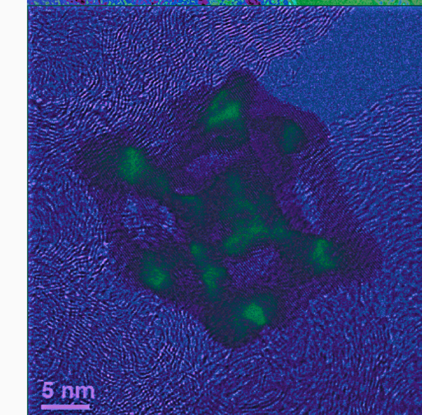
ORNL's Materials Characterization Core (MCC) provides a single source for scientists and researchers from the public and private sectors to access a range of microscopy, spectroscopy, and other characterization techniques and services to obtain insight into the structure and composition of materials at the atomic level.

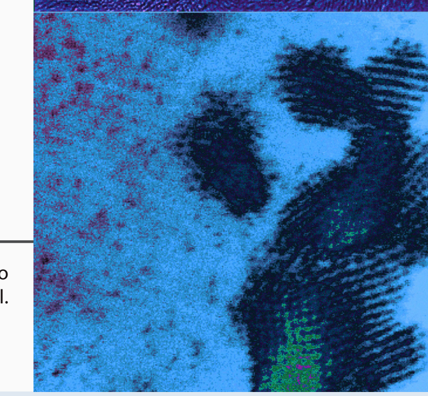
MCC is the DOE Fuel Cell Technologies Office's (FCTO's) leading resource for characterization of fuel cell materials such as catalysts and catalyst supports, membranes, electrodes, and gas diffusion layers.

Through a new cost-share program sponsored by FCTO, a team of MCC scientists led by Dr. Karren More and Dr. David Wood can collaborate directly with organizations on projects that align with the DOE and FCTO missions.

The FCTO program offers a 50% cost share to the organization, which can then work closely with ORNL staff to evaluate new materials, gain insights at the atomic level, and develop solutions to industry challenges. For example, Proton Onsite has worked with MCC on development of their proton exchange membrane electrolysis system.



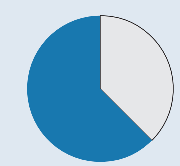




MCC allows scientists to gain insights into materials at the atomic level.

Improving cost, scalability, durability, and safety

40% reduction in cost



- Cost Savings: $.50 per gasoline gallon equivalent
- Pressure Capacity: 875 bar
- Storage Vessel Weight: 90 kg

Hydrogen storage vessel solves embrittlement problem

The stationary storage vessel optimizes cost, scalability, durability, and safety.

A stationary vessel developed by ORNL researchers Dr. Zhili Feng and Dr. Yanli Wang could be the key to less expensive hydrogen storage, making it possible for more hydrogen-powered vehicles to hit the road in the near future.

ORNL researchers have designed a steel-concrete composite vessel that optimizes cost, scalability, durability, and safety by effectively solving the hydrogen embrittlement problem that causes corrosion in conventional stainless steel containers. The steel-concrete composite vessel includes small vents to prevent pressure buildup.

By allowing the hydrogen to migrate through the innermost layer of the vessel through ports, the design of the vessel mitigates hydrogen embrittlement in a layered steel alloy vessel. The design is safer and more cost-effective, making it easier to store hydrogen at the station.

This research was funded by the DOE Fuel Cell Technologies Office.

New perspective on ignition modes opens opportunities

Advanced compression ignition modes are being viewed in a different light thanks to research from ORNL.

Low-temperature combustion (LTC) strategies have been widely studied due to their potential for high efficiency and low emissions of pollutants like NOx. Achieving LTC using gasoline compression ignition engines is a topic of broad interest and considerable efforts on the part of the research community.

Researchers Adam Dempsey, Dr. Scott Curran, and Dr. Robert Wagner provided a new perspective on gasoline compression ignition modes in a paper published in the *International Journal of Engine Research*. The authors used computational fluid dynamics modeling to demonstrate that these modes, which have been previously studied as distinct methods for achieving combustion efficiency, are actually a spectrum driven by fuel stratification or the mix of fuel and air at the time of ignition.

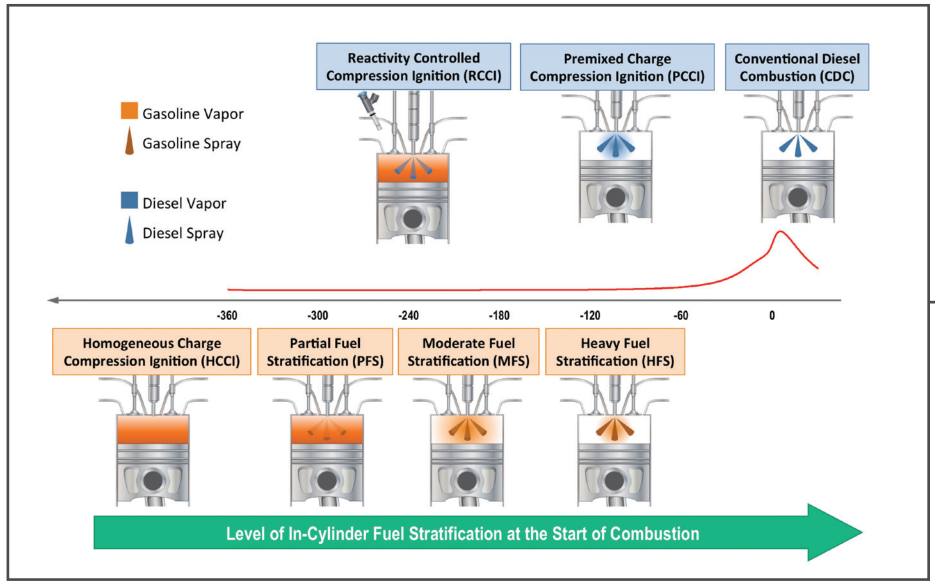
"The level of fuel stratification for these advanced combustion modes is, in reality, a continuum ranging from fully premixed (i.e., homogeneous charge of fuel and air) to heavily stratified, heterogeneous operation," explained Curran. "This perspective changes the way we think about approaches to achieving LTC and provides a missing link for the research community at large."

Researchers from across the national laboratory system are applying this new perspective to the DOE Co-Optimization of Fuels and Engines initiative, which aims to accelerate the introduction of innovative combustion strategies and fuels designed together to maximize performance and energy efficiency.

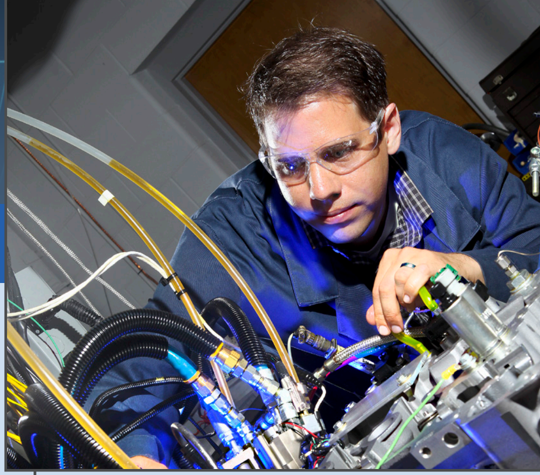
"One thrust of the Co-Optimization initiative is focused on advanced compression ignition strategies, and this new perspective is guiding our approach to this space," said Dr. Robert Wagner, director of ORNL's Fuels, Engines, and Emissions Research Center and steering committee member for the DOE initiative.

> "Looking at gasoline compression ignition as a spectrum rather than a series of separate modes eliminates complexity and opens up new opportunities," said Wagner.

The published findings are among the most-read articles for the journal online. This research was conducted with support from the DOE Vehicle Technologies Office (VTO). The Co-Optimization of Fuels and Engines initiative is supported by both DOE VTO and the DOE Bioenergy Technologies Office.



Advanced compression ignition combustion strategies are shown as a continuum based on the level of fuel stratification at ignition.



ORNL's Dr. Jim Szybist works with a single cylinder engine to measure fuel characteristics.

Discovery will inform future design of fuels and engines

A phenomenon first identified by ORNL researchers Dr. Jim Szybist and Dr. Derek Splitter could have implications for the future design of fuels and engines.

Fuels are commonly given an octane rating, which is a measure of how much compression the fuel can withstand before it ignites. Research octane number, known as RON, is one such measure that has been standard for almost a century.

Enter the new kid on the block, the turbocharged engine. Smaller and lighter than standard gasoline engines, turbocharged engines produce more power by packing more air and fuel into the combustion chamber. These conditions are not well represented by standard ratings like RON.

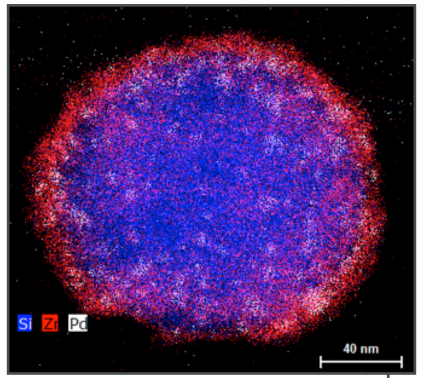
Szybist and Splitter used three different fuels with the same RON and discovered dramatically different fuel behaviors at the higher pressures common in turbocharged engines. For some fuels, burning started before the spark plug triggered ignition without it leading to engine knock.

"Pre-spark heat release under turbocharged conditions is a phenomenon that needs to be taken into account, because it is not being accurately captured by the current models," said Szybist. "We are now operating in a temperature and pressure space outside the bounds that we have historically subjected fuels to and outside where we have a good rating system for fuel quality."

Szybist and Splitter are continuing to examine the relationship between fuel composition and fuel behavior at high pressures as part of the DOE Co-Optimization of Fuels and Engines initiative, which aims to simultaneously accelerate the development of new fuel and engine technologies for maximum efficiency and petroleum displacement. This research was supported by the DOE Vehicle Technologies Office.

Advanced catalyst technology excels at low temperatures

As advanced engines become more efficient, more of the heat generated during combustion is being converted into power, and less heat escapes through exhaust. This improves fuel economy, but it also creates a need for new catalyst technologies that are effective at lower temperatures.



Researchers developed a technique for creating zirconia-coated catalyst supports that enable efficient, durable catalyst operation at low temperatures.

Researchers Dr. Todd Toops, Eleni Kyriakidou, and Dr. James E. Parks, II developed a new synthesis approach that improves low-temperature performance for platinum group metal (PGM) catalysts, the current standard for control of emissions.

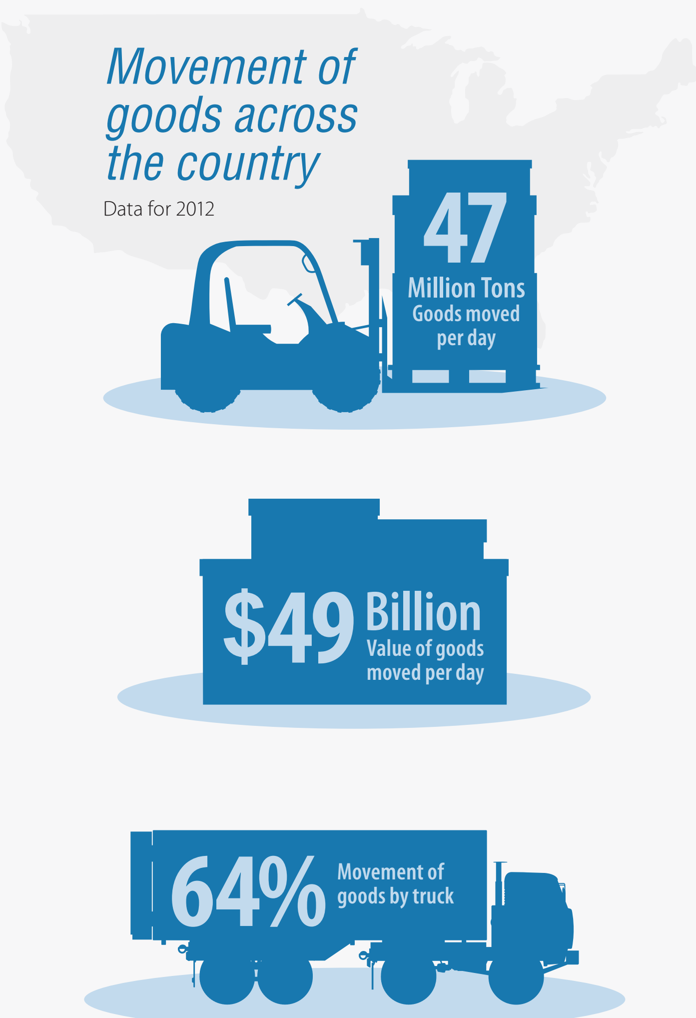
The effectiveness of PGM catalysts can be enhanced by the material that is used to support them in the emissions device. Zirconia is commonly used for supports as it is both durable and known to increase catalyst reactivity, but it also has a low surface area, which can limit overall performance. ORNL researchers took advantage of this enhanced reactivity and solved the surface area issue by coating zirconia like a shell over a high surface area silica support.

This core-shell technique significantly increases the surface area of the zirconia support, providing more opportunity for the PGM catalysts to react efficiently with pollutants.

Working with both Pt and Pd catalysts, researchers demonstrated that supports created with this new coating technique worked efficiently at low temperatures, turning common hydrocarbons such as propane, propylene, and ethylene into benign substances like carbon dioxide and water.

The new catalyst synthesis technique shows great potential to control emissions from advanced combustion engines that have low exhaust temperatures. This research was sponsored by the DOE Vehicle Technologies Office and performed, in part, using instrumentation provided by the DOE Office of Nuclear Energy.

A freight database developed by ORNL helps transportation officials improve highways, railroads, ports, and other trade routes across the country.



Data help officials keep the nation's freight moving

A freight database developed with assistance from ORNL helps transportation officials improve highways, railroads, and other trade routes across the country.

A team of ORNL researchers provided specialized data development, statistical analysis, and modeling support to create the Freight Analysis Framework (FAF), the most comprehensive and widely used freight transportation data source in the United States.

The Department of Transportation updates the framework every 5 years based on numbers from its Bureau of Transportation Statistics (BTS) Commodity Flow Survey, which captures about 70% of freight transportation. ORNL fills in the other 30%, adding data on the domestic movements of foreign trade, as well as crude petroleum and retail services that are not represented in the BTS survey.

Researchers applied modeling techniques to integrate disparate data sources into a comprehensive database that provides a national picture of freight flows.

> "Freight Analysis Framework data help planners in the public and private sectors to better understand freight movement, analyze market trends, and make strategic decisions," said Diane Davidson, leader of ORNL's Transportation Planning and Decision Science Group. "Transportation planners use it to target resources to improve operations or increase capacity."

The database captures freight movement by origin, destination, commodity, mode, trade type, tonnage, and value. Users can determine the amount and type of goods that move by highway, waterway, rail, and other modes of transportation between states, regions, and across the nation. An ORNL-developed data extraction tool makes it easy for users to access the information they need online at http://faf.ornl.gov.

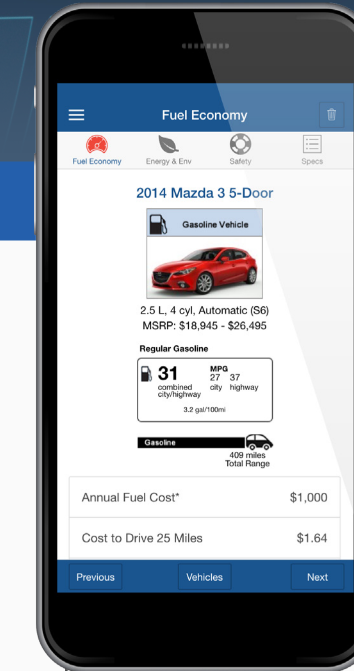
FAF is one of the most used tools in the suite of transportation analytics developed by ORNL. Analytics support vehicle and transportation-system-wide efficiency gains through the development of predictive information, analytical methods, and vehicle systems data. Dr. Ho-Ling Hwang served as ORNL technical lead on the project, which was jointly funded by DOT BTS and the Federal Highway Administration.

Compare vehicles, mileage, and more at fueleconomy.gov

What type of vehicle to purchase depends on a variety of variables including fuel economy ratings, safety, maintenance history, and energy impacts. ORNL, in collaboration with the DOE Vehicle Technologies Office, provides one source for all of this information and more at fueleconomy.gov.

ORNL works with data provided by the US Environmental Protection Agency to offer the latest facts on all vehicles including those that use alternative fuels and electricity.

Consumers can make side-by-side comparisons; view best and worst miles-per-gallon lists; calculate gallons and dollars saved; and estimate, record, and track fuel economies on the site. In addition, ORNL published a downloadable and printed version of the latest data in the Fuel Economy Guide and offered a new, free Find-A-Car app for mobile users to compare vehicles on the go.

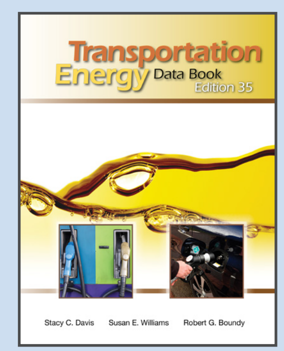


A team led by researcher Rick Goeltz developed the Find-A-Car app as a tool for car buyers to compare vehicles on the go. The free app was downloaded more than 12,504 times in 2016.

Market acceptance modeling tool available online

A MiniTool that offers a web-based lite version of MA^{3}T (Market Acceptance for Advanced Automotive Technologies) has been released and demonstrated by ORNL researchers Dr. Zhenhong Lin, Dr. Fei Xie, and Rick Goeltz. MA^{3}T is a market dynamics model that estimates demands for advanced vehicle powertrain technologies in response to assumptions about technology, infrastructure, consumers, and policies. The MiniTool provides a user-friendly interface for nontechnical users to modify input scenarios such as battery cost or infrastructure deployment and immediately observe the effect on market shares. To view the tool, visit http://teem.ornl.gov/minitool. This research was funded by the DOE Vehicle Technologies Office.

ORNL data support strategic decisions, public outreach

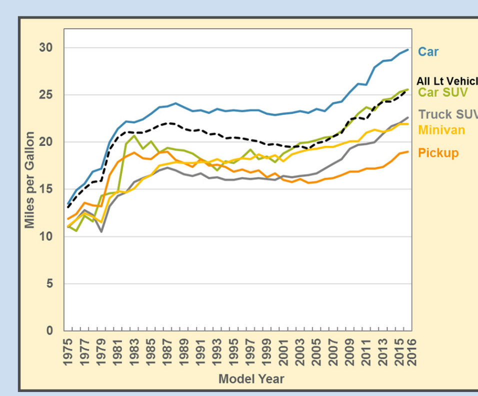


An ORNL team led by Stacy Davis continued its long-standing support of DOE Vehicle Technologies Office (VTO) public communication efforts by publishing the *Transportation Energy Data Book*, the *Vehicle Technologies Market Report*, and the "Fact of the Week" for the VTO home page.

The 35th edition of the *Transportation Energy Data Book* provides a wide range of current and historical transportation data, which serve as a foundation for policymakers, transportation analysts, and VTO staff in making strategic decisions. Approximately 9,100 visitors per month used the resource online, and hard copies were distributed to a nationwide mailing list.

The 2015 *Vehicle Technologies Market Report* was the seventh edition published by ORNL. The colorful graphics-based report details major trends in US transportation, including the use, markets, manufacture, and supply chains for light- to heavy-duty vehicles. Approximately 4,800 visitors per month accessed the report online.

Every Monday morning, ORNL provides a new Fact of the Week for the VTO home page (https://energy.gov/eere/vehicles/current-and-past-years-facts-week) and emails it to a subscriber list of 3,049. The topics align with the VTO mission and offer stakeholders and the general public readily accessible data points on transportation trends.



Fact #955: New light vehicle fuel economy by vehicle class and model year, 1975–2016. For more details, visit https://energy.gov/eere/vehicles/fact-955-december-12-2016-new-light-vehicle-fuel-economy-all-time-high

BUILDING BIOMASS

The *2016 Billion-Ton Report* builds on previous studies and offers updated projections of the economic availability of feedstocks across the nation.

US holds potential to produce a thriving bioeconomy by 2040

From the forests to the fields, the United States is rich in biomass, with the potential to sustain a burgeoning bioeconomy through renewable resources.

The *2016 Billion-Ton Report*, jointly released by ORNL and the US Department of Energy's Bioenergy Technologies Office, provides detailed analyses of what those resources are and where they are located—now and in the future—on a local, regional, and national scale.

The report concludes that the nation has the potential to sustainably produce at least 1 billion dry tons of nonfood biomass resources annually by 2040. Renewable resources include agricultural, forestry, and algal biomass, as well as waste. From currently available logging and crop residues to future available algae and dedicated energy crops, these resources are useable for the production of biofuel, biopower, and bioproducts.

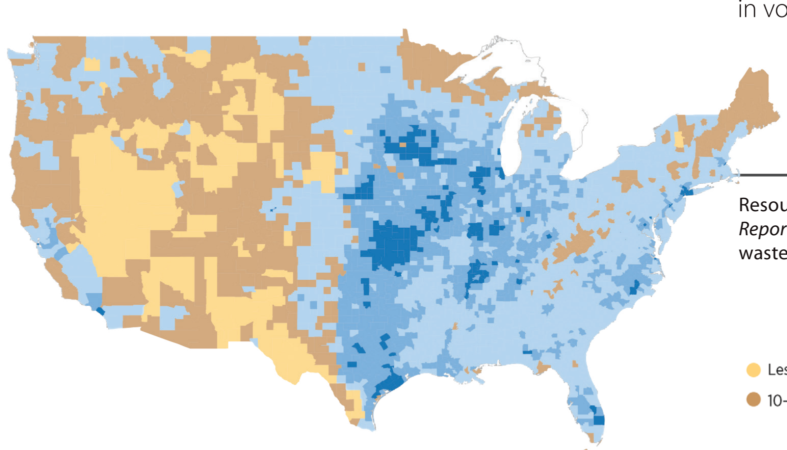
The findings show that the United States could increase biomass production from 365 million dry tons to 1.5 billion dry tons under a high-yield scenario. The report also considers how the cost of preprocessing and transporting biomass to the biorefinery may impact feedstock availability.

Interactive tools available through the Bioenergy Knowledge Discovery Framework (bioenergykdf.net) allow researchers, policymakers, stakeholders, and the public to map and visualize biomass availability scenarios, tailoring the data by factors such as geographic area, biomass source, and price. In 2016, users generated more than 8,000 visualizations.

> "It's our hope that our resource analysis work can inform strategies and contribute to the realization of a billion-ton bioeconomy vision," said ORNL principal investigator Matt Langholtz.

The analysis was led by ORNL with contributions from 65 experts from federal agencies such as the US Forest Service, Department of Agriculture, Environmental Protection Agency, Department of Transportation, and Federal Aviation Administration, as well as other national laboratories, universities, and industry.

ORNL and DOE produced the first billion-ton study in 2005, followed by an update in 2011. The current report updates and expands upon the previous studies and will soon include a first-ever second volume, which will provide analyses of the potential environmental effects of several scenarios presented in volume one.



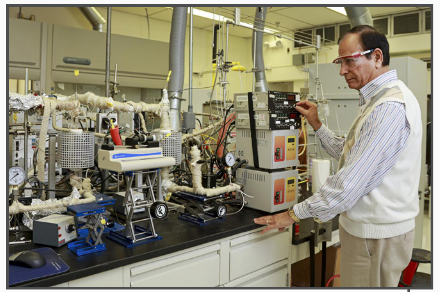
Resource analysis conducted as part of the *2016 Billion-Ton Report* shows the combined potential supplies from forestry, wastes, and agricultural resources for 2040.

Energy-efficient reaction drives ORNL biofuel conversion technology

Researchers are working with licensee Vertimass LLC to scale an ORNL-developed conversion technology to the commercial level. The technology offers a pathway to convert biobased ethanol into hydrocarbon blend-stocks for use with gasoline, diesel, and jet fuels.

As the scientists were developing this new type of catalytic conversion technology, they found that the underlying reaction unfolds in a different manner from what previous studies of similar zeolite catalysts suggested.

It has long been thought that these types of reactions must first go from ethanol to ethylene and then on to form longer chains. In a study published in *Scientific Reports*, ORNL researchers showed that this energy-consuming intermediate step is not necessary for the conversion to happen. Instead, a hydrocarbon pool mechanism allows the zeolite catalysts to directly produce longer hydrocarbon chains from the original alcohols.



Dr. Chaitanya Narula led analysis of an ORNL biofuel-to-hydrocarbon conversion technology to explain the underlying process.

The research, supported by the DOE Bioenergy Technologies Office, has implications for the energy efficiency and cost of catalytic upgrading technologies proposed for use in biorefineries. Uncovering the mechanism behind the reaction helps support the potential economic viability of ORNL's direct biofuel-to-hydrocarbon conversion approach.

World's experts tour region's biomass resources

Bioenergy stakeholders and scientists from across the globe convened at ORNL for the Southeastern United States Bioenergy Study Tour in April 2016. Led by Virginia Dale, the 5-day tour of the Southeast gave guests a first-hand view of the regional bioeconomy and spurred science-based discussions of bioenergy innovations developed by ORNL and the DOE Bioenergy Technologies Office.

Developing international codes and standards for the bioenergy industry

Working closely with industry and the international bioenergy community, researchers are developing codes and standards that facilitate the growth of the bioeconomy.

As part of the Biomass Industry Panel for Codes and Standards, ORNL's Dr. Erin Webb conducted experiments to determine how factors such as feedstock type and bale size, shape, and spacing affect the speed at which a biomass fire can spread. These studies informed the development of standards on the safe handling and storage of biomass to reduce fire risks for the bioenergy industry. The effort has led to five changes to the International Building Code to date.

Studies by Dr. Mike Kass analyzing the compatibility of elastomers, metals, and sealants with ethanol-blended fuel in underground storage tank systems were cited in the federal register for storage standards.

ORNL researchers Maggie Davis and Keith Kline contributed to the development and adoption of a new standard recognized by the International Organization for Standardization (ISO: 13065) that specifies principles, criteria, and indicators for the whole bioenergy supply chain to facilitate assessment of environmental, social, and economic aspects of sustainability.

These research efforts were funded by the DOE Bioenergy Technologies Office.

SUSTAINABLE TRANSPORTATION PROGRAM *by the numbers*

$80 Million R&D Budget

244 2016 Publications

- 9 Books and chapters
- 35 Proceedings of conferences
- 179 Journal articles
- 21 Technical reports

149 Industry Partners

- 30 University Partners
- 25 Collaborative Research and Development Agreements
- 100 Strategic Partnership Projects
- 5 Small Business Voucher Projects

Research Areas

- Bioenergy technologies
- Data science and connected vehicles
- Electric drive technologies
- Energy storage
- Fuel cell technologies
- Fuels, engines, and emissions
- Lightweight materials
- Propulsion materials
- Vehicle systems integration
- Vehicle cyber security

USDRIVE

13 2015 U.S. DRIVE Highlights

Researchers and Fellows

220 Scientists and Engineers

32 Professional Society Fellows

Science Awards

22 R&D 100 Awards

5 2016 SAE Awards

TRANSFERRING TECHNOLOGY TO MARKET

2016 Patents

25 Invention Disclosures

16 Patent Applications

14 Patents Awarded

ORNL technologies licensed in 2016 included the following:

Carbon fiber precursor

LeMond Composites licensed an ORNL process that converts acrylic textile material into carbon fiber, reducing costs by 50%. Four other licenses are pending for the technology.

Carbon fiber production

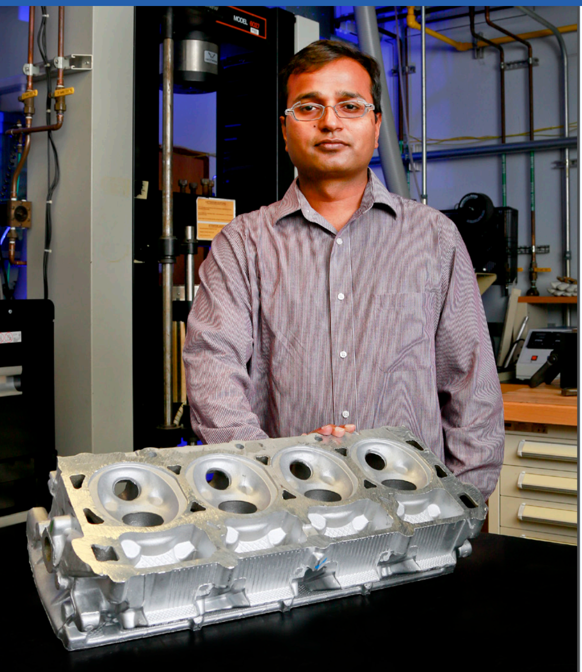
RMX Technologies licensed ORNL plasma oxidation technology that reduces energy consumption by 75%, shortens production time by 2.5–3x, and decreases production costs by 20%.

Lithium-sulfur batteries

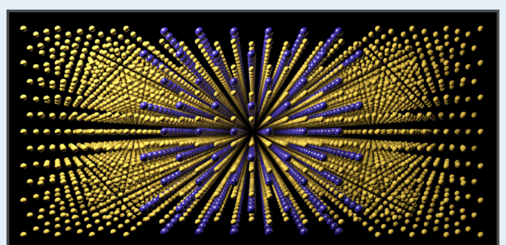
Solid Power, Inc. licensed a portfolio of ORNL battery technologies to develop safe solid-state rechargeable batteries with high energy density.

iDriving real-time data

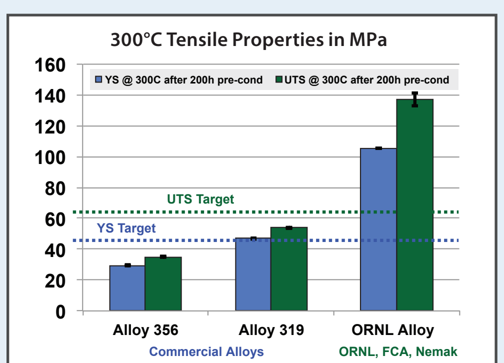
SanTed Project Management LLC licensed technology to determine how driving style factors impact fuel economy in real-time for the trucking industry.



A team of researchers led by ORNL's Dr. Amit Shyam is using high-performance computing to speed the development of new high-temperature aluminum alloys for automotive cylinder heads.



Atomic structure of new aluminum alloy.



ORNL-developed alloy outperformed common aluminum alloys in yield strength and ultimate tensile strength at 300°C.

Atoms to engines:

Accelerating alloy development using high-performance computing

A team led by ORNL material scientist Dr. Amit Shyam has developed a group of stronger, more heat-resistant aluminum alloys for high-efficiency automotive engines.

Automakers need powertrain materials that are not only lighter but also low cost and able to withstand the elevated temperatures and pressures in high-efficiency turbocharged engines.

> "With standard materials development methods, it usually takes 10 to 20 years to deliver new alloys," said ORNL propulsion program manager Dr. Allen Haynes. "The progress this team has accomplished in the past three years is groundbreaking."

Researchers applied the big science capabilities available at ORNL to speed the process of alloy development, taking an integrated computational materials engineering approach. Their methods included development of models based on first-principles quantum mechanics and the scaling of those models for use on the Titan supercomputer.

Models were validated using atom probe tomography and scanning transmission electron microscopy. With these tools at hand, the researchers tailored new alloys at the atomic level to achieve the strength and high-temperature stability necessary for use in automotive cylinder heads for next-generation engines.

Working closely with industry partners FCA US LLC and Nemak, the ORNL-led team made a series of microstructural discoveries that were applied to the design of an affordable new family of cast Al-Cu alloys that are much more heat tolerant than those currently in commercial use.

The team's best performing alloy retained its strength and stability after 200 hours at 300°C and doubled DOE's mechanical properties targets at this temperature.

In the next year, Nemak will cast a full size cylinder head from the alloy for FCA to evaluate on an engine. Microstructural discoveries, methods, and materials genome information will be shared through publication in scientific journals.

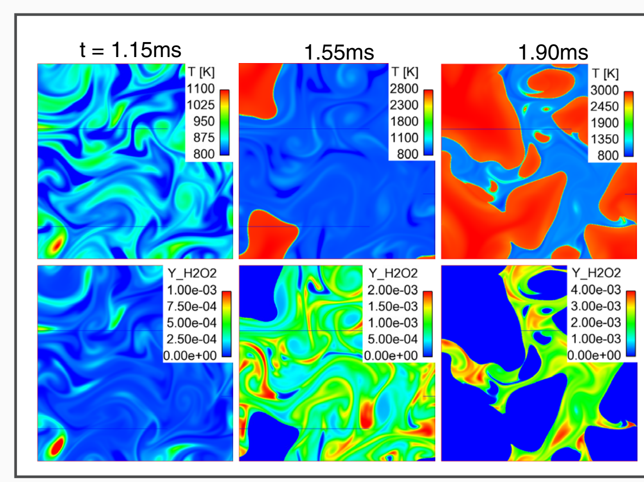
The Oak Ridge Leadership Computing Facility, a DOE Office of Science–funded user facility, approved 6 million hours on Titan for the ORNL alloy development project. The DOE Office of Basic Energy Sciences supports the microscopy equipment used for this project. The research to develop the new cast aluminum alloys is funded by the DOE Vehicle Technologies Office Propulsion Materials Program.

Turbocharging R&D with high-performance computing

ORNL is home to Titan, one of the fastest computers in the world. Using that processing power, scientists are partnering with industry to tackle complex challenges in transportation. Knowledge discovery and technology development are the primary goals of this work, which includes supercomputing projects focused on magnetic materials for advanced electric machines and predictive modeling of energy storage technologies. The projects below are a sampling of computational research led by Dean Edwards and Dr. Charles Finney.

General Electric:
Optimizing dual-fuel combustion

General Electric and ORNL are using high-performance computing to investigate key factors that promote cyclic variability in dual-fuel (natural gas/diesel) engines. These variations in combustion performance limit the potential benefits of dual-fuel operation and can even damage the engine. Using Titan, researchers performed hundreds of simultaneous computational fluid dynamics (CFD) engine simulations to increase understanding of how small changes in engine operation affect combustion. The original project received support through the Oak Ridge Leadership Computing Facility (OLCF), which is funded by the DOE Office of Science. Researchers are continuing the work in collaboration with Argonne National Laboratory and Convergent Science under a DOE ASCR Leadership Computing Challenge (ALCC) award and with support from the DOE Vehicle Technologies Office (VTO).



Direct numerical simulation results showing initiation and progression of end-gas knock.

General Motors:
Developing new fuel injectors

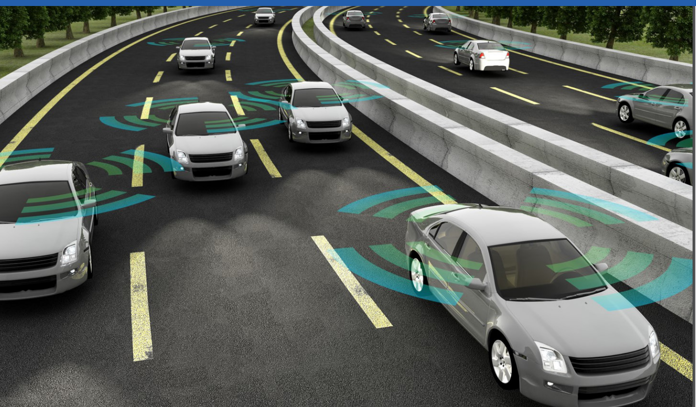
General Motors and ORNL used supercomputing to advance knowledge of spray physics and increase confidence in applying modeling tools to the development of novel fuel injectors and combustion systems that offer improved fuel efficiency. Researchers developed and demonstrated a CFD modeling approach that predicts the structure of gasoline fuel sprays due to fuel temperature and ambient pressure. The method reduced the time to perform these calculations by a factor of three. The project received an ALCC award and support from the DOE VTO.

General Motors:
Modeling engine emissions

General Motors, ORNL, and Lawrence Livermore National Laboratory (LLNL) are developing predictive simulation tools for virtual engine design and calibration that could greatly reduce the number of on-engine experiments required to ensure new engine technologies meet performance and emissions standards. Using a GPU-enabled chemistry solver toolset developed by LLNL with CONVERGE CFD modeling software, the researchers significantly improved emissions predictions across the full operating range of the engine. The project received an ALCC award and support from DOE VTO.

Ohio State University:
Predicting engine knock

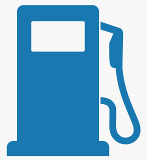
ORNL is assisting Ohio State University in developing models to predict the occurrence of knock in engines. Knock—named for the sound an engine makes when fuel pre-ignites in an uncontrolled state—is a limiting factor for efficient combustion and engine design. Being able to better predict the factors that contribute to knock can speed the development of new engine technologies. Dr. Derek Splitter is the principal investigator for this project, which is supported by DOE VTO.



Researchers are developing controls for CAVs to smooth traffic flow, reduce fuel consumption and emissions, and increase safety on the nation's roadways.

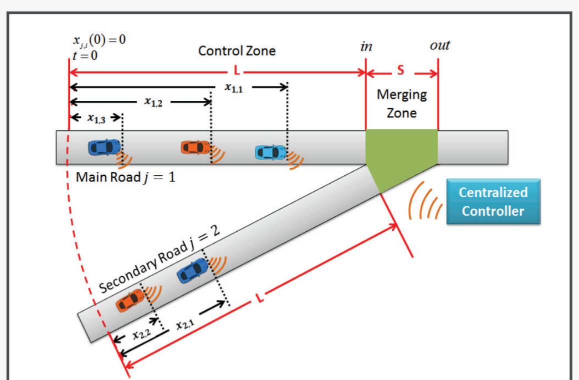
Optimizing traffic flow at highway on-ramps

Simulation results show a potential



50% Reduction in Fuel Consumption

7% Reduction in Travel Time



Simulations using ORNL-developed algorithms showed the potential to reduce fuel consumption by up to 50% and travel time by 7% for CAVs merging at highway on-ramps.

Algorithms rev up fuel efficiency for connected and automated vehicles

A future where vehicles exchange communications with each other and with the infrastructure seems right around the corner. How to take advantage of this emerging connectivity to alleviate traffic congestion, reduce fuel consumption and emissions, and increase safety on the nation's roadways is a complex challenge that researchers at ORNL are investigating.

Scientists Dr. Andreas Malikopoulos and Dr. Jackeline Rios-Torres have developed algorithms and an optimization framework to coordinate traffic flow and increase energy efficiency for connected and automated vehicles (CAVs). One of the scenarios they examined focused on vehicles merging at highway on-ramps.

When implemented in simulations with traffic made up entirely of CAVs, these optimization controls showed the potential to reduce fuel consumption by up to 50% and travel time by 7%.

With near-term traffic more likely to include a mix of CAVs and traditional vehicles, the team also assessed the potential energy efficiency benefits of different numbers of CAVs on the road.

The analysis found fuel consumption is reduced by 40% if only 30% of the vehicles are CAVs, demonstrating that energy savings from CAVs could come relatively early in the consumer adoption process. However, to achieve the 7% savings in travel time, at least 70% of the vehicles on the merging roads must be CAVs.

Malikopoulos and team were awarded a grant from DOE's Advanced Research Projects Agency-Energy (ARPA-E) to advance their algorithm work, with a focus on achieving a 20% improvement in vehicle energy efficiency. The grant challenges the team to develop novel two-level optimization controls for CAVs that coordinate traffic flow and routing while optimizing real-time powertrain efficiency.

The results of ORNL research focused on CAVs have been published in a series of seven papers to date. This research was supported by the DOE Vehicle Technologies Office and through ORNL Laboratory Directed Research and Development funds.

Coming soon to a road near you: safer, more secure vehicles

Connected vehicle technology has the potential to reduce accidents by 81% according to a study by the US Department of Transportation (DOT). With the opportunity to save lives, save money, and even save fuel, Jason Carter of ORNL's Cyber and Information Security Research Group calls this new connectivity "a game changer."

Carter and his team have been assisting DOT on connected vehicle research since 2012. In fact, ORNL's work was cited in DOT's 2014 proposed rulemaking announcement regarding the potential regulation of vehicle-to-vehicle and vehicle-to-infrastructure connectivity.

In the near future, new vehicles will include devices to allow them to communicate (connect) with similar devices in other vehicles, sending basic safety messages with information such as vehicle position, direction, speed, braking status, and size. Similar information will also be transmitted to stationary devices in the infrastructure, such as "smart" traffic lights.

Before this can happen, several challenges associated with the technology must be addressed. Carter is currently working on two interconnected projects with DOT, one addressing security issues, the other privacy.

Authenticating messages

There is a critical need to have a means of ensuring the validity or trustworthiness of the messages exchanged between vehicles and between vehicles and the infrastructure without revealing identifying information. ORNL assessed the feasibility of building an authentication system with the trust/validation function delegated to the vehicles as well as various technical approaches. The team has delivered a concept of operations for this vehicle-based security system and is working on more in-depth modeling and vetting of some of the approaches. When implemented, this security system will be one of the largest of its kind ever.

ORNL is assisting DOT with the development of a vehicle-based credential management system that can increase safety and security while maintaining privacy in connected and automated vehicle communications.

Ensuring privacy

Researchers are looking at technology known as "privacy-preserving data publishing," where certain identifying characteristics are removed or modified so the likelihood of the data being associated with a particular individual is reduced while the usefulness of the data is retained. The ORNL team successfully developed algorithms to do this for vehicle trajectory information collected from pilot studies, and they are applying and further developing this system.

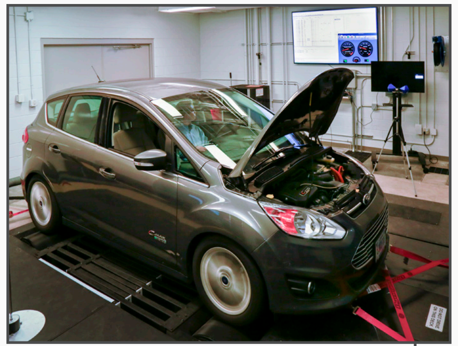
These projects are supported by the National Highway Transportation Safety Administration, the Federal Highway Administration, and the Intelligent Transportation Systems Joint Program Office.

Improving cybersecurity for connected and automated vehicle technologies

Modern vehicles are essentially computers-on-wheels, operating with an average of 100 million lines of code and 150 control units. Those numbers are on the rise as automakers expand safety, entertainment, and autonomous driving features. Each of these sensors and connectivity features—from adaptive cruise control to Wi-Fi and GPS—creates a potential opening for cyberattack.

ORNL is working to address this national transportation challenge through research and development focused on predictive assessment of potential threat vectors—partnering with industry to engineer secure solutions for new vehicles before they hit the road.

In 2016, ORNL augmented long-standing cybersecurity capabilities with a new Vehicle Security Laboratory established at the National Transportation Research Center (NTRC). The facility, with its full vehicle dynamometer and specialized scanning equipment, has been key to recent research into methods of detecting vehicle network intrusions.



The Vehicle Security Laboratory at NTRC integrates ORNL expertise in vehicle systems, cyber security, and predictive modeling.

Researchers Dr. Robert Bridges, Dr. Stacy Prowell, Frank Combs, Michael Moore, and Michael Starr are using the new laboratory to develop a method to detect anomalies in the timing of signals in the onboard vehicle communications network. These variations in signal patterns can indicate cyberattack. The team prototyped a novel aftermarket plug-in detector that alerts the driver to potential attack.

The aluminum–cerium alloy does not require heat treatment and maintains 100% of room temperature mechanical properties after 1,000 hours at 400°C.

Cross-laboratory capabilities speed development of new Al-Ce alloy

Experts in combustion, materials science, and manufacturing came together to accelerate research and development of a new aluminum–cerium alloy created through the Critical Materials Institute (CMI), a DOE Energy Innovation Hub.

Cerium is one of the most abundant rare earth materials, but its usage to date has been limited. Rare earths such as neodymium and dysprosium are frequently used in electronics, electric vehicles, and other modern technologies. Currently, there is no domestic supply chain for these materials, which are imported, primarily from China.

Using cerium in a high-volume application such as cylinder heads for automotive engines could create momentum toward the establishment of a US rare earth industry, increasing energy security.

As part of this CMI initiative, an ORNL research team led by principal investigator Dr. Orlando Rios partnered with Lawrence Livermore National Laboratory and Eck Industries to develop aluminum–cerium alloys that are easier to cast and have higher heat tolerance than common commercial aluminum alloys.

In a matter of months, the aluminum–cerium alloy went from conception to casting to on-engine evaluation. Partner Eck Industries cast a cylinder head from the alloy using 3D printed sand molds. Researcher Dr. Scott Curran conducted experiments with the component on a small four-stroke engine at ORNL's National Transportation Research Center, demonstrating the stable operation of the alloy under full load at temperatures reaching 600°C.

Further evaluations are under way using neutrons to examine residual stress and other indicators of alloy performance while the engine is in operation in the Vulcan beamline at ORNL's Spallation Neutron Source.

CMI is funded by the DOE Advanced Manufacturing Office. The engine experiments were conducted through capabilities supported by the DOE Vehicle Technologies Office. The Spallation Neutron Source is a user facility funded by the DOE Office of Science.

ORNL contributes to standards development for heavy-duty trucks

When heavy-duty and medium-sized trucks traverse the nation's roadways, they're doing so on the wheels of ORNL research.

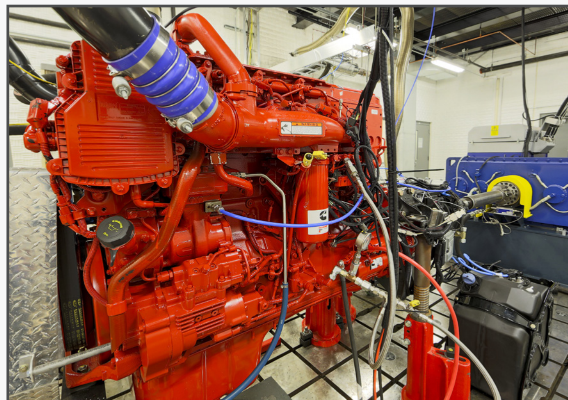
A research team lead by Paul Chambon in the Vehicle Systems Integration (VSI) Laboratory played prominent roles in assisting the US Environmental Protection Agency (EPA) with the development of phase 2 greenhouse gas (GHG) and fuel efficiency standards for medium- and heavy-duty trucks.

ORNL contributed to the development and evaluation of the new engine and powertrain test procedure options associated with the GHG certification process.

In the rulemaking, EPA refers to the new powertrain test procedures that ORNL is helping to develop as having the potential to "become an optimal certification path that leverages the accuracy of powertrain testing along with the versatility of the GHG Model, which alleviates the need to test a large number of vehicle or powertrain variants."

Other ORNL organizations and researchers were involved in corroborating the societal benefits and energy security implications of the new rules. The new standards, jointly proposed by the National Highway Transportation Safety Administration and EPA, are designed to cut carbon pollution by about 1 billion metric tons and save about 1.8 billion barrels of oil (75 billion gallons of fuel) over the lifetime of the vehicles covered by the standards.

ORNL's VSI Laboratory offers unique capabilities to test, simulate, and evaluate conventional and hybrid powertrain components and configurations for vehicles ranging from light-duty cars to Class 8 trucks.



Vehicle Systems Integration Laboratory at the National Transporation Research Center.

Real-time tracking system monitors fuel shipments

Researchers at ORNL and partners from private industry have developed an integrated monitoring system that can track the movement of goods in real time and flag suspicious activity. Developed for the Federal Highway Administration, the proof-of-concept system can be used to identify illegal blending of nontaxable petrochemical products with taxable fuel products and cross-jurisdictional tax evasion.

Devices track the location of the tanker and fuel intake, supplying information to the real-time monitoring system.

The supply-chain-based system tracks fueling stops, loading, and unloading and provides real-time notification of any variation in standard delivery processes (e.g., a hatch or valve left open or an unplanned stop) from the tanker's point of origin to its final destination.

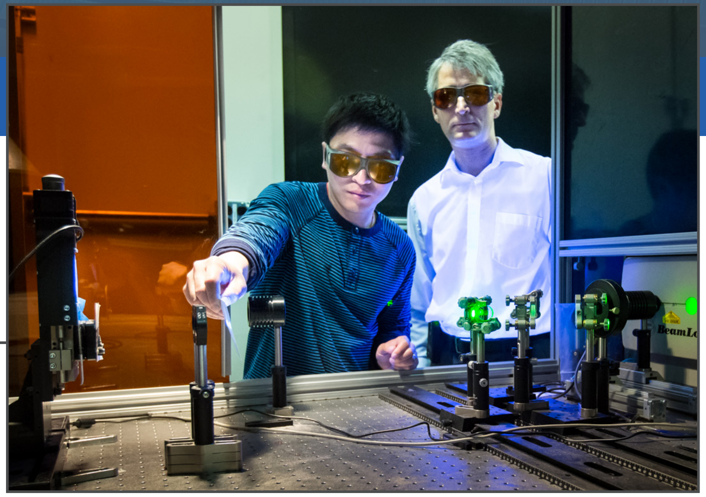
An evidential reasoning system based on ORNL-developed algorithms classifies the tankers' movements as normal or needing further investigation based on information from valve and hatch sensors, vehicle coordinates, carrier-supplied fuel orders and routing details, and the locations of fuel distribution centers.

A custom-developed user interface alerts carriers to possible fuel theft, while a query tool allows trucking companies and state and federal auditors to access records of fuel movements.

An ORNL team led by Dr. Gary Capps and Oscar Franzese conducted a pilot test with three commercial fuel tankers collecting real-world data during normal operations over an 8-month period. During the pilot phase, the vehicles logged a total of 375,000 miles and transported more than 7.5 million gallons of fuel.

Results of the monitoring system study are expected to inform future rulemakings. The system could also be used to track other activities where real-time tracking and flagging of suspicious or unusual activity is needed.

Partners on the project were Barger Transport, Liquid Bulk Tank, Innovative Software Engineering, and Air-Weigh.



Dr. Adrian Sabau and Dr. Jian Chen work with a laser to prepare the surfaces of carbon fiber composites and aluminum to create superior bonds that can absorb 200% more energy than conventional bonds.

Laser treatment creates strong, multimaterial joints for vehicle lightweighting

Joining carbon fiber composites and aluminum for lightweight cars and other high-end multimaterial products could become less expensive and the joints more robust because of a new method that harnesses a laser's power and precision.

An ORNL team led by Dr. Adrian Sabau developed a new process that could replace the practice of preparing the surface of materials by hand using abrasive pads, grit blasting, and environmentally harmful solvents. Using a laser to remove layers of material from surfaces prior to bonding improves the performance of the joints and provides a path toward automation for high-volume use.

> "Our technique is vastly superior to the conventional surface preparation methods," Sabau said. "Combined with the potentially dramatic reduction in the cost of carbon fiber polymer composites, this represents an important step toward increasing the use of this lightweight high-strength material in automobiles, which could reduce the weight of cars and trucks by 750 pounds."

Treating the surface of aluminum and carbon fiber polymer composite is a critical step in the adhesive joining process, which directly affects the quality of bonded joints. Aluminum surfaces contain oils and other contaminants from production rolling operations, while carbon fiber surfaces contain mold releases.

"These surface contaminants affect surface energies and the quality of adhesion, so it is critical that they are removed," said Sabau, adding that the laser also penetrates into the top resin layer, leaving individual carbon fibers exposed for direct bonding to the adhesive and increasing the surface area for better adhesion.

Test results support Sabau's optimism as single-lap shear joint specimens showed strength, maximum load, and displacement at maximum load were increased by 15%, 16%, and 100%, respectively, over those measured for the baseline joints. Also, joints made with laser-structured surfaces can absorb approximately 200% more energy than the conventionally prepared baseline joints, researchers reported.

Sabau noted that the process also doubles the energy absorption in the joints, which has implications for crash safety and potential use in armor for people and vehicles. Tim Skszek of Magna International (Troy, Michigan), a project partner, shares Sabau's enthusiasm.

"The results are most encouraging, enabling the automated processing of a multimaterial carbon fiber–aluminum joint," Skszek said. "With this work, we were able to focus on addressing the gaps in technology and commercial use, and we look forward to applying these findings to products."

This research was funded by the DOE Vehicle Technologies Office.

Lower cost alloys for higher temperature exhaust valves improve vehicle efficiency

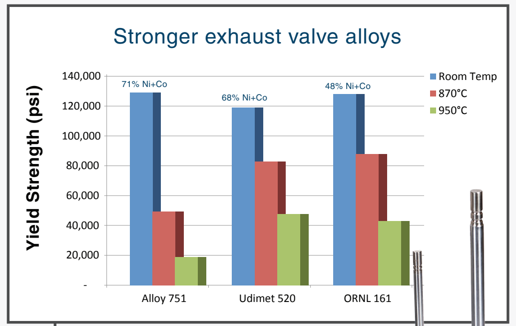
Future high-efficiency engines will require exhaust valves to be able to take the heat—potentially upwards of 950°C by 2025. Alloys that can withstand high temperatures are needed so that car manufacturers can produce vehicles with new engines using advanced internal combustion regimes.

A team led by ORNL's Govindarajan Muralidharan has developed lower cost, higher strength nickel-based alloys capable of withstanding more extreme temperatures than the alloys currently used in exhaust valves. The new alloys have been designed to contain up to 40% less nickel, achieving high strength without the addition of expensive alloying elements. Nickel-based alloys are strong with good oxidation resistance at temperatures up to 950°C.

A computationally guided approach was used to develop this new class of lower-nickel alloys. Several experimental strategies to improve oxidation resistance have also been evaluated.

Oxidation lessened with the addition of trace amounts of reactive elements.

This research was sponsored by the DOE Vehicle Technologies Office.

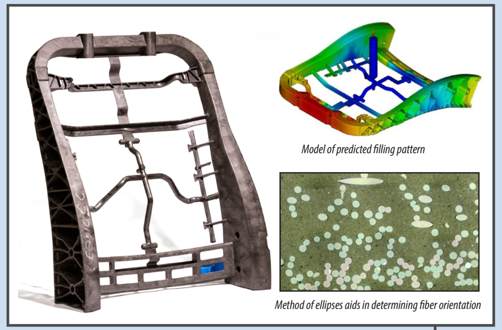


Nickel-based alloys can be used in exhaust valves at temperatures up to 950°C.

Predictive engineering tools for injection-molded carbon fiber composites

Using advanced characterization capabilities and an ORNL-developed process called the "method of ellipses," scientists have validated new 3D models for using long carbon fiber–reinforced thermoplastics in injection molding.

Injection molding with thermoplastics is a common manufacturing method in the automotive industry for fast, economical assembly-line production of nonstructural components such as cup holders and interior trim. Adding long carbon fibers to the thermoplastic resins produces stronger components and presents a potential path for vehicle lightweighting through replacing parts traditionally made with stainless steel and other metals.



An automotive seat frame was used as the test case for the modeling methods because it had the necessary complexity, with changes in thickness, ribs, holes, and changes in flow direction.

Getting the right concentration of carbon fibers is important to the end product's stiffness and strength. If the carbon fiber is not distributed to the critical sections of the component or the fibers are oriented incorrectly, the strength of the resulting product is lessened.

Though models for injection molding existed, there was no previous method that could predict the distribution, orientation, and density of the long carbon fibers in the mold.

Predictive modeling tools developed by ORNL principal investigators Dr. C. David Warren and Dr. Vlastimil Kunc and partners Ford Motor Company, Moldex 3D, BASF, the University of Illinois, Virginia Tech, and PlastiComp provide a solution to the problem.

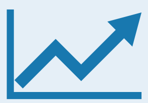
"We've created a model that allows us to understand where the fiber is, what the fiber orientation is, and what the fiber density is," said Warren. "You can then measure on average what the fiber length would be and, with those parameters, identify what the properties are."

The models allow engineers to tailor material properties for new parts, changing processing parameters to produce exactly what is needed and avoiding expensive trial and error. Ford is applying these predictive models to the manufacture of components for new vehicles.

This research was supported by the DOE Vehicle Technologies Office.

XALT Energy and ORNL developed a new coating technology that increases battery energy density, potentially enabling Formula E race cars that currently last only half the race to power through the whole race to the finish line.

Battery Research Objectives



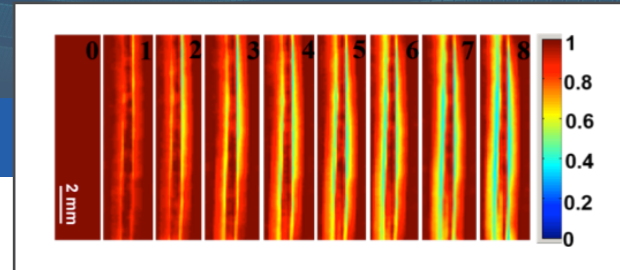
Build a domestic supply chain and create domestic jobs

Advance manufacturing science and production yield

Improve battery performance and safety

Reduce costs of battery production to meet consumer needs

Building better batteries with neutrons and computational modeling



Radiograph shows change in contrast as lithium is incorporated into the graphite electrodes.

Lithium-ion batteries power everything from phones to hybrid electric vehicles, keeping electronics humming along. Dependable and durable, these batteries are gaining traction in the transportation industry. Knowing how well a lithium-ion battery will perform in a vehicle is critical and, as researchers at ORNL have determined, depends largely on the uniformity and distribution of lithium in the electrodes.

ORNL researchers have developed a way to better track the movement and amount of lithium during battery cycling using computational modeling, neutron imaging, and neutron diffraction—all part of an effort to develop more efficient and safer batteries.

> "Inhomogeneity in local lithium concentration and transport across cell thickness is what triggers degradation and ultimately limits battery capacity and lifetime, and this study is a model demonstration which can be easily extended to commercial lithium-ion cells," ORNL lead researcher Dr. Jagjit Nanda said.

To unravel the mechanisms that cause lithium concentration differences, researchers used neutron imaging and neutron diffraction to visualize the distribution of lithium across the cell at various scales (tens of micrometers to nanometers) and to map the position of lithium ions in the crystal lattice and structural changes the lattice undergoes with cycling.

"Neutrons are sensitive to light elements such as lithium and thus can follow its transport evolution in a functioning battery. Neutrons offer unique insights into the battery behavior during charge and discharge," said Dr. Hassina Bilheux, who leads neutron imaging at ORNL for the study.

The neutron data were compared to lithium concentration profiles generated using computational models. These electrochemical transport models were created and made publicly available through AMPERES, a high-fidelity 3D simulation component developed under the Computer-Aided Engineering for Batteries (CAEBAT) project. While the traditional approximate models implemented in AMPERES have been validated previously, this is the first time the more accurate models have been compared with experimental results.

"The ability to more accurately represent the complexities of real materials and behavior is key to improving the performance and safety of batteries," said Dr. John Turner, who leads the CAEBAT project at ORNL.

The project provides a proof-of-principle example for how the combined capabilities of neutron imaging, neutron diffraction, and computational modeling can enable discoveries about chemical and phase transformations within batteries.

"This will no doubt herald a new era in the area of multimodal-multiscale imaging applied to energy storage and conversion systems," said Nanda.

This work was accomplished with funding from the DOE Vehicle Technologies Office using pouch cells created in the DOE Battery Manufacturing R&D Facility supported through the DOE Office of Energy Efficiency and Renewable Energy. Neutron capabilities were provided by the ORNL Spallation Neutron Source and High Flux Isotope Reactor, which are DOE Office of Science user facilities operated by ORNL. CAEBAT models created with funding from the DOE Vehicle Technologies Office were also critical to the success of the study.

Electron beam technology cures cathode coatings instantly

ORNL's Zhijia Du prepares material samples for electron beam curing, which instantly cross-links the binding resins in coating material at a high line speed of 500 feet per minute.

Scientists at ORNL are using the precision of an electron beam to instantly adhere cathode coatings for lithium-ion batteries—a leap in efficiency that promises to save energy, reduce production and capital costs, and eliminate the use of toxic solvents.

Conventional electrode processing uses flammable, toxic N-methylpyrrolidone (NMP) as the solvent, which must be vaporized and recovered during battery production. ORNL's method uses an electron beam to cure coating material as it rolls down the production line, creating instantaneous cross-links between molecules that bind the coating to a foil substrate, without the need for solvents, in less than a second.

"Typical curing processes can require drying machinery the length of a football field and expensive equipment for solvent recovery," said principal investigator Dr. David Wood. "This approach presents a promising avenue for fast, energy-efficient manufacturing of high-performance, low-cost lithium-ion batteries."

This research was supported by the DOE Vehicle Technologies Office and conducted in collaboration with ebeam Technologies USA. Details of the coating technique were published in the *Journal of The Electrochemical Society.*

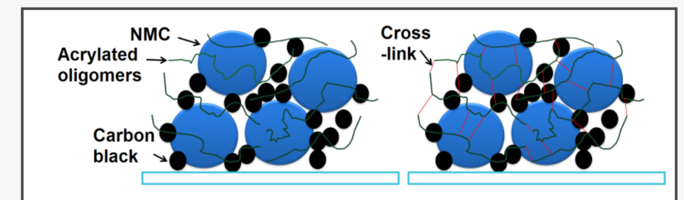
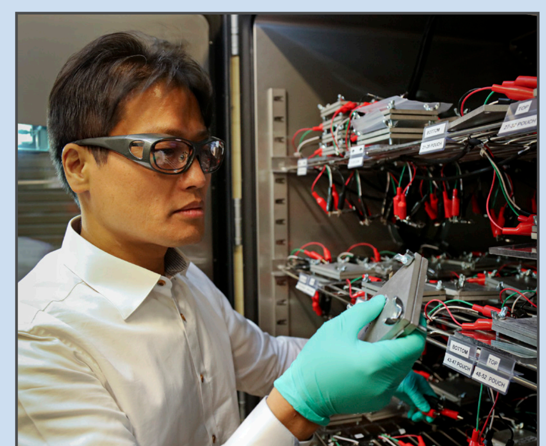


Illustration shows the use of acrylated oligomers as binders in Li-ion battery electrodes.

Fast formation protocol speeds production, improves battery capacity



ORNL's Seong Jin An works with lithium-ion batteries undergoing an ORNL-developed fast-formation protocol that shortens battery production by up to six times.

A new process developed by ORNL could alleviate a bottleneck in battery manufacturing and deliver higher capacity batteries for electric vehicles and consumer devices.

The formation process—where batteries undergo repeated cycling to stabilize and activate them for use—is one of the most time- and energy-intensive production steps. The researchers' new fast-formation protocol could shorten that time frame by six times or more, saving production costs and energy.

The ORNL method, described in the *Journal of Power Sources*, demonstrated the effectiveness of using more numerous and shallow charge-discharge cycles between 3.9 V and 4.2 V and fewer full depth of discharge cycles below 3.9 V.

Evaluation showed the new protocol reduced surface film (electrolyte interphase) resistances and conserved lithium inventory, which improves battery capacity. The process is applicable to all lithium-ion batteries and can be tuned for other chemistries as well.

This research team was led by Dr. David Wood and supported by the DOE Vehicle Technologies Office.

Integrating science capabilities to address national transportation challenges

- BioEnergy Science Center
- Center for Nanophase Materials Science
- High Flux Isotope Reactor
- Manufacturing Demonstration Facility
- Materials Science and Technology Division
- National Transportation Research Center
- Nuclear Science User Facilities
- Oak Ridge Leadership Computing Facility
- Spallation Neutron Source

HONORS AND AWARDS

SAE International honored (from left) Dr. John Storey, Martin Wissink, Dr. Johney Green, Dr. Jim Szybist, and John Thomas at the 2016 SAE World Congress.

DOE Distinguished Achievement Award recipients are (bottom row from left) Cliff White, Madhu Chinthavali, Dr. Omer Onar, Steven Campbell, Larry Seiber; (top row) Dr. Lixin Tang, Paul Chambon, Dr. Burak Ozpineci, Randy Wiles.

Dr. Ron Graves (right) is inducted into the Tennessee Automotive Manufacturers Association's Hall of Fame with fellow honoree, former Tennessee governor Phil Bredesen (left) by TAMA President Rick Youngblood.

USCAR Team Awards

- Advanced Combustion and Emissions Control (ACEC) Fuels Roadmap Subteam – Dr. Ron Graves and Dr. Jim Szybist
- ACEC Low Temperature Aftertreatment Subteam – Dr. James E. Parks, II and Josh Pihl

SAE International

- Forest R. McFarland Award – Dr. John Storey, Dr. Jim Szybist, John Thomas
- Myers Award – Martin Wissink

Newly Elected Fellows

- American Society of Mechanical Engineers – Dr. Robert Wagner
- ASM International – Dr. Michael Brady
- ORNL Corporate Fellow – Dr. Nancy Dudney
- SAE International – Dr. Johney Green

DOE Distinguished Achievement Awards

- ORNL wireless power transfer team – Steven Campbell, Paul Chambon, Dr. Madhu Chinthavali, Dr. Omer Onar, Dr. Burak Ozpineci, Larry Seiber, Dr. David Smith, Dr. Lixin Tang, Cliff White and Randy Wiles
- H2 at Scale – ORNL's David Wood participates on the team led by Dr. Brian Pivovar of National Renewable Energy Laboratory

National and Regional Awards

- Gilbreth Lectureship Award from the National Academy of Engineering – Dr. Claus Daniel
- Biodiesel Researcher of the Year Award from the National Biodiesel Board – Dr. Michael Lance
- Tennessee Automotive Manufacturers Association (TAMA) Hall of Fame – Dr. Ron Graves

R&D 100 Awards

- R&D 100 Award Winner

  Waste tire derived carbon

  ORNL material chemists devised a proprietary process for repurposing discarded car tires as a source of carbon powder, a sooty hydrocarbon byproduct that can be modified to incorporate into anodes of lithium-ion batteries.

  Research team: ORNL's Dr. Parans Paranthaman and partner RJ Lee Group

  Funding for this project was provided by the DOE's Office of Science and ORNL's Technology Innovation Program.

- Special Recognition Award Winner

  Wireless power transfer based electric and plug-In vehicle charging system

  Researchers developed the world's first 20-kW wireless charging system for passenger cars and achieved 90% efficiency at three times the rate of the plug-in systems commonly used for electric vehicles today.

  Research team: ORNL's Steven Campbell, Paul Chambon, Madhu Chinthavali, Dr. Omer Onar, Dr. Burak Ozpineci, Larry Seiber, Dr. David Smith, Dr. Lixin Tang, Cliff White, and Randy Wiles, as well as retired staff members Curt Ayers, Chester Coomer, and Dr. John Miller, with partners Toyota Motor Engineering & Manufacturing North America, Cisco Systems, and the International Transportation Innovation Center

  Funding for this project was provided by the DOE's Energy Efficiency and Renewable Energy Office, Vehicle Technologies Office.

- R&D 100 Award Finalists

  Plasma oxidation for rapid processing of carbon fiber

  Plasma oxidation technology developed by ORNL and RMX Technologies accelerates the oxidation stage of carbon fiber production. The innovation cuts processing time by a factor of 2.5 to 3 times, reduces energy consumption by 75%, and lowers production costs by 20% while maintaining or improving carbon fiber quality.

  Research team: ORNL's Felix Paulauskus and Dr. C. David Warren with partner RMX Technologies

  Funding for this project was provided by the DOE's Energy Efficiency and Renewable Energy Office, Vehicle Technologies Office.

  SHARP-ion battery

  ORNL assisted Sharp in the development of low-cost sodium-ion battery technology. This technology provides comparable performance and safety with the potential of lowering costs by 25% and lasting 10 times longer than lithium-ion batteries.

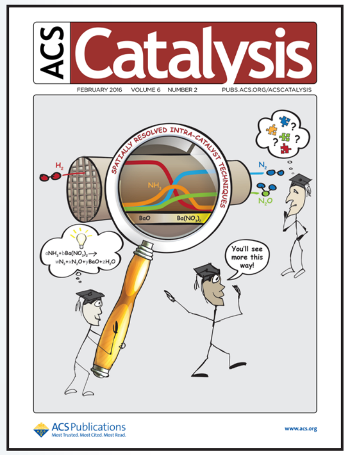
  Research team: ORNL's Jianlin Li, David Wood, and Claus Daniel assisted Sharp

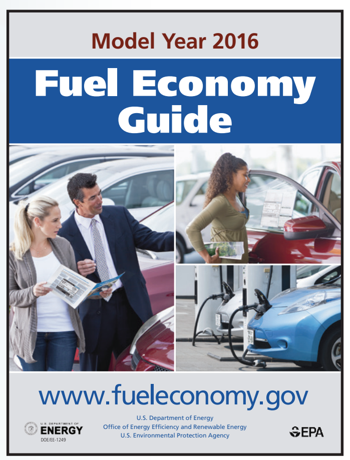
  This research was conducted as part of a strategic partnership project.

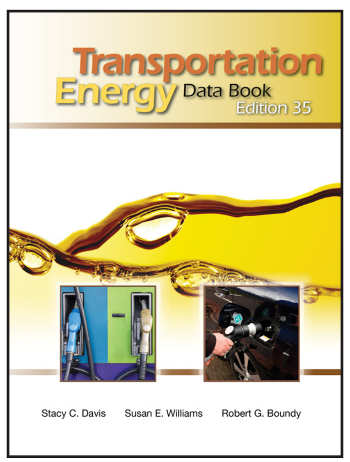
PUBLICATIONS

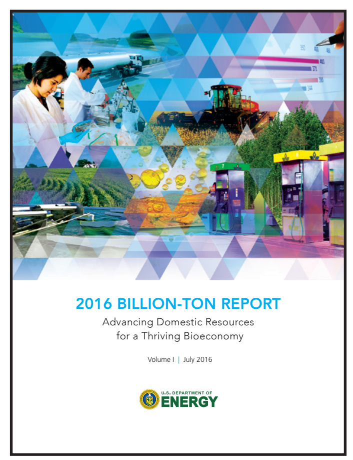
The Sustainable Transportation Program published 244 publications in fiscal year 2016, including 179 journal articles, nine books and book chapters, 35 proceedings of conferences, and 21 technical reports.

Publication highlights









Most downloaded article of 2016 for *GCB Bioenergy*:

"Reconciling food security and bioenergy: priorities for action," authored by K. Kline, S. Msangi, V.H. Dale, J. Woods, G. Souza, P. Osseweijer, J. Clancy, J. Hilbert, H. Mugera, P. McDonnell, and F. Johnson, *GCB Bioenergy*, **9**, 557, 2016.

Top 10 all-time most-cited articles in *Tribology Letters*:

"Ionic liquids with ammonium cations as lubricants or additives," authored by J. Qu, J.J. Truhan, S. Dai, H. Luo, and P.J. Blau, *Tribology Letters*, **22**, 207, 2006.

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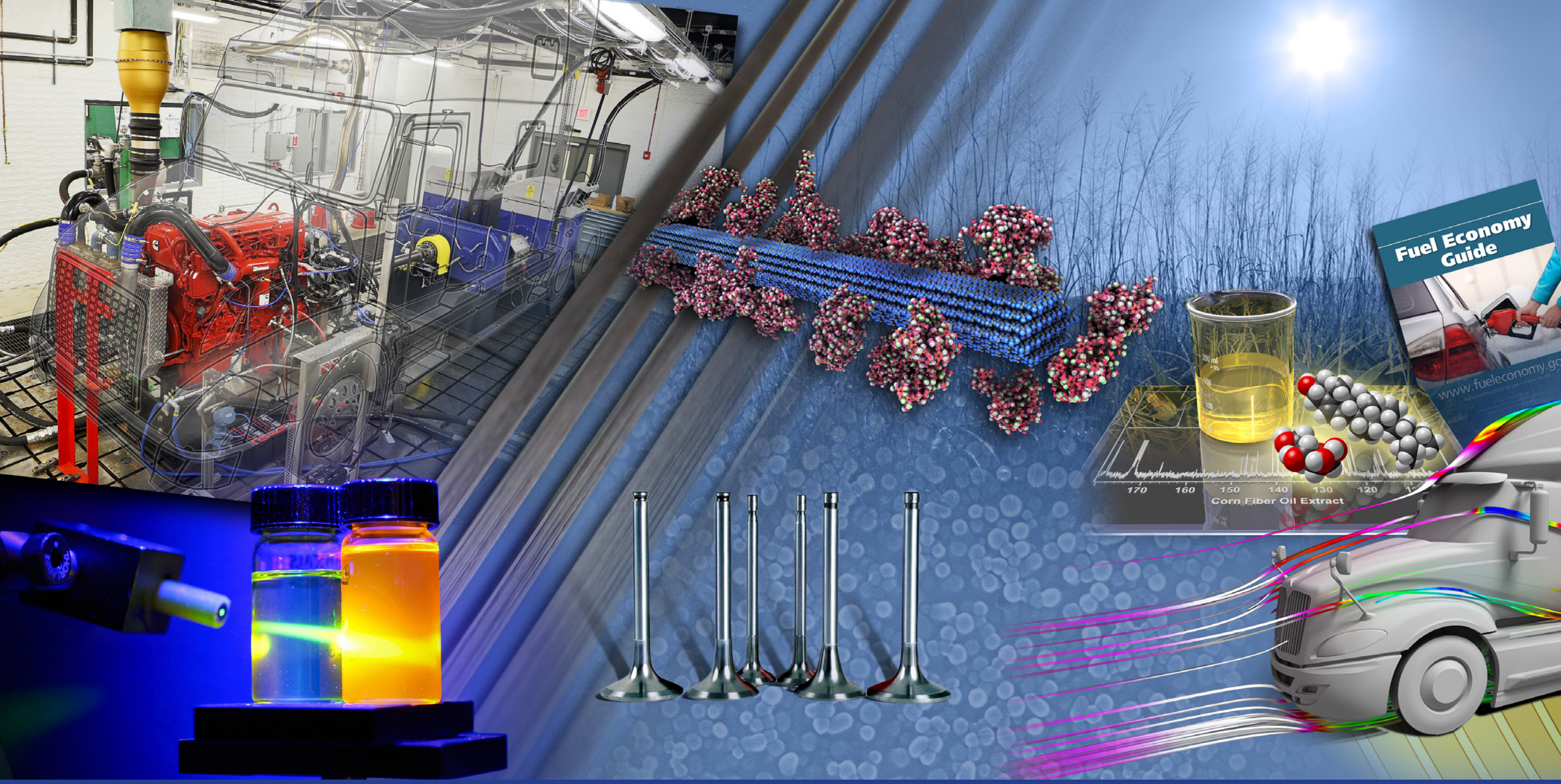

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