Sustainable Transportation Program

2014 Annual Report

Oak Ridge National Laboratory

ORNL/SPR-2014/57

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Sustainable Transportation Program
2014 Annual Report

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Introduction

Oak Ridge National Laboratory's (ORNL's) Sustainable Transportation Program (STP) brings together science and technology experts from across scientific disciplines to partner with government and industry in addressing national transportation challenges. STP develops knowledge and technologies that accelerate the deployment of new vehicles and efficient transportation systems powered by domestic, renewable, clean energy.

The Program's research and development portfolio includes vehicle systems integration, fuel and lubricant technologies, advanced combustion engines, innovative materials, intelligent transportation systems and operations, efficient vehicle components, and transportation electrification. Millions of vehicles on the road today are more durable and more efficient because of ORNL-developed materials technologies.

ORNL also provides data and analysis to guide policies and strategic decisions of the Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) and the Department of Transportation (DOT). In addition to government agencies, industry leaders and consumers make transportation decisions every day using data collected and analyzed by ORNL.

The Program's primary support comes from DOE EERE through three technology development offices: Vehicle Technologies (VTO), Fuel Cell Technologies (FCTO), and Bioenergy Technologies (BETO). Support also comes from DOT, other federal agencies, and the private sector. ORNL supports the US DRIVE (Driving Research and Innovation for Vehicle efficiency and Energy sustainability) and the 21st Century Truck government–industry partnerships, as well as DOE's EV Everywhere Grand Challenge and other sustainable transportation efforts.

The Sustainable Transportation research program pursues an "all of the above" strategy that incorporates

- accelerating widespread use of electric vehicles (EVs) powered by both batteries and fuel cells
- increasing the efficiency of all types of vehicles through lighter materials and advanced combustion and power train technologies
- enabling widespread use of cleaner fuels such as biofuels and natural gas
- collecting, analyzing, and disseminating data to support efficient commercial fleet operation, intelligent systems, congestion management, and informed decision-making.

These efforts are directed toward attaining

- efficient, secure, affordable vehicles for passengers and freight
- domestic production of transportation fuel
- reduction of the environmental impacts of transportation
- predictability and reliability in transport scheduling.

Transportation is a key factor in the energy and environmental future of the United States. Highway transportation (light-, medium-, and heavy-duty vehicles) accounted for about 28% of US greenhouse gas emissions and about 60% of US petroleum consumption in 2012. Although energy use by light-duty passenger vehicles is projected to decline by about 20% by 2040—largely as a result of more stringent greenhouse gas and corporate average fuel economy regulations—light commercial trucks and heavy trucks are projected to use 37% more energy in 2040 than in 2012.

A sustainable transportation system that increases efficiency, cuts pollution associated with vehicle use and production, relies more on renewable fuels, and increases highway safety is an indispensable part of a sustainable future.

With funding from BETO in FY 2014, ORNL researchers developed HiPAS (High Performance Architectured Surface Selective) membranes—inorganic membranes consisting of a micrometer support layer, a nanoporous working layer, and a superhydrophobic or superhydrophilic surface layer. The membranes are an enabling technology that will be commercialized to increase efficiency and reduce costs in the biorefinery and biofuel production and processing industries. Another BETO-funded project used the Soil Water Assessment Model to assess the potential for growing bioenergy crops in the transition zone of the Arkansas-White-Red River basin between the semi-arid western and more humid eastern zones. The study results indicate that bioenergy crops could be grown sustainably there and could reduce erosion and improve water quality. ORNL and the University of Tennessee collaborated to complete an update of the *Feedstock Supply and Price Projection* report to BETO, which provides data for decisions about commercialization of cellulosic biomass feedstocks. The report evaluates feedstock prices at the farm level and presents the data by county to aid local and regional projections.

In research supporting the DOT, ORNL and its industry partners developed and demonstrated an onboard monitoring system for fuel trucks to prevent fuel tax evasion. It tracks the movements of fuel tankers from bulk storage to final destination in real time to prevent blending of taxable and non-taxable fuels and other tax evasion attempts. ORNL also worked with the Federal Motor Carrier Safety Administration to reduce crashes at roadway work zones involving commercial motor vehicles (CMVs). ORNL hosted a workshop to identify needed research on reducing work zone crashes and is developing methods for alerting CMV drivers that they are approaching work zones that may have stalled traffic.

ORNL research sponsored by FCTO continued to advance techniques for characterizing materials for fuel cell membrane electrode assemblies from the micrometer to the angstrom scale. In 2014, ORNL identified microscopy conditions for characterizing ionomer distributions at nanometer lengths within catalyst layers. An ORNL project developed a model to analyze the economics of providing hydrogen refueling infrastructure for fuel cell vehicles (FCVs), indicating where and when to build hydrogen stations and the size to build for commercial viability, and how long it will take stations to turn a profit. ORNL researchers also conducted a sensitivity analysis to evaluate the optimum pressure for delivering hydrogen to FCVs. Another project related to fueling infrastructure validated the design for a steel/concrete composite vessel (SCCV) for high-pressure hydrogen, showing that the SCCV can meet the 2015 DOE cost target and reduce the cost of stationary hydrogen storage by 15%. In a project to develop carbon fiber vessels for hydrogen storage, ORNL and Virginia Tech University produced melt-spun carbon fibers of up to 25 Msi modulus and 250 ksi strength, and ORNL combined the fibers to produce small tows for progressive tensioning and shrinkage management. In addition, ORNL and its commercial partner SGL analyzed 11 different chemical formulations for carbon fibers made from textile-grand polyacrylonitrile precursor (a comparatively low-cost precursor) and selected the best polymer composition and manufacturing methods for producing carbon fibers from the precursor.

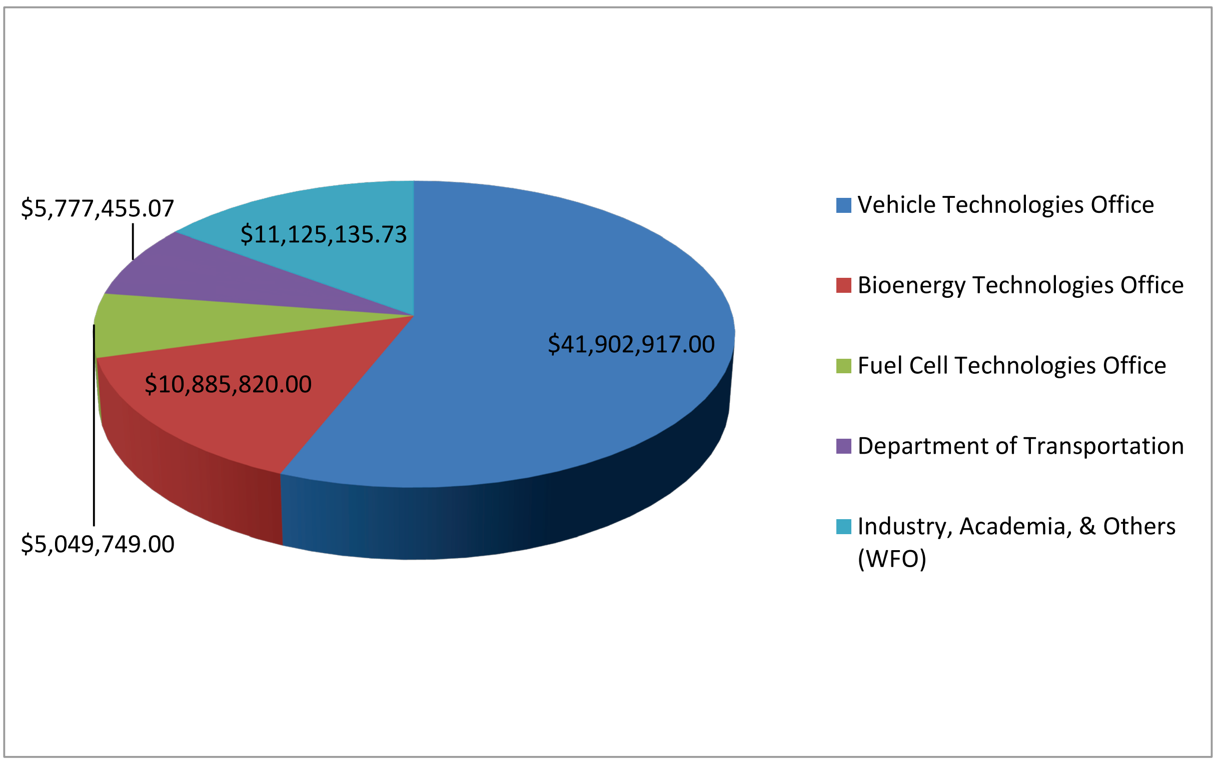
With funding from VTO, ORNL researchers conducted an analysis indicating that until the cost of EV batteries drops to $100/kWh or less, battery electric vehicle (BEV) models with a range below 100 miles would be the best choice for most consumers. In another VTO project, ORNL researchers developed a new type of catalyst that improves emissions control at low temperatures without using precious metals. A new version of the software VIBE (Virtual Integrated Battery Environment) provided a platform that anyone can use to advance battery development. In lightweight materials research, ORNL is developing a plasma processing technique for rapid, inexpensive oxidation of polyacrylonitrile precursor fibers that could boost throughput and lower fiber costs. Power electronics researchers used additive manufacturing to produce a power inverter for use in EVs that is lighter, more efficient, and more rugged against harsh operating conditions. Using advanced hybrid technologies and control systems, ORNL researchers are taking a multi-faceted approach to developing an advanced heavy-duty powertrain system that will decrease energy consumption and criteria emissions in Class 8 line haul vehicles. Another ORNL team funded by VTO developed and demonstrated a stationary wireless charging system that operates at the same efficiency as plug-in charging.

Highlights of these and other STP research and development (R&D) efforts begin on page 11.

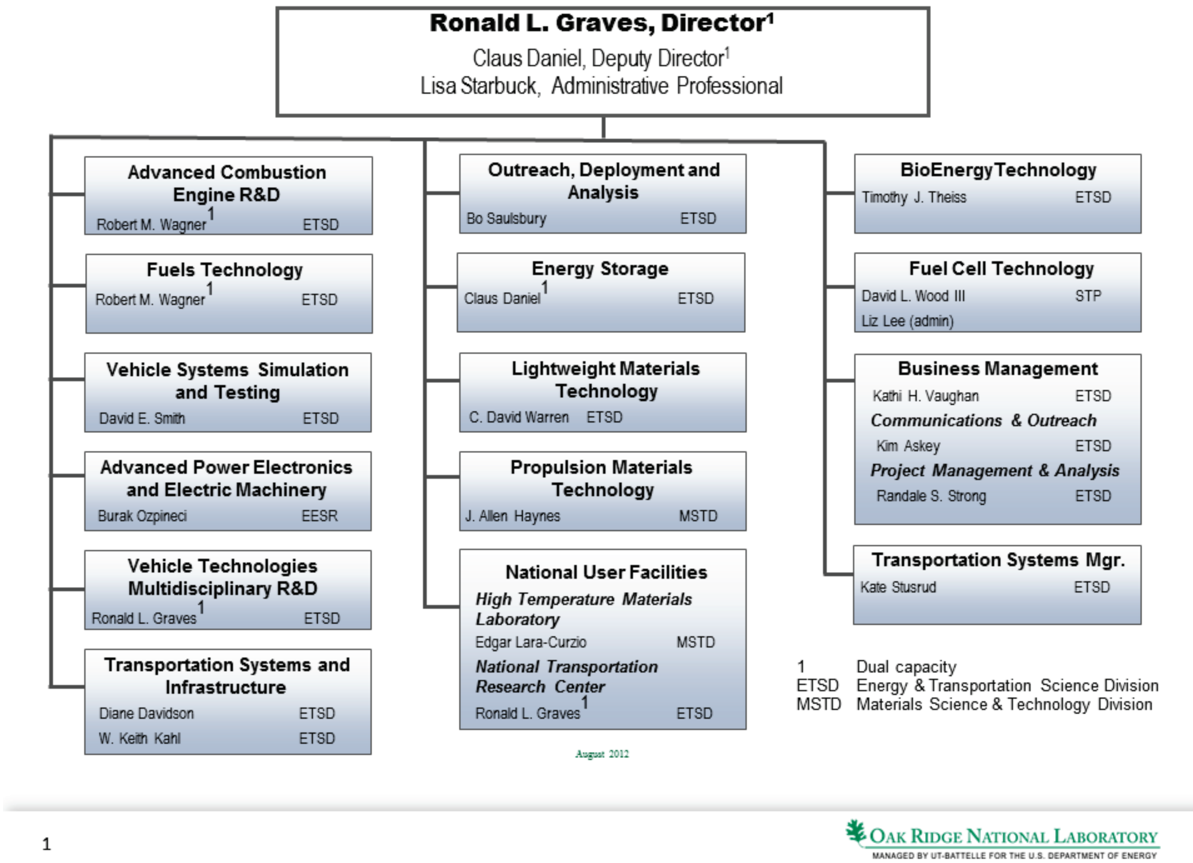
Program Metrics

Funding

The STP received $74.7 million in new budget funding in FY 2014. Approximately $16.8 million or 22.4% is funding competitively awarded through Funding Opportunity Announcements. DOE VTO was the largest sponsor of the ORNL program. Funding from industry, academia, and other nongovernment partners increased in FY 2014 compared with the previous year.



Program funding provided significant support for 170 scientific and technical staff in 10 technical divisions, reflecting the multidisciplinary character of the ORNL program. STP team leaders are shown in the following organizational chart.



Industry Impact

ORNL's STP conducts most of its R&D in collaboration with industry so that pathways to commercialization are built into projects from the beginning. Industry partnerships are carried out through a variety of mechanisms, including Cooperative Research and Development Agreements (CRADAs), Work for Others (WFO) agreements, technology licensing, User Facility Agreements, and informal collaborations and information exchanges at technical conferences and workshops.

CRADAs

STP researchers supported 23 CRADAs in FY 2014 with 17 different companies, developing an array of transportation-related technologies. Industry partners contributed about $6.6 million in materials and services to those efforts.

WFO Agreements

ORNL worked with 57 industrial companies, 18 federal and state government entities, and 8 universities under 108 separate WFO agreements in FY 2014. Those agreements were valued at about $11.1 million in total.

Laboratory-directed Research and Development

STP staff were granted funding for four projects through the ORNL Laboratory-directed Research and Development (LDRD) program. Those projects are listed in Table 1.

Table 1. FY 2014 LDRD awards

Project Type/ID No.	Principal Investigator	Initiative	Title
Director's R&D 7457	T. Toops $388,900	Next Generation Neutron Source Instrumentation	Dynamic Neutron Imaging of Intra-nozzle Fluid Dynamics of Fuel Injectors
Director's R&D 7396	A. Malikopoulos $385,000	Science and Informatics for Energy and Urban Infrastructure	Scalable Data and Informatics for Connected Vehicles Leveraged to Enhanced Efficiency
Director's R&D 6923	N. Ericson $330,000	Integrated Energy Systems	Complementary Silicon Carbide Wide Band Gap Integrated Circuits for Bidirectional Electric Vehicle Chargers
Director's R&D 6928	B. Ozpineci $330,000	Integrated Energy Systems	Next Generation Compact and Reliable WBG-Based Inverter Breakthrough with Additive Manufacturing and High Performance Computing

Patents and Patent Applications

Sustainable Transportation Program research at ORNL resulted in 15 patent applications. Ten patents were granted based on earlier filings (Table 2). Patent applications filed in FY 2014 are shown in Table 3.

Table 2. Patents awarded during FY 2014

Inventor	Title	Patent Number
M. P. Brady, Y. Yamamoto, and G. Muralidharan	Alumina Forming Iron Base Superalloy	8,815,146
D. L. Wood, III, H. M. Meyer, J. Y. Howe, E. A. Payzant, N. C. Gallego, and C. I. Contescu	Forming Gas Treatment of Lithium Ion Battery Anode Graphite Powders	8,834,829
J. R. Mielenz, R. E. Norris, Jr., C. C. Eberle, A. K. Naskar, F. S. Baker, and J. M. Pickel	Lignin-Derived Thermoplastics Co-Polymers and Methods of Preparation	8,748,537
A. P. Borole	Microbial Fuel Cell Treatment of Fuel Process Wastewater	8,597,513
R. R. Bhave, B. L. Bischoff, C. K. Narula, and J. Nanda	Multi-Layered, Chemically Bonded Lithium-Ion and Lithium/Air Batteries	8,722,256
Goyal, Amit	Nanocomposites for Ultra High Density Information Storage Devices, Including the Same and Methods of Making the Same	8,685,549

Table 2. Patents awarded during FY 2014 (continued)

Inventor	Title	Patent Number
L. C. Maxey, J. E. Parks, II, W. P. Partridge Jr., and S. A. Lewis Sr.	Optically Stimulated Differential Impedance Spectroscopy	8,653,830
S. V. Kalinin, N. J. Dudney, S. Jesse	Real Space Mapping of Ionic Diffusion and Electrochemical Activity in Energy Storage and Conversion Materials	8,719,961
P. J. Blau, J. Qu, H.-T. Lin	Titanium Aluminide Intermetallic Alloys with Improved Wear Resistance	8,771,439
A. A. Wereszczak	Sintered Silver Joints via Controlled Topography of Electronic Packaging Subcomponents	8,822,036

Table 3. Patent applications filed during FY 2014

Inventor	Title	Application Number
C. J. Janke, F. L. Paulauskas, A. K. Naskar, and C. D. Warren	Sulfonated Polyolefin-Based Flame Retardant Material	14/175,218
J. M. Pickel, R. E. Norris Jr., C. C. Eberle, A. K. Naskar, F. S. Baker, and J. R. Mielenz	Lignin-Derived Thermoplastics Co-Polymers and Methods of Preparation	14/058,657
M. Keller, B. H. Davison, and C. K. Narula	Zeolite Catalytic Conversion of Alcohols to Hydrocarbons	14/293,248
A. Goyal	Scalable Fabrication of One-Dimensional and Three-Dimensional Conducting, Nanostructured Templates for Diverse Applications such as Battery Electrodes for Next Generation Batteries	14/448,625
C. A. Bridges, G. M. Veith, and M. Paranthaman	Nitride- and Oxide-Modified Electrode Compositions and Their Methods of Making	14/473,099
A. Malikopoulos	Driver Feedback for Fuel Efficiency	14/323,875
J. Nanda and N. J. Dudney	High-Energy-Density Multivalent Conversion-Based Cathodes for Lithium Batteries	14/047,722
G. M. Veith, B. L. Armstrong, N. J. Dudney, and W. E. Tenhaeff	Impact-Resistant Electrolytes	14/497,667
S. Ozcan	Multifunctional Curing Agents and Their Use in Improving Strength of Composites Containing Carbon Fibers Embedded in a Polymeric Matrix	14/107,416
H. Luo and J. Qu	Corrosion Prevention of Magnesium Surfaces via Surface Conversion Treatments Using Ionic Liquids	14/044,248
V. Schwartz, B. L. Armstrong, and J. S. Choi	Method of Synthesizing Bulk Transition Metal Carbide, Nitride, and Phosphide Catalyst	14/069,514
C. Liang, N. J. Dudney, and A. Rondinone	A High Conducting Oxide–Sulfide Composite Lithium Superionic Conductor	14/104,803

Table 3. Patent applications filed during FY 2014 (continued)

Inventor	Title	Application Number
B. H. Davison and C. K. Narula	Catalytic Conversion of Alcohols Having at least Three Carbon Atoms to Hydrocarbon Blendstock	14/321,012
H. Wang	Thermal Management for High-Capacity Large-Format Li-ion Batteries	14/150,154
A. K. Naskar	Polymer Blend Compositions and Methods of Preparation	14/311,893

Staff Awards and Honors

Research staff working on STP projects were recognized with a number of awards and professional honors reflecting significant contributions to research, technology development, and service to professional societies. A selection of the most prominent awards is presented in Table 4.

Table 4. Significant awards and honors received by STP researchers

ORNL Awardee Name(s)	Name/Type of Award
S. Curran	Best Presentation at the 2013 American Society of Mechanical Engineers Internal Combustion Engine Fall Conference
	Outstanding Oral Presentation Award for 2014 SAE World Congress
C. Daniel, D. Wood III, W. Porter, A. Shyam, C. Contescu, R. Tejo, E. Lara-Curzio, J. Howe, H. Meyer, J. Li, R. Dinwiddie, C. Maxey, H. Wang, B. Armstrong	Federal Laboratory Consortium Excellence in Technology Transfer Award for Symmetrix HPX-F
S. Das	Appointed to the Transportation Research Board Committees on Transportation Economics and Alternative Transportation Fuels and Technologies
D. Davidson	Appointed to the Transportation Research Board Committee on Critical Transportation Infrastructure Protection
S. Davis	Special Recognition Award, DOE Vehicle Technologies Office
	Appointed to the Transportation Research Board Transportation Energy Committee
M. Hu, M. Sturgeon, R. Bhave, B. Bischoff, T. Aytug, T. Theiss	R&D 100 Award for Super-hydro-tunable HiPAS Membranes
P. T. Jones	Invited to coordinate the Wireless Charging for Electric Vehicles task for the International Energy Agency Hybrid and Electric Vehicle Implementing Agreement
K. Kahl	Appointed to the Task Force on Automated Driving and Platooning for the American Trucking Association Truck Maintenance Council

Table 4. Significant awards and honors received by STP researchers (continued)

ORNL Awardee Name(s)	Name/Type of Award
M. Kass	Appointed to the Advisory Committee for the University of California-Riverside College of Engineering Center for Environmental Research and Technology
	Appointed to the SAE Task Force on Automotive Security Guidelines and Risk Development
J.-M. Li	Invited panel member for Transit Cooperative Research Synthesis Study SA-34 on Open Data and Open Government for Transit Agencies
H.-T. Lin	Appointed to the Advisory Board of the World Academy of Ceramics
Z. Lin	Appointed to the Transportation Research Board Committee on Alternative Transportation Fuels and Technologies
C. Liu	Appointed to the Transportation Research Board Transportation Energy Committee
L. Marlino, N. Ericson, S. Frank, C. Britton and partners from Toyota, Arkansas Power Electronics International, and the University of Arkansas	R&D 100 Award for High Performance Silicon Carbide-based Plug-In Hybrid Electric Vehicle Battery Charger
P. Maziasz	2014 AIME Champion H. Mathewson Medal from The Minerals, Metals, and Materials Society
C. Narula	ORNL Inventor of the Year
O. Onar	Associate Editor, IEEE *Transactions on Transportation Electrification* journal
J. Parks II, V. Prikhodko, J. Storey and partners from Filter Sensing Technologies Inc. and Massachusetts Institute of Technology	R&D 100 Award for RF-DPF Diesel Particulate Filter Sensor
Jun Qu	R&D Award, DOE Vehicle Technologies Office
J. Qu, H. Luo, S. Dai, P. Blau, T. Toops, B. West, B. Bunting, and partners from General Motors Research and Development Center, Shell Global Solutions, and Lubrizol Corp.	R&D 100 Award for Ionic Liquid Anti-wear Additives for Fuel-efficient Engine Lubricants
S. Sluder	Fellow, SAE International
	Forest R. MacFarland Award, SAE International
	Outstanding Oral Presentation Award for 2014 SAE World Congress
J. Storey	Fellow, SAE International
	Outstanding Oral Presentation Award for 2014 SAE World Congress
R. Wagner	2014 International Leadership Citation, SAE International
	2014 Internal Combustion Engine Award, American Society of Mechanical Engineers
A. Wereszczak	R&D Award, DOE Vehicle Technologies Office
B. West	Appointed to the Fellows Committee, SAE International

Infrastructure and Facility Investments

Commercial Motor Vehicle Roadside Technology Consortium. ORNL's technical management of the Commercial Motor Vehicle Roadside Technology Consortium (CMVRTC), with strong ties to the Tennessee Department of Safety and Homeland Security and the Tennessee Department of Transportation, was enhanced by the availability of a new "first-of-its-kind" resource. In 2014, the Tennessee Highway Patrol completed a new Incident Management Training Facility outside Nashville that is used to teach best practices for safe, quick clearance of major highway incidents. Creation of the facility was supported by Federal Highway Safety Improvement project funds. ORNL used the facility in creating a new promotional video for the Federal Motor Carrier Safety Administration's CMV Work Zone safety technology initiative. It features an 1,800 ft section of interstate-like roadway ranging from two to six lanes, a guardrail, a two-way interchange, and a concrete barrier rail, as well as a section of two-lane highway and a full four-way intersection. The facility can be used to simulate collisions and roadside incidents, which allows emergency responders to realistically simulate and train for safe, efficient crash clearance and roadside investigation techniques. Future activities involving its use for wireless CMV enforcement technology testing and evaluation are anticipated.

Vehicle Systems Integration Laboratory. The Powertrain Research Cell of the Vehicle Systems Integration (VSI) Laboratory was fully commissioned through demonstration of powertrain-in-the-loop capabilities using a full Class 8, 15 L engine coupled to a ten-speed automated manual transmission. The powertrain was subjected to a host of duty cycles and vehicle configurations and met research cell performance expectations. In addition, a full Class 8 hybrid powertrain was installed in the Powertrain Research Cell (using the same 15 L engine) that made use of the AVL powertrain dynamometer system and the AVL battery emulator. The full range capability of the AVL battery emulator was proved at up to 400 kW in both motoring and regeneration modes, and it completed full commissioning in early FY 2014. The VSI Component Test Cell was also fully commissioned using a 105 kW traction motor mated to the AVL high-speed, double-ended dynamometer and the battery emulator. Full range speed and torque capabilities of the dynamometer were proved, and it completed full commissioning later in FY 2014.

Fuels, Engines, and Emissions Research Center. A new capability was added to the Fuels, Engines, and Emissions Research Center. The multicylinder combustion research engine will enable direct comparisons of dual-fuel reactivity-controlled compression ignition combustion modes with different fuel and additive chemistries. This capability will accelerate research into advanced combustion regimes.

Aberration-Corrected Electron Microscope. ORNL's aberration-corrected electron microscope was upgraded with a Protochips fourth-generation catalyst specimen holder and control system, making it a one-of-a-kind instrument. It is one of the world's most powerful microscopes for characterization of catalyst materials at the single-atom level under simulated real-world conditions. Protochips developed the new technology in partnership with ORNL.

Power Electronics and Electric Machinery Laboratory. A unique facility for evaluating and benchmarking wide-bandgap components used in inverters, converters, and onboard vehicle chargers was added to ORNL's Power Electronics and Electric Machinery Laboratory. The new facility can autonomously evaluate any wide-bandgap device in any package for any power level. Results covering a variety of performance and efficiency metrics are available to research partners, academia, and industry through the Sustainable Transportation website at www.ornl.gov/transportation.

HiPAS Membranes to Improve Biofuel Processing Efficiency

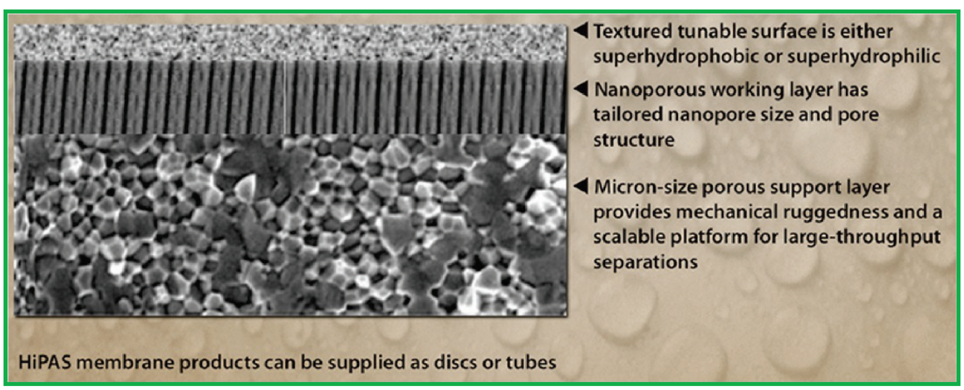
Contact: Michael Z. Hu, hum1@ornl.gov, 865-574-8782

ORNL researchers have developed a new class of robust inorganic materials called HiPAS (High Performance Architectured Surface Selective) membranes with high potential to improve the efficiency of bio-oil processing and other applications important to the biofuels industry.

Begun as a seed project in FY 2014, the project has completed proof-of-principle studies with an ethanol-water mixture system. In addition, with ORNL Laboratory Directed Research and Development funding, the project generated results for a new membrane material that led to successful licensing of one coating material technology to Surface Dry Coatings, LLC.

Effective separations using high-performance membrane processes have the potential to improve bio-oil processing efficiency and economy via their enhanced carbon recovery and separation efficiency as well as reduced bio-oil acidity. The membrane technology is an enabling technology potentially applicable to several different separation steps relevant to biomass and biofuel conversion and production. Good examples are oil/water separation, dewatering of ethanol or bio-oils, and pyrolysis vapor upgrading and fractionation.

HiPAS membrane development builds upon three key ORNL capabilities: (1) inorganic membrane tubular support technology, (2) materials science and engineering of nanoporous working layer materials, and (3) superhydrophobic/superhydrophilic coatings. HiPAS membranes consist of three layers: a micrometer porous support layer, a nanoporous working layer, and a surface layer nanoscale-textured/functionalized to be superhydrophobic or superhydrophilic.



HiPAS membranes consist of a porous support layer, a nanoporous working layer, and a textured superhydrophilic or superhydrophobic surface layer.

The key outcomes of this project development are new membrane products and processes that enable high-throughput processing while maintaining desirable separation selectivity. The improved separation process will lower system material costs, improve the lifetimes of structural containment materials, and reduce biomass or bio-oil processing costs as a result of the higher separation efficiency. This membrane technology will ultimately be commercialized to benefit the efficiency and economy of biorefinery and biofuel production/processing industries.

The new membrane materials development effort has won a 2014 R&D100 Award. Work in FY 2015 will begin optimizing the membrane structures and process development. Through the project, ORNL has initiated a collaboration with National Renewable Energy Laboratory for vapor-phase separation and processing of pyrolysis oil compositions (crude or upgraded).

Publications and Presentations

1. M. Z. Hu, D. Shi, and D. A. Blom. 2014. " Nano-structured mesoporous silica wires with intra-wire lamellae via evaporation-induced self-assembly in space-confined channels," *Journal of Nanomaterials*, article 932160.

2. M. Hu. 2014. "High-performance super-hydro-tunable membranes for advanced separations in biofuel processing," presented at the 18th Symposium on Separations Science and Technology, Oak Ridge, Tennessee, October 28.

3. M. Hu. 2014. "Chemical processing and chemical manufacturing of nanomaterials with engineered nanostructures and properties," invited presentation at Honeywell Process Solutions, Houston, March 30–31.

ORNL Finds Switchgrass Farming Opportunity in Transition Zone in Southwest

Contact: Yetta Jager, jagerhi@ornl.gov, 865-574-8143

ORNL research indicates that bioenergy crops grown in the transition zone between semi-arid western and more-humid eastern portions of the Arkansas–White–Red river basin of the US Southwest could improve water quality in addition to producing feedstocks for biofuels.

ORNL is seeking locales where cellulosic feedstocks can be economically competitive and provide water quality improvements. ORNL researchers used the Soil Water Assessment Model (SWAT) to compare water quality (nitrate, total phosphorus, and sediment loadings) under two scenarios: a business-as-usual future baseline and an economic scenario that assumes a farmgate price of $50/dry ton of switchgrass and 1% annual yield increases.

In the Arkansas–White–Red river basin, a strong increasing precipitation gradient exists from west to east. SWAT showed opportunities for improved sustainability—in terms of both water quality and productivity indicators—in the transitional longitudinal band where conventional crops require irrigation but perennial feedstocks, such as switchgrass, do not.

A pilot study showed that the region identified in the Arkansas–White–Red basin may become even more valuable under climate change in the future. Growing deep-rooted perennials presents an opportunity for sustainable bioenergy crop production— their roots will prevent soil erosion and protect rivers even as they produce biomass for biofuels to replace fossil fuels.

The US public and markets abroad have concerns about the sustainable use of land to produce bioenergy crops. Political and social acceptance of bioenergy depends on shifting from producing feedstocks in ways that harm water quality in US rivers and estuaries. This research is part of a larger collaboration with Argonne National Laboratory to address concerns about the impacts of bioenergy crops on the incidence of hypoxia (reduced oxygen concentrations) in the Gulf of Mexico. SWAT is being used to model the Mississippi River basin.

Publication

1. H. I. Jager, L. M. Baskaran, P. E. Schweizer, A. F. Turhollow, C. C. Brandt, and R. Srinivasan. 2014. "Forecasting changes in water quality in rivers associated with growing biofuels in the Arkansas–White–Red river drainage, USA," *GCB Bioenergy*. Published online at DOI: 10.1111/gcbb.12169.

ORNL Provides 2014 Supply, Price Projections for Bioenergy Feedstocks

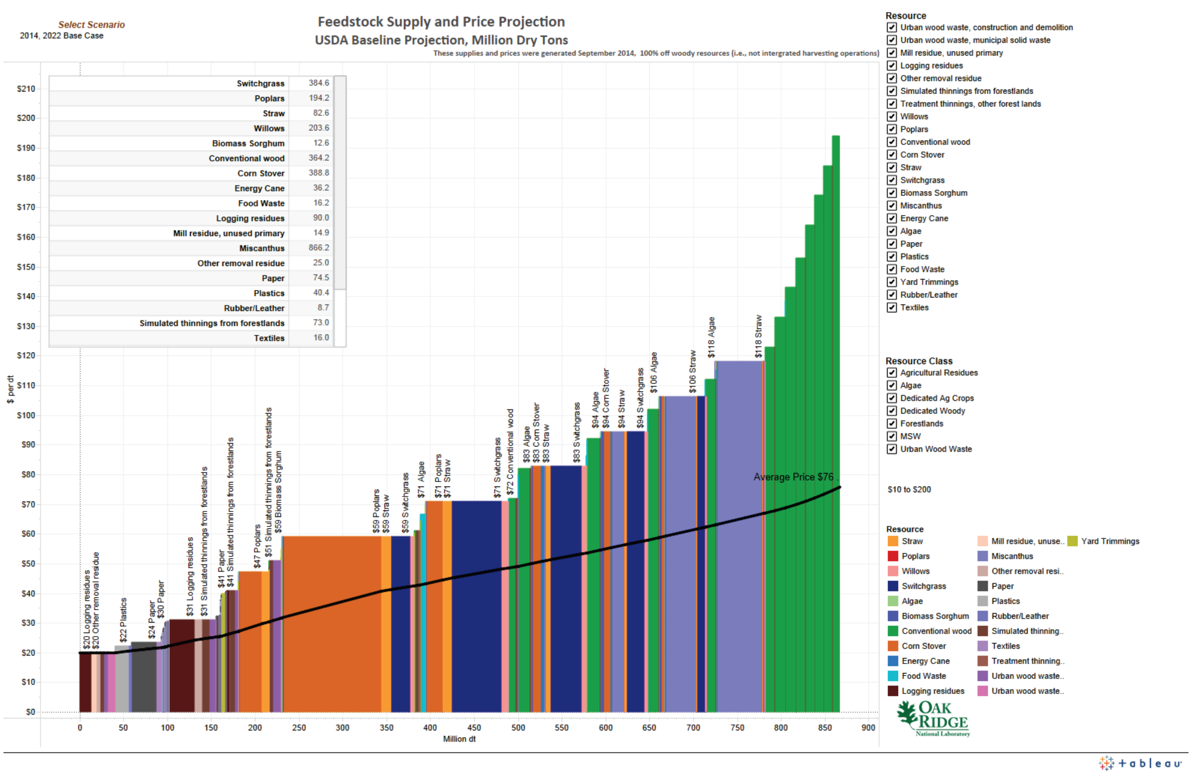
Contact: Matt Langholtz, langholtzmh@ornl.gov, 865-574-6520

ORNL researchers developed and submitted an update of the report *Feedstock Supply and Price Projection* (FSPP) to DOE BETO in 2014. Following on the 2011 *Billion-Ton Updat*e and the 2013 FSPP, the 2014 FSPP informs BETO strategies on commercialization and deployment of second-generation cellulosic biofuels.

Current, robust price projections are essential for the success of the emerging US biofuels industry. ORNL and the University of Tennessee Agriculture Policy Analysis Center were partners in developing the FSPP, which evaluates feedstock "farmgate" prices (i.e., the prices of feedstocks ready to load and transport from the farm) as a part of the total delivered cost of cellulosic biofuels.

ORNL provides relevant, up-to-date information essential to effective policy development and support of the evolving bioenergy industry. These data facilitate informed decision making and commercialization strategies as leaders in government and industry work toward goals set out in the Energy Independence and Security Act of 2007.

It is essential that the advanced biofuels industry and the US government be able to project realistic quantities of various biomass feedstocks and the likely costs of those feedstocks. The data in the FSPP are available at a county-wide level suitable for local or regional supply projections. Under current projections, feedstock costs make up about 1/3 of the price of cellulosic biofuels at the pump. The feedstock price can fluctuate with economic and technological changes within and beyond the agricultural sector, warranting annual monitoring and reporting of FSPPs.



Supply projections, base case scenario, 2022, all resources, dry tons, nominal 2022 dollars.

The 2014 FSPP includes enhanced reporting through dynamic interactive visualization tools. Lessons learned in the 2014 FSPP and the associated visualizations are expected to aid in the development of the 2016 Billion Ton Report, which will build on the national resource analysis work established by the 2005 *Billion Ton Study* and the 2011 *Billion Ton Update*.

Additional feedstocks, such as algae and municipal solid waste will be included in future price projections. Monitoring and evaluation will continue, with assessments leading up to the detail required for the 2016 *Billion Ton Report*.

ORNL Develops System to Thwart Fuel Tax Evaders

Contact: Gary Capps, cappsgj@ornl.gov, 865-946-1285

Revenues from motor fuel and other highway use taxes are the primary source of funding for the US transportation system; and ensuring all of these taxes are collected, remitted, and credited to the Highway Trust Fund is a priority for the DOT Federal Highway Administration (FHWA). However, an estimated $10 billion in revenue is lost each year to fuel tax evasion (FTE).

To prevent such losses, ORNL researchers and partners from private industry have developed an integrated monitoring system that can track the movement of fuel tankers in real time and flag any suspicious activity. The goal of this research is to provide a proof-of-concept system to prevent illegal blending of non-taxable petrochemical products with taxable fuel products and cross-jurisdictional tax evasion.

For federal tax purposes, the point of taxation for gasoline and diesel fuel is the point of removal from bulk storage at the terminal rack. Approximately half of the states in the United States have the same point of taxation. However, for the remaining states, the point of taxation is at the wholesaler/distributor level or below. This presents additional challenges in tracking untaxed fuel after it leaves bulk storage. Current approaches to preventing FTE are time-consuming and attempt to discover and investigate evasions after the fact.

Using evidential reasoning techniques, ORNL researchers developed a supply-chain–based system that tracks fueling stops, loading, and unloading and provides near-real-time notification of any variation in standard delivery processes (e.g., a hatch or valve left open) from the tanker's point of origin to its final destination.

Three fuel tankers were equipped with the systems for an 8 month pilot test beginning in October 2014. Data from the systems are processed daily. Data collection will be completed in summer 2015, and a final report of the results will be drafted in early FY 2016. The results of the pilot test will inform possible FHWA rulemaking on tracking and monitoring equipment.

Stakeholder meeting participants examine monitoring equipment on a fuel tanker.

The system integrates sensor technology, wireless communications, vehicle tracking, and information analysis using a custom-developed sensor system, telematics, and sophisticated software. A user interface was developed to alert carriers to possible fuel theft, as well as a query tool for use by state and federal auditors.

The ORNL Commercial Motor Vehicle Roadside Technology Consortium team led a demonstration of the system for sponsors and industry partners at the beginning of the pilot test. As part of the project closeout, ORNL will host a meeting of potential users and manufacturers of the technology to gauge interest in tech transfer and deployment. If implemented, this monitoring system would make fuel movements transparent for carriers and auditors and help eliminate FTE and fuel theft.

ORNL Working to Prevent Accidents at Highway Work Zones

Contact: Gary Capps, cappsgj@ornl.gov, 865-946-1285

ORNL is working with the Federal Motor Carrier Safety Administration (FMCSA) to develop and implement strategies to reduce commercial vehicle accidents in roadway work zones on US highways. FMCSA statistics show that almost 600 fatalities occurred in work zones in 2013, with 25% of those involving commercial motor vehicles (CMVs).

As a part of this effort, ORNL is participating along with the Commercial Motor Vehicle Roadside Technology Consortium states of Tennessee, Mississippi, Georgia, North Carolina, and Kentucky. The Consortium is working with FMCSA to harness new safety and communication technologies to reduce injuries and loss of life in work zones.

Federal statistics show that after dropping steadily over the past decade, the incidence of work zone accidents involving CMVs is plateauing.

In November 2014, ORNL hosted the first-ever workshop on methods reducing work zone crashes, with a focus on CMVs. It included FMCSA and Federal Highway Administration staff and representatives from departments of transportation in Consortium member states and three non-member states. The meeting was focused on reviewing state efforts to address the issue of work zone crashes, understanding how commercial mobile radio systems in CMVs could be used to avoid accidents, and identify specific research areas to be addressed to deploy solutions.

ORNL maintains a website for the Consortium (ornl.gov/cta/CMVRTC) and has developed an educational video about using advanced communication technologies to alert CMV drivers that they are approaching work zones (www.youtube.com/crash mitigation) that have potential slow or stalled traffic queues.

ORNL researchers are currently working to define the messages that will be used to provide real-time alerts to CMV drivers about pending traffic issues at work zones and developing methodologies for implementing the messaging.

ORNL is working to prevent crashes due to traffic congestion at highway work zones like this one.

FMCSA launched the predecessor to the Consortium in 2007, in partnership with ORNL, the Tennessee Departments of Safety and Transportation, and the University of Tennessee, to further enable FMCSA testing of current, new-to-market, and emerging CMV safety technologies and to promote their usage and acceptance by stakeholders. The Consortium has since expanded to include Georgia, North Carolina, Kentucky and Mississippi. It provides a series of specially equipped testing facilities at inspection stations to demonstrate, test, evaluate, and showcase innovative CMV safety technologies under real-world conditions to improve commercial truck and bus safety.

Publications

1. National Transportation Research Center. 2014. *Technologies to Reduce Commercial Motor Vehicle Crashes in Work Zones*, Federal Motor Carrier Safety Administration.
2. M. B. Lascurain, O. Franzese, and G. Capps. 2015. *Heavy and Overweight Vehicle Brake Testing: Six-Axle Combination Vehicle Final Report*.
3. M. B. Lascurain. 2015. *Low Rolling Resistance Tire Stopping Distance Testing*.

Development of Strong, Low-Cost Commercial Textile Precursor

Contact: C. D. Warren, warrencd@ornl.gov, 865-574-9693

The cost of the carbon fiber in a hydrogen storage system is 60–80% of the total system cost, and the polyacrylonitrile (PAN) carbon-fiber precursor is about half of that cost. To preserve the cost advantages of using a high-volume PAN fiber—and simultaneously meet the needs of higher-performance applications with fiber strengths in the range of 650–700 ksi—ORNL researchers are developing the capability to use methyl-acrylate–based, textile-grade PAN as a much less expensive carbon fiber precursor.

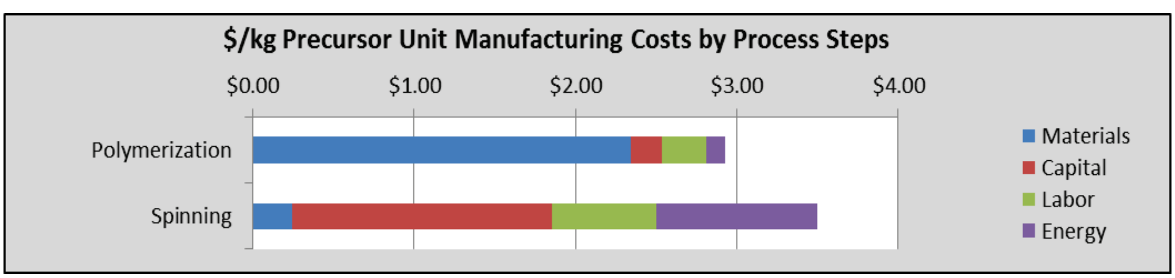
VTO research has developed technologies for producing lower-cost carbon fiber for use in automobile body and chassis applications. Fibers previously developed had strengths slightly below 500 thousand pounds per square inch (ksi), which is well above strengths suitable for automotive structural applications but insufficient for many high-demand applications with higher performance requirements, such as hydrogen storage tanks for fuel cell electric vehicles.

This project determined the ideal polymer formulation and conversion protocol (time–temperature–tension profiles) to produce the best carbon fiber using a precursor manufactured inexpensively in existing textile PAN plants. Successful completion of the project resulted in defining the precursor formulation and manufacturing methods to produce carbon fiber. SGL Group—The Carbon Company (SGL), ORNL's partner in the effort, is committed to commercializing the technology.

SGL and ORNL defined and analyzed candidate precursor formulations, down-selected to 11 candidate formulations, and selected the 3 most promising for testing. SGL determined how to spin each formulation into precursor fiber tows and sent them to ORNL for conversion trials. Critical parameters included uniformly round fibers and consistency from fiber to fiber and along the length of each fiber.

ORNL conducted thermal evaluations to pinpoint conversion temperatures of the precursor. The next step—determining the limits of fiber stretching in each stage during oxidative stabilization—was completed by systematically adding tension to precursors that have been processed through all earlier stages until reaching the breaking point of the precursor at the next temperature.

Another task was to develop a baseline cost model for production of high-strength carbon fiber (700 ksi) based upon the technologies currently employed in industry today. The expected cost benefits of using this precursor will be evaluated using that cost model and the processing conditions determined in this project. The baseline cost model is nearing completion.



Baseline precursor cost ($6.40/Kg [$2.91/lb]) for high-performance carbon fiber (2.1 lb of precursor is required to make 1.0 lb of carbon fiber).

Publications and Presentations

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2. A. Wheatley, C. D. Warren, and S. Das. 2013. “Low-cost Carbon Fibre: Applications, Performance and Cost Models,” pp. 405–434 in *Advanced Composite Materials for Automotive Applications: Structural Integrity and Crashworthiness*, John Wiley & Sons.

ORNL Characterizes Microstructures of Fuel Cell Materials

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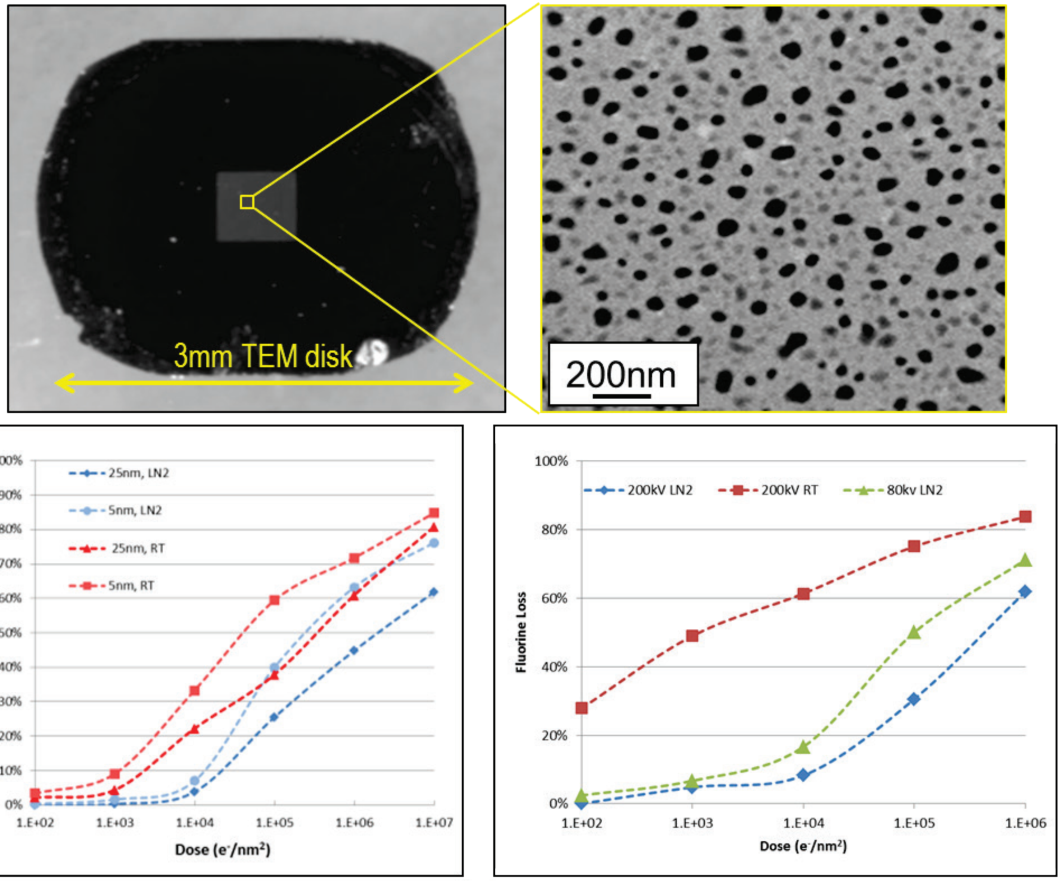
ORNL is identifying and optimizing novel high-resolution imaging and compositional/chemical analysis techniques, and developing unique specimen preparation methodologies, to characterize the constituent materials in fuel cell membrane electrode assemblies (MEAs) from the micrometer to the Angstrom scale. ORNL will make the techniques and expertise available to fuel cell researchers outside ORNL via Work for Others (proprietary) research, ORNL user facilities, and collaborative non-proprietary research projects.

Polymer electrolyte membrane fuel cells (PEMFCs) are being developed for use as efficient, zero-emission power sources. However, PEMFC performance degrades over time at high temperatures and relative humidity during electrochemical aging in automotive and stationary applications. The performance degradation can be attributed to the durability of individual materials that make up the MEA, including the electrocatalyst, catalyst support, recast ionomer, polymer membrane, and gas diffusion layer/microporous layer.

ORNL has focused on forming relationships with numerous industrial PEMFC developers and manufacturers, universities, and national laboratories to apply ORNL’s advanced electron microscopy techniques and expertise to characterize as-fabricated (fresh) fuel cell materials, MEAs subjected to accelerated stress tests designed to degrade specific components, and field-aged MEAs. The goal is to establish critical processing–microstructure–performance correlations to elucidate changes in individual materials that contribute to measured MEA degradation, performance loss, and failure. The results will enable faster commercialization of fuel cell electric vehicles.

The primary focus of research conducted in FY 2014 was identifying the proper microscopy conditions to characterize ionomer distributions at multiple length scales (on the 100 nm scale and the ~5 nm scale) within catalyst layers. Model substrates were prepared to identify ideal microscopy imaging and analysis conditions to minimize electron beam damage during evaluation. The primary microscope variables assessed were the effects of accelerating voltage, electron dose, and specimen temperature on fluorine loss. The through-electrode-loading variation in the ionomer distributions was studied for two different electrode geometries to understand the effects of underlying microporous layers on the ionomer distribution.

This case study demonstrates that quantitative ionomer measurements can be performed in scanning transmission electron microscopy by mitigating electron beam damage through controlled electron beam dose, sample cooling, and high accelerating voltages. This result is comparable to scanning transmission x-ray microscopy performed using a synchrotron source.



Flourine loss as a function of electron dose @ 60kV during STEM-EELS

Flourine loss as a function of voltage and specimen cooling during STEM-EDS

A study of thin Nafion films (5–25 nm thick) shows that analysis of ionomer films to minimize fluorine loss should be conducted at higher voltages (200 kV) and low electron doses and with cryogenic cooling (temperatures less than −100°C). Under these combined conditions, beam damage can be reduced by two to three times.

Publications and Presentations

1. C.-N. Sun, K. L. More, G. M. Veith, and T. A. Zawodzinski. 2013. "Composition dependence of the pore structure and water transport of composite catalyst layers," *Journal of the Electrochemical Society* **160**(9), F1000–F1005.

2. M. Li, D. A. Cullen, K. Sasaki, N. S. Marinkovic, K. L. More, and R. R. Adzic. 2013. "Ternary electrocatalysts for oxidizing ethanol to carbon dioxide: Making Ir capable of splitting C-C," *Journal of The American Chemical Society* **135**(1), 132–141.

3. K. A. Perry, K. L. More, E. A. Payzant, R. A. Meisner, B. G. Sumpter, and B. C. Benicewicz. 2014. "A comparative study of phosphoric acid-doped m-PBI membranes," *Journal of Polymer Science B* **52**(1), 26–35.

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Hydrogen Station Economics and Business Model Development

Contact: Zhenhong Lin, linz@ornl.gov, 865-946-1308

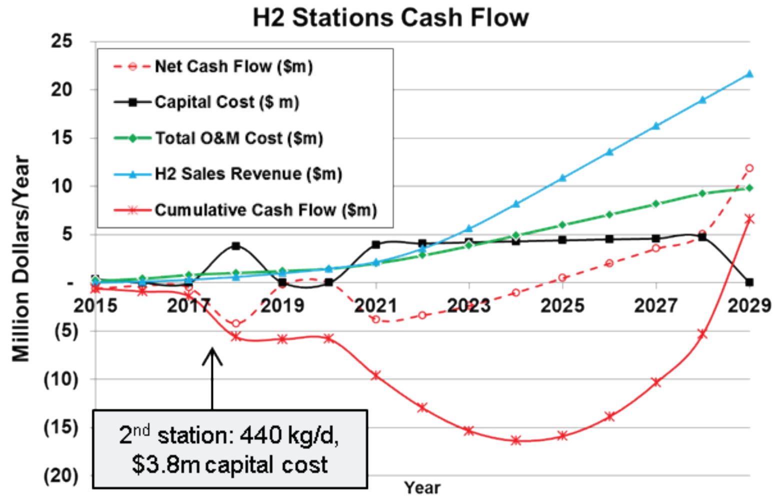
A sufficient hydrogen supply infrastructure is a critical issue in influencing drivers to purchase and use fuel cell electric vehicles (FCVs). Hydrogen refueling infrastructure must be constructed and must be commercially viable, with affordable hydrogen retail prices, to encourage continued expansion of the FCV market. ORNL research is addressing the issue by developing a station deployment optimization model and analysis of station network economics, risk of investment, viable business strategies, and public–private partnerships.

The Hydrogen Station Economics and Business model optimizes key deployment decisions to meet fuel demand by trading off costs for infrastructure and fuel accessibility. Variables include station size, location, and building schedule. Early FCV buyers seem to prefer high fuel availability (measured by the ratio of the number of hydrogen stations and the number of gasoline stations); however, high fuel availability during early commercialization may result in deploying more small stations and/or lower station utilization, which in turn leads to the loss of station scale economy and increased hydrogen cost.

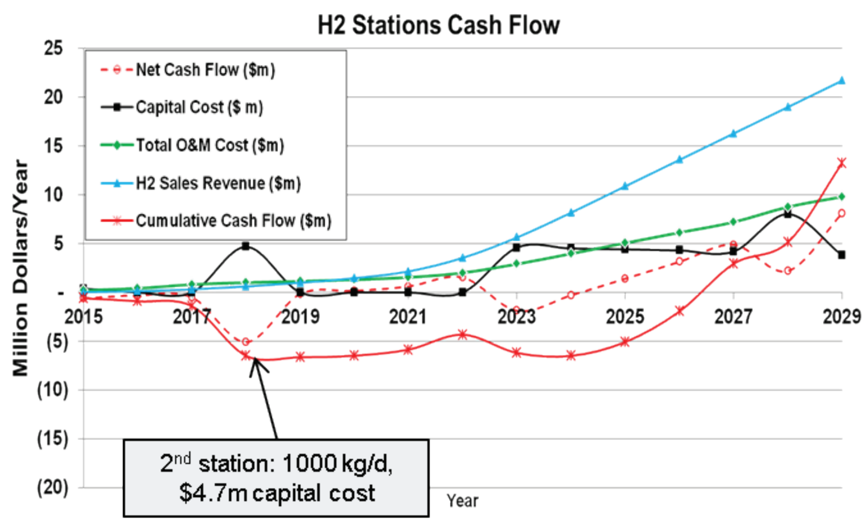
The project developed an Excel-based model, which takes as input FCV attributes and penetration assumptions; driver characteristics, including driving pattern, value of time, and discount rate; and infrastructure assumptions, including station capital cost and operation and maintenance (O&M) cost. The model outputs station deployment solutions (when and where to build and station size) and calculates cash flow and total system cost (infrastructure cost plus fuel accessibility cost).

In FY 2014, the project evaluated and conducted cash flow analysis for three station build-out scenarios: small station first (SSF), uniform-size station, and large station first (LSF). The SSF scenario refers to initially building small stations, followed by medium-size stations, and finally large stations. By contrast, the LSF scenario deploys larger stations first and smaller stations later. Large stations have a better scale economy in terms of both capital cost and O&M cost, but they have lower utilization rates, particularly in the early market.

Positive cash flow includes hydrogen sales revenue, and negative flow includes capital cost as a lump sum payment and annual O&M costs. Station owners endure net loss for about a decade before the break-even point. SSF annual cash flow becomes positive around 2025, but cumulative flow is negative until 2029. The LSF scenario shows better station economics: cumulative cash flow is positive by 2027.



Hydrogen station cash flow for small station first strategy.



Hydrogen stations cash flow for large station first strategy.

Publications and Presentations

1. Z. Lin, C. Liu, and D. Greene. 2014. "Hydrogen Station Economics and Business (HySEB)—Preliminary results," presented at the 2014 DOE Fuel Cell Technologies Program Annual Merit Review, Washington, D.C., June 17.

Melt-Processable PAN Precursor for High Strength, Low-Cost Carbon Fibers

Contact: Bob Norris, norrisrejr@ornl.gov, 865-576-1179

ORNL is developing advanced approaches to manufacturing high-strength carbon fiber that could yield significant cost savings.

High-strength carbon fiber enables the manufacture of durable, lightweight, compressed hydrogen vessels for high-pressure storage. However, current high-strength carbon fiber products are too expensive to meet DOE goals for storage system costs. Developing and demonstrating a melt-spun polyacrylonitrile (PAN) approach to producing precursor for carbon fiber will provide a more cost-effective route to achieving the performance necessary for high-pressure storage.

Melt spinning removes significant costs in handling and recovering solvents involved in solution spinning; it also eliminates a significant bottleneck in production rates required by the time, space, and energy used in the multistep solvent recovery process. Although somewhat similar processes have been demonstrated previously, no PAN-based carbon fiber currently is produced this way. The melt-spinning approach could save 25% of the costs involved in producing carbon fiber for high-pressure gas storage systems; additional savings may be possible in combination with advanced conversion approaches developed at ORNL.

The PAN precursor project is being conducted in multiple phases. Phase II is now under way. During the latter portion of Phase I, a milestone was achieved with a demonstration of carbon fiber properties exceeding the go/no-go point established at 15 Msi modulus and 150 ksi strength. Properties meeting follow-on milestone levels of up to 25 Msi modulus and 250 ksi strength also were achieved with melt-spun PAN produced at Virginia Tech University using a conversion protocol previously developed at ORNL. The conversion protocol's multiple steps simulate oxidation with differential scanning calorimetry testing, and then preliminary tensioning experiments in batch mode use the customized ORNL precursor evaluation system. Small tows spun at Virginia Tech were combined at ORNL to obtain a tow with an ample number of filaments (~100) to enable progressive tensioning during multiple oxidative stabilization steps and specific shrinkage management in low- and high-temperature carbonization.

This project's tasks focus on precursor development and conversion process improvements, and the primary precursor option is development and demonstration of melt-spinnable PAN. If successful, melt spinning is projected to be significantly less costly than wet spinning and will offer the capability to produce high-quality, relatively defect-free precursor. Concurrent activities in development of melt-stable PAN copolymer and blends, as well as in the processes necessary to spin the formulations successfully into tows made of filament, will be required.

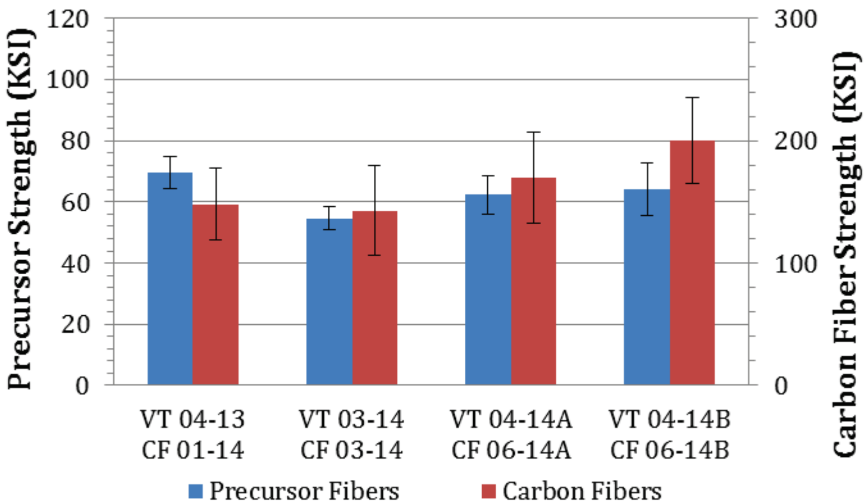
Publications and Presentations

1. J. Huang, D. G. Baird, and F. L. Paulauskas. 2014. "Thermal and rheological behavior of plasticized polyacrylonitrile and melt spinning of precursor fibers," *ANTEC 2014—Proceedings of the Technical Conference and Exhibition*, April 28–30, 2014.

2. F. L. Paulauskas and R. Norris. 2014. "Melt processable PAN precursor for high strength, low-cost carbon fibers," presented at 2014 DOE Hydrogen Program and Vehicle Technologies Annual Merit Review and Peer Evaluation Meeting, June 17.

3. R. Norris, S. Ozcan, and F. L. Paulauskas. 2014. "Carbon fiber and nanostructured material systems for manufacturing for high pressure hydrogen and natural gas storage," presented at Nanomaterials for Industry Conference, April 6–9.

4. F. L. Paulauskas and R. Norris. 2014. "Melt processable PAN precursor for high strength, low-cost carbon fibers," presented at Hydrogen Storage Tech Team Meeting, April 17.



Tensile strength of carbonized Virginia Tech PAN fibers.

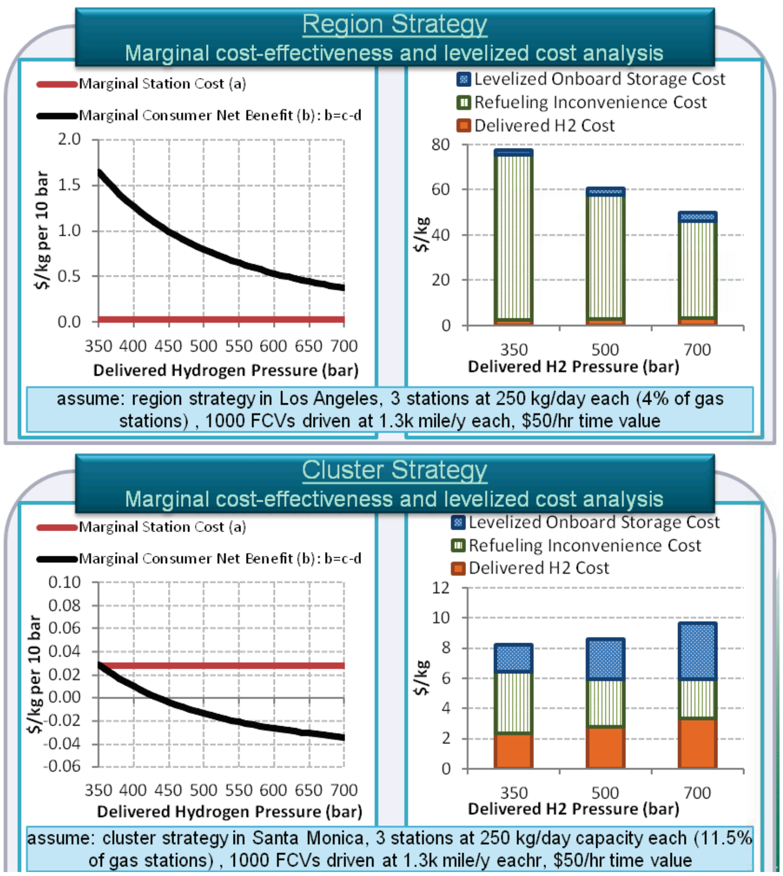
Randcastle 5/8 in. screw extruder in the processing lab at Virginia Tech.

Analyzing Optimal Onboard Storage Pressure for Hydrogen FCVs

Contact: Zhenhong Lin, linz@ornl.gov, 865-946-1308

Cost is an ongoing challenge in the development and widespread acceptance of vehicles powered by alternative fuels, such as hydrogen fuel cell vehicles (FCVs). The pressure at which hydrogen is delivered to hydrogen vehicles can affect the delivered cost of the fuel and the vehicle's range. A higher hydrogen pressure allows more hydrogen to be stored on board, enabling a longer driving range between refills; but it increases the cost of the hydrogen supply infrastructure—and therefore the delivered cost of hydrogen. Lower hydrogen pressure shortens the vehicle driving range and results in higher refueling frequency but may reduce the delivered hydrogen cost.

It is necessary, therefore, to find a balance among consumer refueling convenience, onboard storage costs, and infrastructure costs for refueling facilities. ORNL researchers are evaluating both region-wide optimal infrastructure rollout strategies and clustering strategies to find the most cost-effective balance for the location of hydrogen fueling stations. The optimal storage pressure (OP) is lower with a cluster strategy than with a regional rollout strategy. Clustering allows a small number of stations to achieve a high level of refueling convenience.



Optimizing pressure for region and cluster strategies.

Under scenarios constructed to reflect compliance with the zero-emission vehicle mandate in California, lower pressure is desirable for a cluster strategy, whereas higher pressure is desirable for a regional strategy. As indicated in the table, in the regional strategy, the vehicles and stations are assumed to spread over the Southern California region. In the cluster strategy, the vehicles and stations are assumed to concentrate in 4, 6, and 12 representative areas similar to Santa Monica during three periods, respectively. Although the total numbers of vehicles and stations are the same, the refueling convenience differs between the two rollout strategies, which leads to OP differences.

Zero emission vehicle (ZEV) compliance assumptions

	ZEV Years 1–3	ZEV Years 4–6	ZEV Years 7–9
FCVs on road	636	3,442	25,000
Average station size (kg/d)	100	200	350
Station utilization	47%	85%	88%
Cluster Strategy			
Clusters	4	6	12
FCVs on road/cluster	159	574	2,083
Stations/cluster	2	2	4
FA (% of gas stations)	7.7%	7.7%	15.4%
Region Strategy			
Stations in the region	8	12	48
FA (% of gas stations)	0.13%	0.20%	0.80%

Notes: FCV = fuel cell electric vehicle; FA = fuel availability.

The OP sensitivity analysis was completed using seven parameters—time value, driving intensity, time to nearest station, onboard storage cost, station cost, pressure incremental station cost, and station scaling factor. There is a tradeoff between delivered pressure and fuel availability. A larger number of stations shortens each refueling trip and thus can reduce the need for the longer range enabled by higher pressure.

Going forward, in-depth OP analysis for early adopters and integration with consumer choice models is recommended. More research is needed to identify the OP for early adopters, for maximizing FCV market acceptance, and for standardization concerns.

Publications/Presentations

1. Z. Lin, C. Liu, and D. Greene. 2014. "Analysis of optimal onboard storage pressure for hydrogen fuel cell vehicles," presented at the 2014 DOE Annual Merit Review meeting, Washington, D.C., June 16–20.

Vessel Design and Fabrication Technology for Stationary Hydrogen Storage

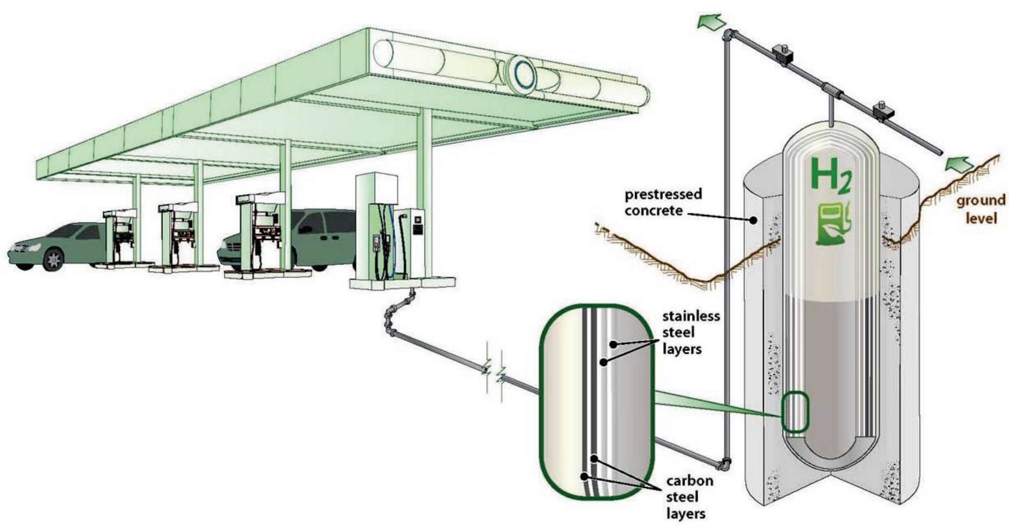
Contact: Zhili Feng, fengz@ornl.gov, 865-576-3797

Low-cost infrastructure is critical to successful market penetration of hydrogen-based transportation technologies such as off-board bulk stationary hydrogen storage, which is needed in locations ranging from hydrogen production plants to refueling stations. However, design capacity and pressure needs are expected to vary considerably depending on the intended use, the location, and other economic and logistic considerations.

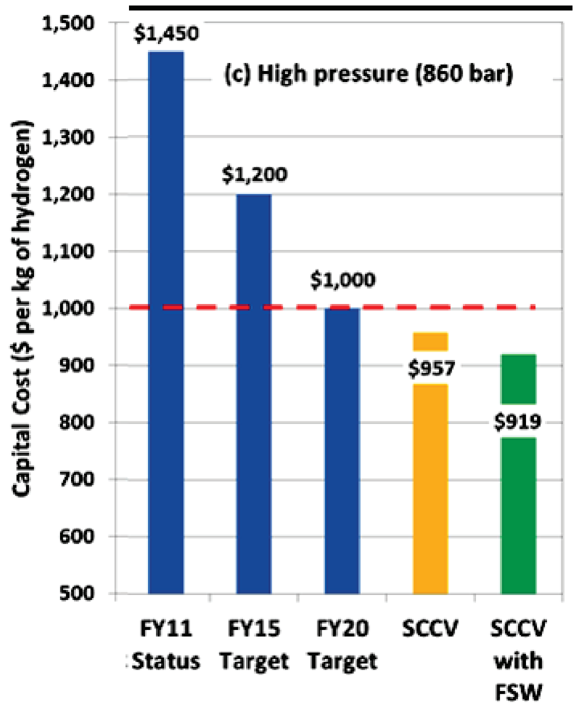
For the past several years, ORNL has led a diverse multidisciplinary team from industry and academia to develop and demonstrate an integrated design and fabrication technology for a cost-effective, high-pressure steel/concrete composite vessel (SCCV) that can meet different stationary hydrogen storage needs. The SCCV has several inherent features aimed at solving the two critical limitations and challenges of today's high-pressure hydrogen storage vessels—the high capital cost and the safety concerns regarding hydrogen embrittlement of high-strength steel vessels.

The SCCV comprises four major innovations: (1) flexible modular design to meet varying storage pressure and capacity needs, cost optimization, and system reliability and safety; (2) composite design and construction with an inner steel vessel encased in a pre-stressed outer concrete reinforcement; (3) a layered steel vessel wall and vent holes to solve the hydrogen embrittlement problem; and (4) an integrated sensor system to monitor the system's structural integrity and operation status. The novel SCCV design allows for the stresses or the structural load from the high-pressure hydrogen to be shared between the inner steel vessel and the pre-stressed outer concrete reinforcement, thereby offering flexibility to optimize low-cost commodity materials (such as structural steels and concretes) and industry-accepted fabrication technologies for cost reduction.

The major tasks in FY 2014 included validating that the SCCV design can reduce the cost of stationary hydrogen storage by more than 15% and meet the DOE 2015 cost target; demonstrating ORNL-patented multipass, multilayer friction-stir welding for joining a multiple-layer steel to a thickness of 1.5 inches; and designing and fabricating a quarter-size mock-up composite vessel capable of storing 90 kg of gaseous hydrogen at 430 bar. Because SCCVs can be fabricated with relatively mature technologies, cost figures for fabrication of SCCVs were available from commercial vendors. Through a survey of a number of industry manufacturing vendors, researchers obtained a detailed cost breakdown that assumed moderate- to high-volume production. The results show that the design is economically viable and technically feasible for storing compressed gaseous hydrogen.



Schematic showing the design of a steel/concrete composite vessel comprising inner layered steel tanks and outer pre-stressed concrete confinement



Comparison between steel/concrete composite vessel unit costs and DOE technical targets for hydrogen pressures of 860 bar.

Publications and Presentations

1. Y. C. Lim, S. Sanderson, M. Mahoney, X. Yu, Y. Wang, and Z. Feng. “Characterization of multilayered multipass friction stir weld on ASTM A572 G50 Steel,” *Welding Journal*, in press.

2. Y. Wang, Y. C. Lim, F. Ren, W. Zhang, M. Jawad, F. Vossoughi, and Z. Feng. 2014. “Steel-concrete composite vessel for stationary high-pressure hydrogen storage,” presented at ASME 2014 12th Fuel Cell Science, Engineering and Technology Conference, Boston, June 30–July 2.

3. Y. Wang, Y. C. Lim, J.-A. Wang, L. Anovitz, W. Zhang, and Z. Feng. 2014. “Evaluation of mechanical property testing procedures and techniques for materials used for hydrogen storage and distribution,” presented at ASME 2014 12th Fuel Cell Science, Engineering and Technology Conference, Boston, June 30–July 2.

4. Y. C. Lim, S. Sanderson, M. Mahoney, Y. Wang, and Z. Feng. 2014. “Friction stir welding high strength low alloy steel using a multilayer approach,” presented at 10th International Friction Stir Symposium, Beijing, China, May 20–23.

Analysis

Study Indicates Optimum BEV Driving Range May Be Below 100 miles

Contact: Zhenhong Lin, linz@ornl.gov, 865-946-1308

Until the cost of an electric vehicle battery is cut to $100/kWh or less, most US consumers considering a battery electric vehicle (BEV) would be better off with a model with a range below 100 miles, according to ORNL research.

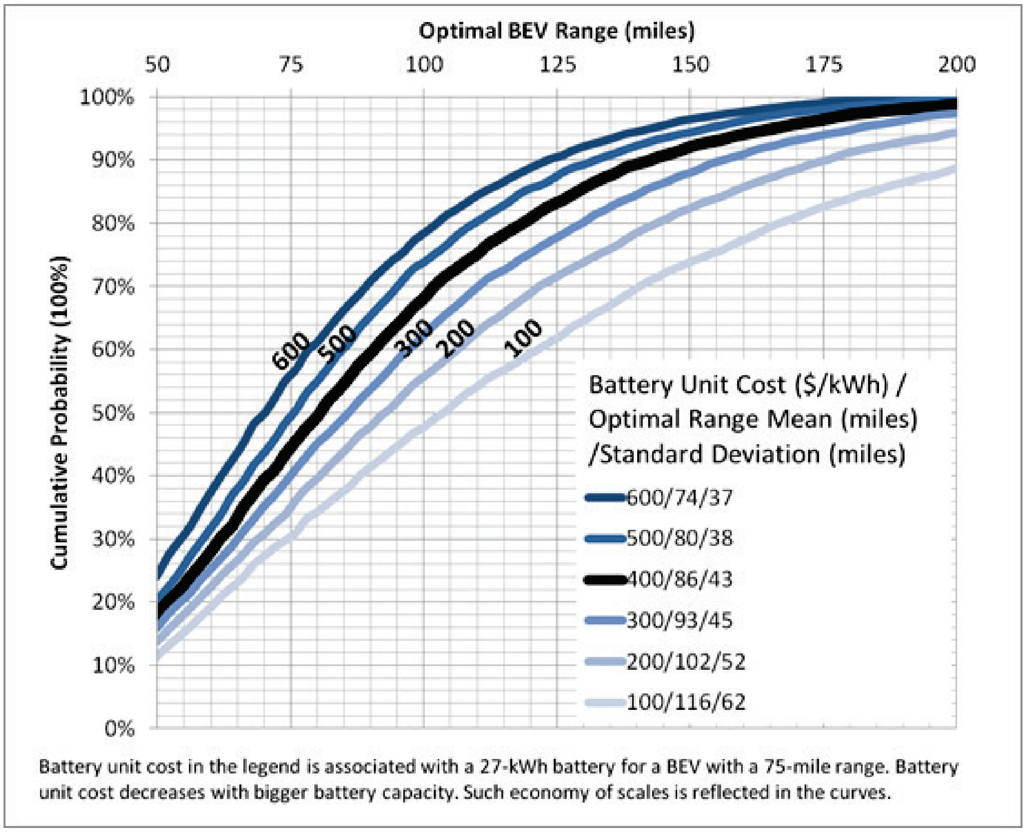
The research, published in *Transportation Science*, suggests reconsidering the R&D goal of attaining a driving range (distance the vehicle can travel between charges) for BEVs comparable to that of a conventional vehicle. It also implies that policy and R&D should focus on continuing to reduce battery cost to make short-range BEVs more price-competitive, and on widely deploying charging infrastructure to improve their usability.

Properly determining driving range is critical for accurately predicting the market potential of BEVs and their societal benefits, such as reducing petroleum use and greenhouse gas emissions.

ORNL proposes a framework for optimizing the BEV driving range by minimizing the sum of battery price, electricity cost, and range limitation cost, which serves as a measure of range anxiety. The range optimization framework is linked to policy-relevant parameters, including battery cost and price markup, battery utilization, availability of charging infrastructure, vehicle efficiency, electricity and gasoline prices, household vehicle ownership, daily driving patterns, discount rate, and perceived vehicle lifetime.

The electric driving range of a BEV was optimized separately for each of 36,664 sample drivers representing new car drivers in the United States. The results showed the distribution of optimized BEV ranges among US consumers, as well as changes in the distribution in response to battery cost reductions and charging infrastructure improvements.

The quantitative results strongly suggest that ranges of <100 miles are likely to be more popular in the BEV market for a long time. The average optimal range among US drivers was found to be largely inelastic. However, a lower battery cost was found to significantly drive BEV demand toward longer ranges, whereas charging infrastructure improvements drive demand toward shorter ranges. The bias of a single-range assumption, and the effects of range optimization and diversification in reducing such biases, were both found to be significant.



Cumulative share of optimal range by battery cost

The study findings explain why products with a range below 100 miles dominate the BEV market. Before the introduction of the Nissan Leaf (certified with a 73-mile electric range) in December 2010, BEV ranges were often assumed to be between 150 and 200 miles. Now, ~80% of the BEV products on the US market have a driving range of <100 miles.

Publication

1. Z. Lin. 2014. “Optimizing and diversifying electric vehicle driving range for US drivers,” *Transportation Science* **48**(4), 635–650. http://dx.doi.org/10.1287/trsc.2013.0516

Combustion Engines and Fuels

ORNL Catalyst Controls Emissions at Low Exhaust Temperatures

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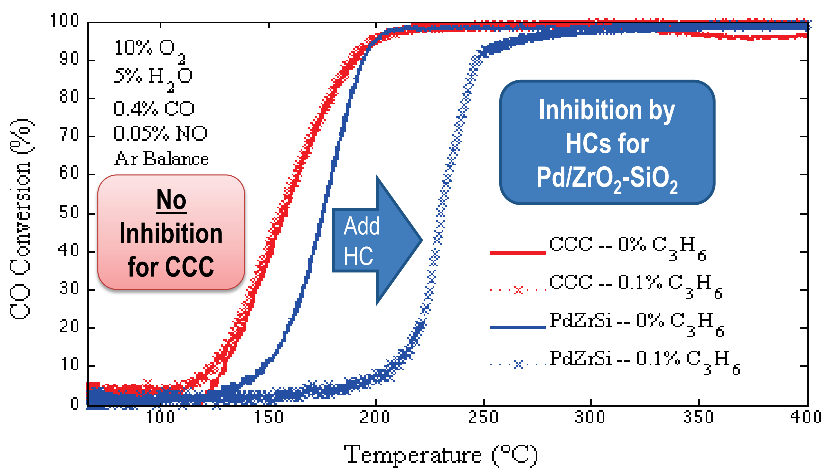
Advanced, more fuel-efficient combustion engines are creating challenges for emission control systems because their efficiency leads to lower exhaust temperatures. The oxidation of carbon monoxide (CO) and other pollutants by catalysts becomes more difficult at lower temperatures. However, a new type of catalyst developed at ORNL is enabling improved low-temperature performance without employing precious metal catalysts.

This catalyst has great potential as an emissions control component that enables the use of advanced combustion engines that reduce petroleum consumption.

Platinum group metal (PGM) catalysts are the current standard for controlling pollutants in automotive exhaust streams, but their high cost and their susceptibility to inhibition at low temperatures are barriers to the use of more fuel-efficient engines. Inhibition occurs when one pollutant fills the active catalyst sites and prevents other pollutant species from being oxidized. Of particular concern is the inhibition between CO and hydrocarbon species, since both CO and hydrocarbon emissions are higher for advanced combustion engines.

ORNL has developed a ternary mixed-oxide catalyst consisting of copper oxide, cobalt oxide, and ceria (dubbed CCC) as an alternative to PGM-based catalysts for low-temperature CO oxidation (90% conversion at 170°C). The innovative CCC catalyst outperforms PGM catalysts for CO oxidation in simulated exhaust streams while showing no signs of inhibition by nitrogen oxides or the model hydrocarbon, propene (C_3H_6).



CO light-off curves of CuO_x–CoO_y–CeO_2 (CCC) and Pd/ZrO_2–SiO_2 catalysts in simulated exhaust conditions. The graph illustrates that the CO reactivity on CCC is unaffected by the presence of C_3H_6.

The surprising chemical behavior of the low-cost CCC catalyst could be a key to preventing the inhibiting behavior of CO and allowing other catalysts to oxidize hydrocarbons at lower temperatures.

A typical PGM-based catalyst must be heated to over 235°C to convert 50% of the C_3H_6 in the presence of CO; however, if the CO is removed, the conversion can occur at significantly lower temperatures. Furthermore, the heat generated from the combustion of CO over the CCC catalyst would be beneficial in activating the traditional PGM catalysts used for hydrocarbons. Therefore, if used in harmony, these two catalysts have the potential to oxidize both CO and C_3H_6 when the exhaust temperatures are on the order of 150°C. These factors illustrate that this catalyst has great potential as a low-cost component in the exhaust streams of advanced combustion vehicle engines with low-temperature exhaust.

Publications, Presentations, and Patents

1. T. J. Toops, J. E. Parks, J.-S. Choi, M. Kim, C. Bauer, and A. Binder. 2014. "Investigation of low temperature emissions control catalysts to enable fuel-efficient engine commercialization," presented at 2014 Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Workshop, Dearborn, MI, May 1.

2. J. E. Parks, T. Toops, J.-S. Choi, M. Kim, C. Bauer, and A. Binder. 2014. "Low temperature emission control to enable fuel-efficient engine commercialization," presented at DOE Vehicle Technologies Office 2014 Annual Merit Review and Peer Evaluation Meeting, Washington D.C., June 19.

3. A. J. Binder, T. Toops, S. Dai, and J. E. Parks. 2014. "CO oxidation over CuO_x-CoO_y-CeO_2 ternary oxide in simulated exhaust conditions: Comparison to platinum-group metal catalysts," presented at Eighth International Conference on Environmental Catalysis, Asheville, NC, August 24–27.

Higher EGR Levels Could Significantly Improve Engine Efficiency

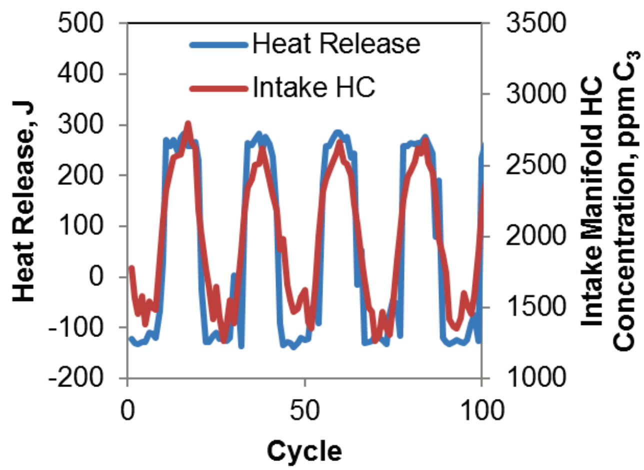
Contact: Brian Kaul, kaulbc@ornl.gov, 865-46-1299

Experiments at ORNL with high levels of external exhaust gas recirculation (EGR) in vehicle engines reveal the importance of two different timescales of deterministic feedback that drive cycle-to-cycle variations. The findings provide insight into new control approaches for improving the stability of high-efficiency combustion.

The new insights into the two interplaying timescales of combustion feedback will be used to develop intelligent control systems with the goal of extending the EGR dilution limit, which could lead to estimated engine efficiency improvements of up to 10%.

Cyclic variations in dilute combustion are known to exhibit identifiable, repeating patterns, indicating that they are driven by deterministic (non-random) processes and thus are potentially controllable. Previous research examining dilute combustion, for both lean (excess air) and inert diluents, has shown that the composition of the residual gases in the cylinder is a dominant mechanism by which cycle-to-cycle effects are carried forward, and that the previous cycle has the strongest effect.

The ORNL experiments and analysis identified the existence of both short- and long-timescale patterns in cyclic dispersion for an engine running with external EGR. The short-timescale dynamics are due to the internal residual gases, while the long-timescale dynamics are due to the external EGR loop. At high EGR rates, this feedback mechanism dominates, and there is a strong correlation between the time it takes for EGR to recirculate through the system and the period of combustion variations. This correlation is caused by the effect of the EGR composition on combustion.



A time series of heat release and intake hydrocarbon concentration for 55% EGR shows the onset of multi-cycle dynamics in combustion variations.

EGR has been used for emissions control since the 1970s, but it has been limited to low levels because of cycle-to-cycle variations in engine performance that degrade drivability and engine efficiency. Significant thermodynamic efficiency gains could be achieved by operating with higher levels of EGR because it would enable higher compression ratios and more optimal combustion phasing; this is especially the case for the turbocharged direct-injection engines becoming more common in the market. Reducing cyclic variations to acceptable levels is necessary to enable these gains.

Publications, Presentations, and Patents

1. B. C. Kaul, C. E. A. Finney, R. M. Wagner, and M. L. Edwards. 2014. "Effects of external EGR loop on cycle-to-cycle dynamics of dilute SI combustion," *SAE Int. J. Engines* **7**(2).

2. C. E. A. Finney, B. C. Kaul, D. A Splitter, C. S. Daw, and R. M. Wagner. 2014. "Long-timescale combustion instabilities in spark-ignited engines," presented at the 2014 Spring Technical Meeting of the Central States Section of the Combustion Institute, Tulsa, Oklahoma, March 16–18.

3. C. E. A. Finney, B. C. Kaul, D. A. Splitter, C. S. Daw, and R. M. Wagner. 2014. "Engines on the edge: Long memory and mode switching in internal combustion engines," poster presented at XXXIII Dynamics Days US, Atlanta, January 2–5.

Ionic Liquid Lubricant Additives Improve Fuel Economy

Contact: Jun Qu, qujn@ornl.gov, 865-576-9304

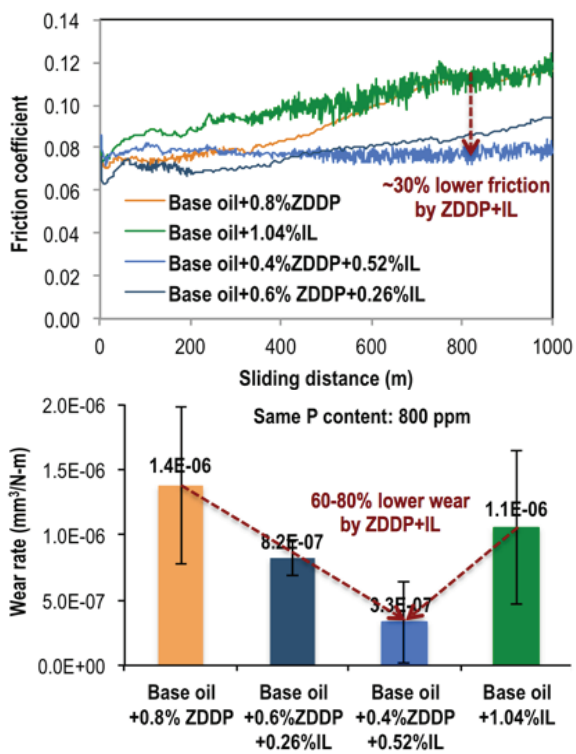
ORNL and its partners have developed lubricant additives with superior friction and wear reduction characteristics that could mean billions of gallons of annual fuel savings if they were deployed across the US vehicle fleet.

Parasitic friction generally consumes 10–15% of the energy generated in an internal combustion engine. Since cars and trucks account for 70% of the annual oil consumption in the United States, that friction penalty represents a large amount of wasted energy. Lubricants such as motor oil are critical in mitigating friction and wear in vehicles. One path to lowering friction and increasing fuel economy is lowering oil viscosity to reduce hydrodynamic drag; but if the viscosity is too low, the lubricant may not offer enough wear protection for the engine.

ORNL researchers, in cooperative research and development agreements with General Motors and Shell and in partnership with Lubrizol, have developed novel ionic liquids (ILs) as next-generation anti-wear lubricant additives to meet targets for lower viscosity combined with improved wear protection. The ILs offer good oil miscibility, high thermal stability, noncorrosiveness, excellent wettability, and effective anti-wear and friction reduction qualities. In FY 2013, a prototype low-viscosity (SAE 8) engine oil containing the IL additives demonstrated 2% higher fuel efficiency while providing wear protection and aging performance comparable to a commercial SAE 5W-30 engine oil in multi-cylinder engine dynamometer studies.

In FY 2014, a new group of phosphonium-organophosphate ILs with symmetric cation structures (IL-C) were invented at ORNL, and they have demonstrated even better anti-wear performance than the earlier compounds. Furthermore, the new ILs show synergistic effects in combination with the conventional anti-wear additive ZDDP. The ZDDP+IL combinations outperformed either ZDDP or the IL-C alone by ~30% for friction and 60–80% for wear. Surface characterizations revealed interesting changes in the tribofilm composition: addition of the IL promotes zinc compounds and metal-phosphates but reduces sulfur compounds and metal oxides. The latest experimental results and in-depth fundamental understanding are promising.

In FY 2015, the researchers will formulate a low-viscosity engine oil using ZDDP+IL-C as an antiwear additive and conduct engine tests to demonstrate its effects on engine efficiency and emission catalysts. The mechanisms behind the synergism between the IL and ZDDP also will be further investigated.



Synergistic effects of combining an IL and ZDDP (maintaining 800 ppm of phosphorus in oil). Friction was reduced by 30% (upper) and wear by 60–80% (lower).

Publications, Presentations, and Patents

1. J. Qu and H. Luo. 2014. “Ionic liquids containing symmetric quaternary phosphonium cations and phosphorus-containing anions, and their use as lubricant additives,” US Patent Application 14/184,754, filed February 20.

2. W. C. Barnhill, J. Qu, H. Luo, H. M. Meyer III, C. Ma, M. Chi, and B. L. Papke. 2014. “Phosphonium-organophosphate ionic liquids as lubricant additives: Effects of cation structure on physicochemical and tribological characteristics,” *ACS Applied Materials & Interfaces* **6**(24), 22585–22593.

3. J. Qu. 2014. “Ionic liquids as next generation anti-wear additives: Molecular design to engine dynamometer testing,” invited presentation at 38th Automotive/Petroleum Industry Forum (Detroit Advisory Panel), Dearborn, April 16.

4. J. Qu. 2014. “Ionic liquid-additized engine oil for improved fuel efficiency,” invited presentation at SAE 2014 High Efficiency IC Engine Symposium, Detroit, April 6–7.

5. J. Qu, B. L. Papke, W. C. Barnhill, B. Kheireddin, H. Luo, C. Chen, P. J. Blau, B. H. West, M. Richard, S. Mercer, and S. Dai. 2014. “Ionic liquids as ashless oil additives: Correlations between molecular structures and oil-solubility and lubricating characteristics,” presented at STLE 69th Annual Meeting, Orlando, May 18–22.

6. J. Qu. 2014. “Oil-soluble ionic liquids as next-generation lubricant anti-wear additives,” presented at 248th ACS National Meeting, San Francisco, August 10–14.

ORNL Demonstrates Novel Route to Onboard Hydrogen Generation

Contact: James Szybist, szybistjp@ornl.gov, 865-946-1514

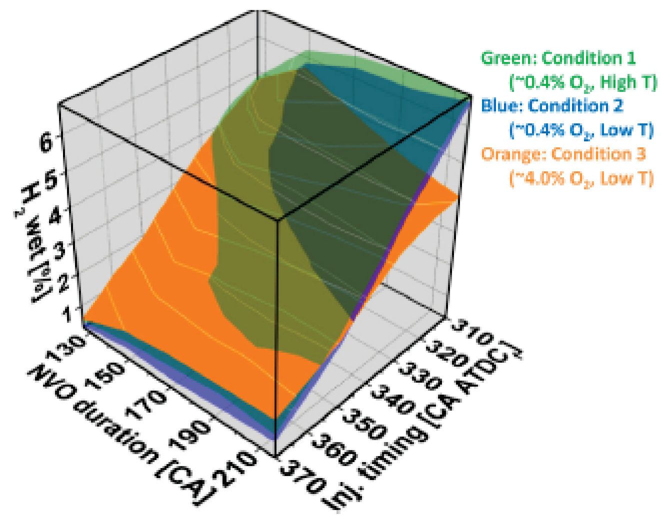
Researchers at ORNL have developed a novel in-cylinder reforming route to generate hydrogen (H_2) aboard a vehicle with a reduced fuel energy penalty, or even a fuel energy benefit in some cases.

Hydrogen can be used to enable high-efficiency, lower-temperature gasoline combustion. However, methods of reforming fuel to generate H_2 onboard an engine typically incur significant fuel energy penalties.

Increasing the level of exhaust gas recirculation (EGR) on spark-ignited (SI) gasoline engines is a well understood pathway to increasing engine efficiency. However, the amount of EGR dilution that is feasible is limited, because a high level of EGR adversely affects combustion stability and ultimately efficiency. Introducing small amounts of H_2 during combustion can help stabilize combustion under highly dilute conditions, primarily by increasing the flame speed.

The ORNL strategy injects fuel into recompressed hot exhaust gases, and the waste heat from the exhaust drives the fuel reforming reactions to produce H_2 and other products. The conditions conducive to H_2 generation were characterized, and H_2 levels exceeding 6% were measured.

The research was performed on a single-cylinder experiment at ORNL using a unique engine cycle. It is currently being scaled up to multi-cylinder research. The way the H_2 is being used is similar to dedicated-EGR research being performed at Southwest Research Institute, but the way that the H_2 is being generated at ORNL is unique.



Surface response of H_2 generation as a function of fuel injection timing and duration of the engine recompression event.

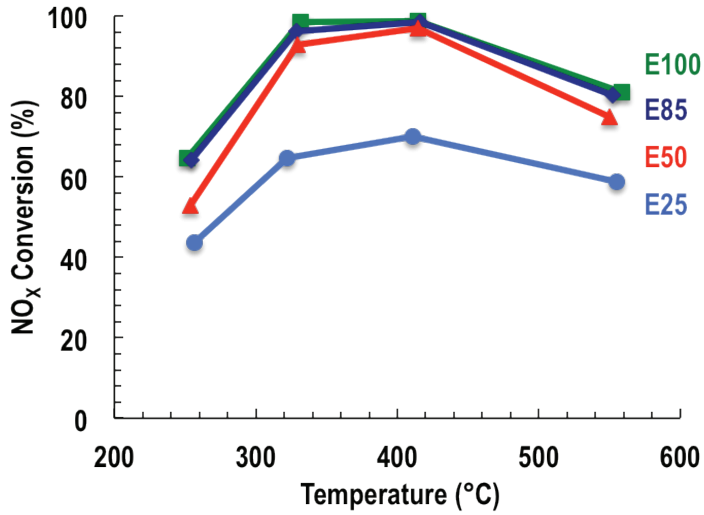
High-Ethanol Blends Improve Catalyst Control of NOx Emissions

Contact: Jim Parks, parksjeii@ornl.gov, 865-946-1283

ORNL research shows that adding high levels of ethanol to gasoline can greatly benefit silver–alumina catalyst control of nitrogen oxides (NOx) emissions from lean-burn gasoline engines. The findings demonstrate a synergistic approach by which the NOx emission issues posed by more fuel-efficient lean gasoline engines can be better controlled by fuels with more biofuel content. Thus the benefits of the approach include reduced petroleum consumption via two pathways: greater fuel efficiency and higher renewable biofuel use.

Fuel-efficient lean gasoline engines and the use of high-ethanol fuel blends (such as E85) could significantly reduce US petroleum consumption, but issues associated with both strategies must be resolved before they can be widely adopted. Lean gasoline engines are more fuel-efficient than the common stoichiometric gasoline engine that dominates the US passenger car fleet; however, NOx emissions produced by lean engines are difficult to cost-effectively control because of the excess oxygen in the exhaust from lean operation. E85 directly replaces petroleum with a biomass-derived fuel, but its adoption is hindered by the lower density of ethanol, which causes it to have lower tank mileage than gasoline.

ORNL researchers have found a synergy between the lean-engine and high-ethanol fuel strategies by exploiting the unique chemical reactivity of ethanol to facilitate cost-effective NOx control for lean-burn engines. Prior work at ORNL and elsewhere has demonstrated that ethanol is an effective reductant for removing NOx from engine exhaust when it is introduced upstream of a silver/alumina catalyst. This work was extended in FY 2014 to evaluate the NOx reduction efficiency of market-feasible ethanol/gasoline blends over a silver/alumina catalyst.



NOx conversion in relationship to temperature for four different ethanol/gasoline fuel blends. The fuels were sprayed upstream of a silver/alumina catalyst in the exhaust of a lean gasoline engine.

The study showed 98% NOx conversion in lean gasoline engine exhaust with ethanol–gasoline blends containing at least 50% ethanol. These results demonstrate the capability for ethanol from realistic fuel blends to reduce NOx in real engine exhaust. They also illustrate the potential benefits of an ethanol separation strategy for applications with lower-ethanol-content fuel blends.

The goal is to enable more use of vehicles with emissions-compliant, high-efficiency lean gasoline engines that consume less petroleum and go farther on a tank of fuel when running on high-ethanol blends.

Future work will focus on catalyst durability, minimizing hydrocarbon emissions, and evaluating other bio-derived alcohols for NOx reduction using the same catalyst.

Publications, Presentations, and Patents

1. V. Y. Prikhodko, J. A. Pihl, T. J. Toops, J. Thomas, J. E. Parks II, and B. West. “Selective catalytic reduction of oxides of nitrogen with ethanol/gasoline blends over a silver/alumina catalyst on lean gasoline engine,” accepted by SAE Technical Paper Series.

2. V. Y. Prikhodko, J. A. Pihl, T. J. Toops, J. Thomas, J. E. Parks II, and B. West 2014. “Selective catalytic reduction of oxides of nitrogen with ethanol/gasoline blends over a silver/alumina catalyst on a lean gasoline engine,” presented at 8th International Congress on Environmental Catalysis, Asheville, NC, August 24–27, 2014.

RCCI–GCI Strategy Demonstrates Higher Efficiency, Lower Emissions

Contact: Scott Curran, curransj@ornl.gov, 865-946-1522

Reactivity-controlled compression ignition (RCCI) and gasoline compression ignition (GCI) combustion strategies tested on a common multi-cylinder engine platform yielded a brake thermal efficiency (BTE) equivalent or superior to that of diesel engines while producing ultra-low NOx and soot emissions.

The experiments at ORNL demonstrate the potential of these advanced combustion modes to meet the long-term engine efficiency goals of the US DRIVE partnership.

RCCI is a combustion regime in which first a low-reactivity fuel is injected into the engine cylinder and premixed with air, and then a high-reactivity fuel is injected into the cylinder before ignition. GCI fires gasoline by compression ignition, rather than spark ignition, to increase engine efficiency. BTE is a measure of how efficiently an engine converts the energy in a fuel into mechanical energy to drive a vehicle.

The ORNL engine experiments used a dual-fuel RCCI/majority-premixed GCI strategy on production-viable engine hardware: a turbocharged direct-injection light-duty diesel engine, equipped with 15:1 compression ratio pistons designed for premixed combustion, and stock diesel injection and air-handling systems. A 68 research octane number gasoline-range fuel was used. A wide range of gasoline-like fuels is under investigation in the literature for GCI strategies, and the optimal strategy for the highest efficiency and lowest emissions will depend on both the fuel and the combustion chamber geometry.

2000 rpm, 4.0 bar brake mean effective pressure comparison of diesel combustion, RCCI, and majority-premixed GCI

	CDC	RCCI	GCI LTC
BTE (%)	33.4	35.8	34.7
NOx (ppm)	96	26	10
HC (ppm)	161	2164	2615
CO (ppm)	322	1733	2100
FSN (-)	1.02	0.01	0.01

The results showed a BTE improvement on the order of 4–7% at 2000 RPM, 4.0 bar brake mean effective pressure. They approach the Advanced Combustion and Emissions Control 2020 stretch goal of 36% BTE at 20% of peak load at 2000 RPM. (Modern conventional diesel engines can achieve a BTE of 34% at 20% peak load.)

The tests demonstrated that both of the low-temperature combustion strategies were able to achieve the BTE improvements while simultaneously producing engine-out NOx emissions of less than 0.2 g/kW h and soot emissions of 0.00 FSN (filter smoke number) on a common engine platform.

These results are the first from a larger study comparing dual-fuel RCCI and the spectrum of low-temperature GCI concepts with conventional diesel combustion on the same engine platform. Both the dual-fuel RCCI and single-fuel GCI concept were shown to have elevated CO and hydrocarbons compared with diesel combustion, which will be an issue for currently available exhaust aftertreatment systems.

The next steps of the study will compare RCCI with more stratified GI strategies using a variety of gasoline-range fuels and a stock diesel piston.

Publications, Presentations, and Patents

1. S. Curran, Z. Gao, and R. Wagner. 2014. "Reactivity controlled compression ignition drive cycle emissions and fuel economy estimations using vehicle systems simulations with E30 and ULSD," *SAE International Journal of Engines* **7**(2), 902–912.

2. B. Dempsey, S. J. Curran, R. M. Wagner, and W. Cannella. 2014. "Effect of premixed fuel preparation for partially premixed combustion with a low octane gasoline on a light-duty multi-cylinder compression ignition engine," paper ICEF2014-5561, V001T03A012 in *ASME 2014 Internal Combustion Engine Division Fall Technical Conference*, ASME.

3. S. Curran, A. Dempsey, R. Wagner, and Z. Gao. 2014. "Efficiency and emissions comparison of single and dual-fuel low temperature combustion on a light duty multi-cylinder diesel engine," presented at 2014 SAE High Efficiency Engine Symposium, Detroit, April.

Engine Simulations Show 25% Better Fuel Economy for RCCI Operation

Contact: Scott Curran, curransj@ornl.gov, 865-946-1522

Simulations conducted at ORNL show a 25% improvement in fuel economy for a vehicle using reactivity-controlled compression ignition (RCCI) operation, compared with a gasoline engine baseline. Data from experiments on a multi-cylinder engine were used to model vehicle fuel economy and emissions for three fuel combinations in an RCCI cycle.

In-cylinder blending of gasoline and diesel for RCCI combustion can reduce NOx and particulate matter emissions while maintaining or improving brake thermal efficiency (a measure of how efficiently fuel energy is converted to mechanical energy) compared with conventional diesel combustion (CDC). In RCCI, the fuel reactivity can be tailored to the engine speed and load, allowing the extension of stable low-temperature combustion over more of the light-duty drive cycle load range.

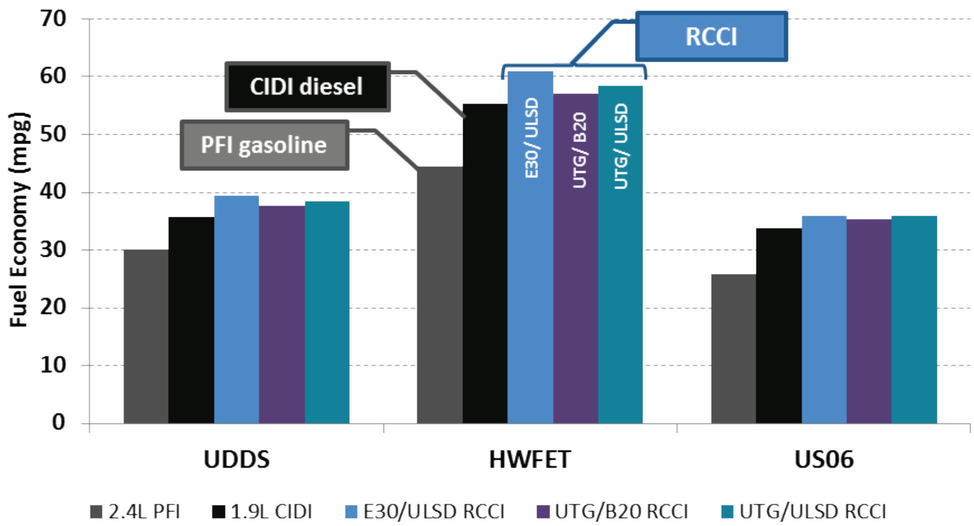
Researchers explored the potential for advanced combustion concepts such as RCCI to improve drive cycle fuel economy by simulating a multi-mode RCCI-enabled vehicle operating over multiple US drive cycles. Experimental engine maps for multi-mode RCCI with three fuel combinations were explored: E30 and ultra-low-sulfur diesel (ULSD), gasoline and ULSD, and gasoline and B20 (20% biodiesel/80% ULSD).

The modeled fuel economy results were compared with 2009 port-fuel-injected gasoline engines ranging from 1.8 to 4.0 L, allowing for comparisons to both best-in-class (2.4 L) and matched vehicle performance baselines (2.7 L). Simulations assumed a conventional mid-size passenger vehicle with an automatic transmission matched to each engine.

In all three cases, the RCCI strategy allowed for at least 25% improvement in modeled fuel economy compared with a representative 2009 gasoline baseline, and 6–10% improvement compared with a CDC baseline. The modeling showed that nearly equal amounts of diesel and gasoline would need to be carried on-board. Differences in fuel reactivity (cetane and octane numbers) and fuel properties were also shown to enable larger loads or improvements in drive cycle coverage.

Although the simulation showed lower NOx emissions for RCCI, increases in CO and unburned hydrocarbon emissions and lower engine exhaust temperatures associated with RCCI may challenge conventional exhaust aftertreatment systems. Other research is addressing reducing CO and unburned hydrocarbon emissions, as well as novel catalysts.

The current range of the experimental RCCI engine map investigated in this effort does not allow for RCCI operation over some entire drive cycles. RCCI limitations were dictated by noise and CO and unburned hydrocarbon emission constraints imposed on the experiments. Full coverage of a drive cycle may require a multi-mode strategy in which the engine switches from RCCI to CDC when speed and load fall outside the RCCI range.



RCCI fuel economy simulations show potential for more than 25% improvement in fuel economy compared with a gasoline baseline.

Publications

1. S. Curran, Z. Gao, and R. Wagner. 2014. "Reactivity controlled compression ignition drive cycle emissions and fuel economy estimations using vehicle systems simulations with E30 and ULSD," *SAE Int. J. Engines* **7**(2), 902–912.

2. S. Curran, Z. Gao, and R. Wagner. 2014. "Reactivity-controlled compression ignition drive cycle emissions and fuel economy estimations using vehicle system simulations," *Int. J. Engine Research*.

Computer Models Help Develop Strategies for Managing Ammonia Inventories on Catalysts

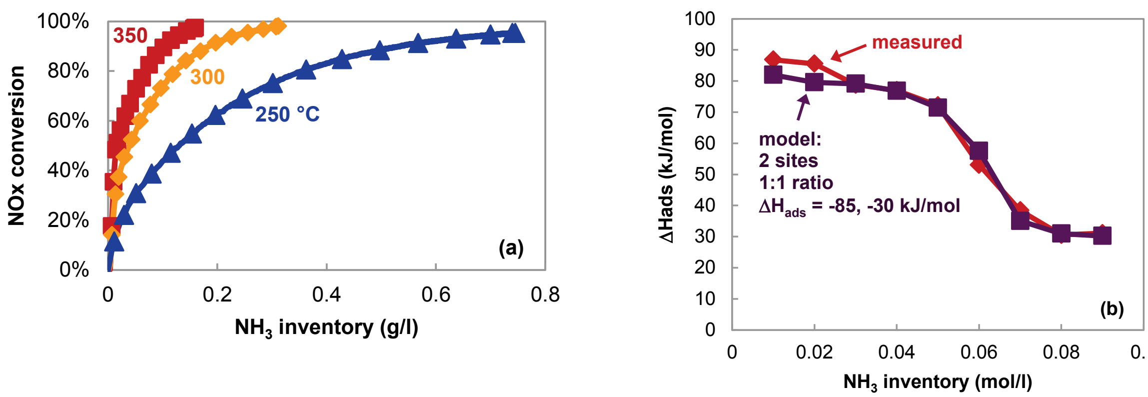
Contact: Josh Pihl, pihlja@ornl.gov, 865-946-1524

ORNL has devised new methods of measuring NH_3 (ammonia) storage on selective catalytic reduction (SCR) catalysts that support more accurate computer simulation tools to improve emissions control strategies for highly efficient lean-burn engines.

Simulation tools based on ORNL's data will help engineers design emissions control systems and associated operating strategies needed for vehicles to comply with strict new emissions regulations while achieving fuel efficiency goals.

Advanced lean-burn engines are designed to burn fuel in excess air to achieve high efficiency; however, these engines require effective removal of NOx from their exhaust to meet current and future emissions standards. State-of-the-art lean NOx control systems rely on SCR technologies in which ammonia reacts with NOx over a catalyst to form harmless nitrogen and water.

How efficiently SCR catalysts remove NOx depends largely on the amount of ammonia that adsorbs on the catalyst surface. Thus the ammonia inventory must be carefully managed to achieve maximum NOx conversion while minimizing the amount of ammonia used and the amount that passes through the catalyst unreacted. The development and optimization of exhaust system configurations and control strategies increasingly relies on computer simulations; therefore, accurate models of ammonia storage on SCR catalysts are needed to predict ammonia inventories under realistic driving conditions. The fidelity of current SCR computer models is limited by uncertainties surrounding key catalyst parameters, such as the number of distinct ammonia storage sites and the binding energy associated with ammonia adsorption at each site.



(Left) NOx conversion as a function of ammonia (NH_3) inventory for a commercial SCR catalyst. (Right) Measured and modeled NH_3 adsorption enthalpy as a function of the NH3 inventory for the same catalyst.

Researchers at ORNL have developed new techniques for quantifying and analyzing ammonia storage that minimize these uncertainties. The measurement of ammonia storage isotherms isolates the energetics of adsorption and eliminates the confounding effects of kinetics and mass transport. Thermodynamic analysis techniques allow researchers to extract key catalyst parameters, including the number of distinct sites, the relative abundance of those sites, and the energetics of adsorption at each site. Having accurate data for these parameters will enable modelers to generate more accurate predictions of ammonia inventories from SCR models, especially for aged catalysts.

Publications, Presentations, and Patents

1. J. Pihl and S. Daw. 2014. "NH_3 storage isotherms: A path toward better models of NH_3 storage on zeolite SCR catalysts," presented at *2014 DOE Crosscut Workshop on Lean Emissions Reduction Simulation* (available at www.cleers.org), April 29.

Energy Storage

ORNL Releases Battery Modeling Software

Contact: John A. Turner, turnerja@ornl.gov, (865) 241-0212

The ORNL Electrical Energy Storage Modeling and Simulation team has released a new version of the Virtual Integrated Battery Environment (VIBE), a software environment for research, analysis, and design of electrical energy storage devices such as batteries. VIBE was developed as part of the VTO Computer Aided Engineering for Batteries (CAEBAT) program.

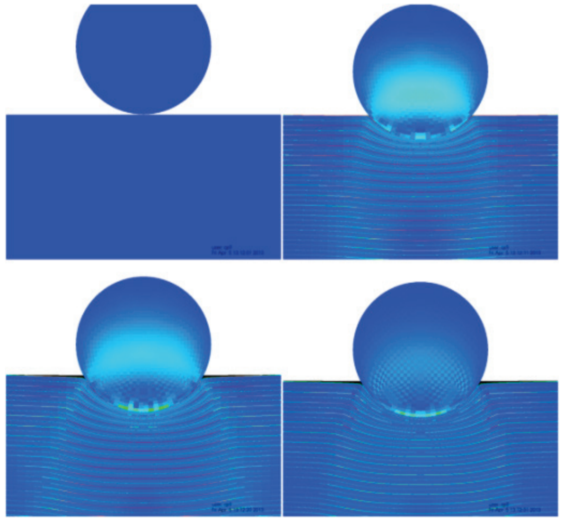
The new release has the following features:

- VIBE: Flexible integrated environment for coupled simulation of cell sandwich, cells, modules, and packs using a range of electrochemistry models (from fast-running approximate models to high-fidelity 3-dimensional [3D] models), optionally coupled to electrical and thermal models
- AMPERES: Advanced fully-coupled 3D single-domain electrical-electrochemical-thermal capability
- Open Architecture Software (OAS): Robust Python infrastructure for coupling physics components and orchestration of simulations
- BatML and BatState: Standards for input and information exchange between components
- ICE: User interface to simplify configuration, setup, launch, and post-processing

A hierarchical process was developed to construct meshes for battery packs. In the automated script-based geometry and mesh construction procedure, a single prismatic cell is replicated to form a module, which in turn is replicated to obtain a battery pack. This produces significant savings in time and effort in creating geometry for simulations.

To demonstrate the mechanics capabilities of VIBE, simulations were performed to replicate the ORNL pinch test, in which a battery cell is crushed against a flat plate by a rigid sphere. Unlike other approaches for modeling battery response to an external load, in which cell properties are homogenized over multiple domains, the ORNL approach resolves all layers. This allows failure criteria to be specified for each of the domains (electrode, current collector, separator, pouch material) independently, greatly improving the accuracy of short circuit location predictions.

OAS integrates open-source computational tools and facilitates interoperability with commercial and proprietary battery design software. This enables battery designers to use the best available tools to accelerate development of high-performing, safe batteries for next-generation plug-in electric vehicles.



Example VIBE simulation results showing Von Mises stress distribution on a deformed mesh in different domains of a pouch cell under external mechanical loading.

Publications, Presentations, and Patents

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2. S. Allu, S. Kalnaus, W. Elwasif, S. Simunovic, J. A. Turner, and S. Pannala. 2014. “A new open computational framework for highly-resolved coupled 3D multiphysics simulations of Li-Ion Cells,” *J. Power Sources* **246**, 876–886.

Water-Based Processing Delivers High-Performing LIB Cells

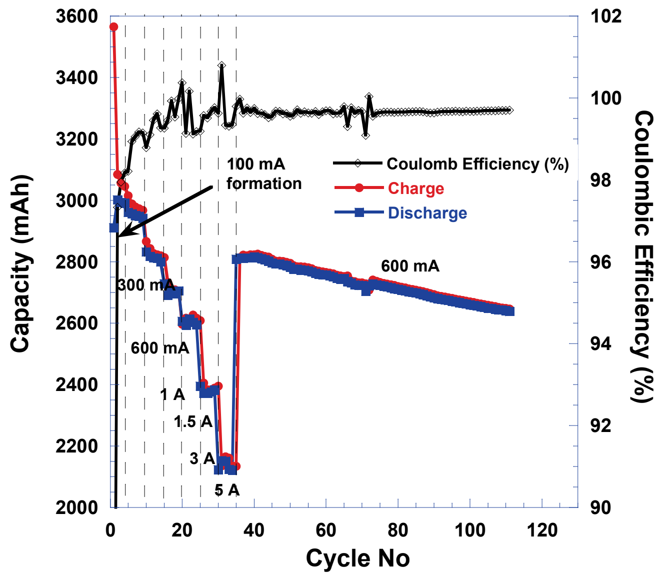
Contact: David L. Wood, III, wooddl@ornl.gov, 865-574-1157

ORNL has achieved excellent performance in a lithium ion battery (LIB) manufactured using aqueous processing, which lowers the production cost and increases the sustainability of LIBs.

DOE is targeting a 74% reduction in the cost of LIBs for electric vehicles (EVs), from the current ~$500/kWh to $125/kWh, by 2020. To meet this goal, substantial progress is required in cutting the costs of both materials and their processing, since they make up over 80% of the total costs of EV batteries. The organic solvent N-methyl-2-pyrrolidone (NMP) used in conventional electrode manufacturing is expensive and toxic and produces flammable vapors during electrode manufacturing that require costly solvent recovery.

ORNL has developed an aqueous process for LIB manufacturing in which NMP (costing >$1.25/L) is replaced with deionized water ($0.015/L). The technology enables further significant cost reductions for electrode processing and eliminates the need for NMP treatment and recovery. In addition, it can reduce carbon dioxide emissions in LIB manufacturing and is more environmentally benign, a critical issue in future mass production of LIBs. This novel processing route is estimated to reduce the full battery pack cost by as much as 8–10%.

In FY 2014, ORNL further demonstrated the excellent performance of composite cathodes from aqueous processing in large-format pouch cells. The pouch cell exhibits excellent rate performance and Coulombic efficiency. The capacity retention in long-term cycles is identical to that in pouch cells with NMC 532 cathodes from conventional NMP-based processing, which indicates aqueous-processed electrodes can deliver the desired performance.



Battery performance from a pouch cell with a graphite anode and a composite cathode manufactured through aqueous processing.

Currently, over 70% of graphite anodes are manufactured through aqueous processing. However, aqueous processing remains challenging for the diverse array of LIB cathodes. ORNL tackled the challenge by optimizing water-soluble binder and mixing sequences, developing a stable and uniform slurry, designing electrode formulas, improving the electrode coating, and optimizing drying procedures. Great progress has been demonstrated in half and full coin cells in the past few years.

Publications, Presentations, and Patents

1. J. Li, B. L. Armstrong, J. Kiggans, C. Daniel, and D. L. Wood. 2013. “Optimization of multicomponent aqueous suspensions of $LiFePO_4$ nanoparticles and carbon black for lithium ion battery cathodes,” *Journal of Colloid and Interface Science* **405**, 118–124.

2. J. Li, B. L. Armstrong, J. Kiggans, C. Daniel, and D. L. Wood. 2013. “Lithium ion cell performance enhancement using aaqueous $LiFePO_4$ cathode dispersions and polyethyleneimine dispersant,” *Journal of The Electrochemical Society* **160**, A201–A206.

Resolving Voltage Fade in LMR-NMC Composite Electrodes

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High-voltage lithium- and manganese-rich layered oxides with the composition $xLiMO_2 \cdot (1-x) Li_2MnO_3$ (LMR-NMC) are potential cathode materials for high-energy-density lithium-ion batteries. However, voltage fade during cycling impedes their usage. A layered-to-spinel (LS) structural rearrangement in LMR-NMC oxides has been identified as a principal cause of voltage fade;

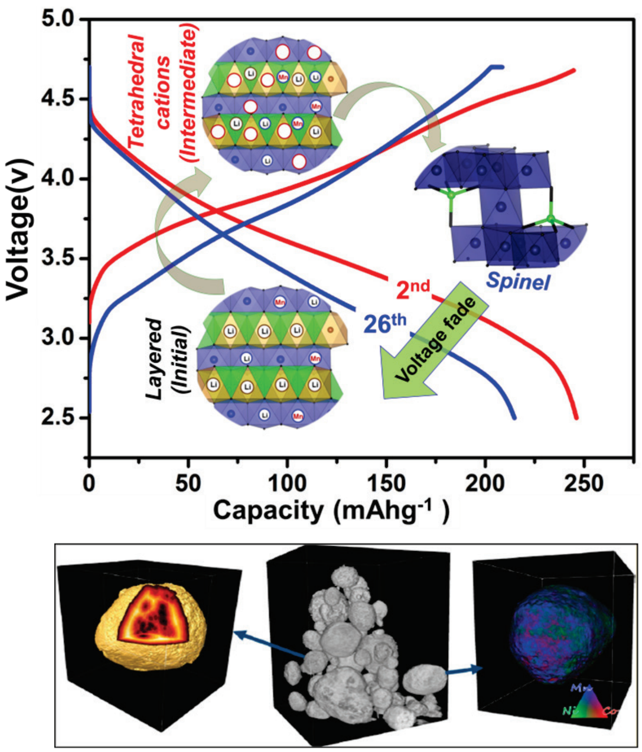
therefore, the LS conversion mechanism needs to be confirmed so that the composition and structure of the oxides can be manipulated to suppress voltage fade.

ORNL researchers used neutron scattering to unravel the unique cation migration paths and key mechanisms for LS transformation in LMR-NMC oxide cathodes. They conducted neutron diffraction experiments on LMR-NMC oxides at different states of charge (3.2, 3.5, 4.1, and 4.5 V) to explore the atomic occupancies in different crystallographic sites to uncover the root cause of voltage fade. The neutron diffraction analysis provided evidence that LMR-NMC transforms to a spinel phase via an intermediate structure with tetrahedral cation occupancies that blocks lithium diffusion pathways. It serves as a "building block" for the creation of a spinel-like framework.

The experiments showed two key cation migration paths for LS transformations:

1. Lithium atoms diffuse from octahedral to tetrahedral sites of the lithium layer [(Li_{Li}oct → Li_{Li}tet]. Subsequently, lithium ions from the adjacent octahedral sites of the metal layer diffuse to the tetrahedral sites of the lithium layer [Li_{TM}oct→Li_{Li}tet].
2. Manganese atoms migrate from the octahedral sites of the transition-metal layer to the "permanent" octahedral site of the lithium layer via the tetrahedral site of the lithium layer [Mn_{TM}oct → Mn_{Li}tet → Mn_{Li}oct)].

Complementing the results from neutron studies, the researchers used x-ray tomographic reconstruction of individual aggregated LMR-NMC cathode particles—derived from their corresponding Mn, Co, and Ni K XANES (x-ray absorption near-edge structure spectroscopy) edges—to obtain a 3-dimensional picture of transition-metal segregation upon cycling. The reconstructions were used to probe changes in the internal morphologies of the particles, as well as their porosities under continuous high-voltage cycling.



(Upper panel) Voltage and capacity curves from a LMR-NMC high-energy cathode showing voltage fade phenomena after 26 cycles and the LS transformation mechanism deduced from neutron diffraction. Insets demonstrate initial layered structure transforms to spinel via an intermediate structure that has cations on tetrahedral sites. (Lower panel) Tomographic reconstruction of LMR-NMC cathode particles showing internal voids (left) and a 3-dimensional rendering of the corresponding Mn, Ni and Co from x-ray absorption near-edge structure spectra.

These findings suggest that the efforts to suppress or eliminate voltage fade should be directed toward minimizing the transition-metal and/or lithium migration using methods such as revisiting the compositional phase space or dopant substitution to stabilize the lattice against excess delithiation.

Publications, Presentations, and Patents

1. D. Mohanty, J. Li, A. Huq, D. P. Abraham, A. Sefat, E. A Payzant, D. L. Wood, and C. Daniel. 2014. "Unraveling the voltage fade mechanism in high-energy-density lithium-ion batteries: Origin of the tetrahedral cations for spinel conversion," *Chemistry of Materials* **26**, 6272−6280.

2. F. Yang, Y. Liu, S. K. Martha, Z. Wu, J. C. Andrews, G. E. Ice, P. Pianetta, and J. Nanda. 2014. "Nanoscale morphological and chemical changes of high voltage lithium–manganese rich NMC composite cathodes with cycling," *Nano Letters* **14**, 4334–4341.

Polyanion Glasses as High-Capacity Lithium Ion Battery Cathodes

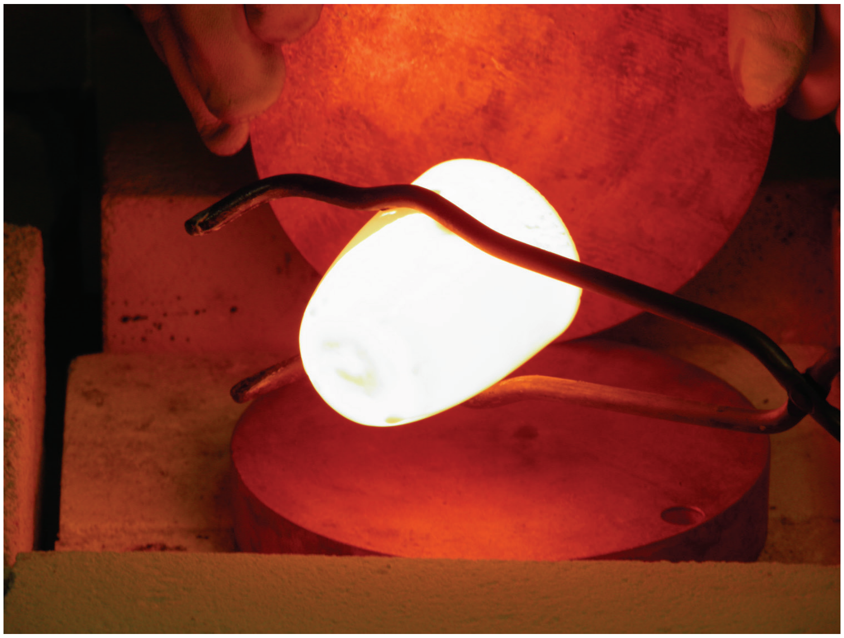
Contact: Andy Kercher, kercherak@ornl.gov, (865)-576-5252

Scientists at ORNL are developing new battery cathode materials with the potential for better performance than those currently used in lithium ion batteries for electric vehicles. Hybrid and electric vehicles are central to the US strategy to reduce oil dependence and greenhouse gas emissions. One of the challenges to increasing their market penetration is that the specific capacities of lithium ion batteries—specifically their cathodes—are too low for widespread public acceptance of electric vehicles.

Polyanion materials, such as lithium cobalt phosphate and lithium manganese silicate, theoretically have the specific capacity to be excellent candidate cathodes for automotive lithium ion batteries. But experimentally, their capacity and/or cyclability is poor because of their low electrical conductivity ($<10^{-12}$ S/cm) or irreversible crystalline phase transformations.

ORNL researchers are developing glass polyanion cathode materials that not only have high theoretical capacity but also can experimentally achieve high capacity by overcoming the key problems of crystalline polyanion materials. Their amorphous structure and mixed polyanion content can provide dramatically higher electrical conductivities (10^{-7} S/cm) and can potentially be structurally stable through multiple valence changes. In addition, these glass materials are produced by low-cost conventional glass processing techniques, such as mold casting and splat quenching.

The polyanion glasses developed at ORNL have demonstrated high-capacity intercalation and conversion reactions. For iron phosphate vanadate glasses, the intercalation reaction achieved full theoretical capacity and good cycling for 100 cycles. Particle size reduction was shown to improve the capacity and high-power performance. However, intercalation in non-iron glasses has been limited (< 30% theoretical capacity), and intercalation involving a multi-valent transition has not yet been demonstrated. Reversible conversion reactions in polyanion glasses were an unexpected result of the ORNL research. The glass-state conversion reaction mechanism was confirmed using x-ray absorption spectroscopy, x-ray diffraction, and electron microscopy of ex-situ cathodes from coin cells at key states of charge.



ORNL glass cathode materials are usually formed by splat quenching, in which molten glass is cooled rapidly between two copper plates.

Conversion reactions in polyanion glasses have been found in silver, cobalt, copper, iron, and nickel phosphate vanadate glasses. These have voltages up to 2.9V, specific capacities up to 500 mAh/g, and good capacity retention at specific currents up to 2,000 mA/g. During a glass-state conversion reaction, lithium cations react with the cathode to produce a lithium polyanion glass and metal nanoparticles. Thus far, glass-state conversion reactions have shown the large hysteresis and cycling fade similar to conversion reactions in crystalline oxides and halides. Ongoing research seeks to improve the electrochemical performance of glass cathodes through intercalation or conversion by compositional changes aimed at improving key physical properties.

Lightweight Materials

Advanced Oxidative Stabilization of Carbon Fiber Precursors

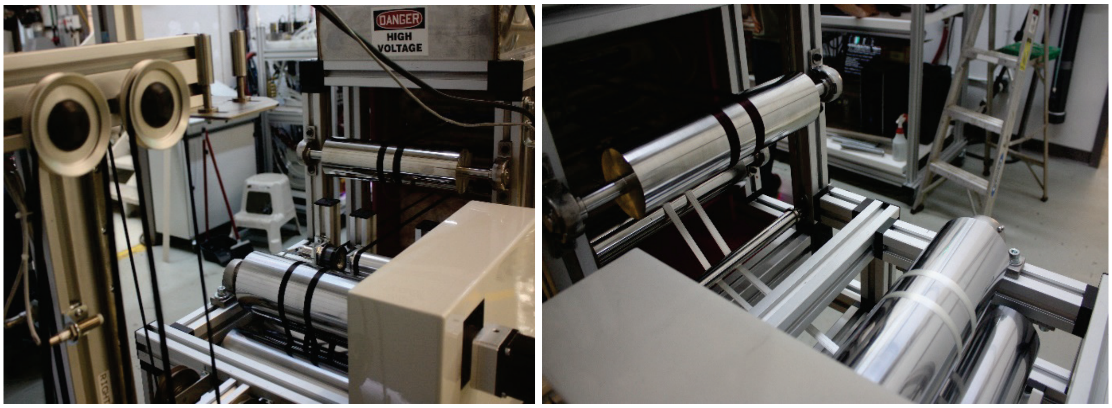
Contact: Felix L. Paulauskas, paulauskasfl@ornl.gov, 865-576-3785

The cost of producing carbon fiber (CF) is the single largest obstacle to its incorporation in future automotive systems. The bulk of expenses are tied to the cost of the precursor as well as to conversion of the precursor into CF and activation of the surface for resin compatibility. Conversion work includes development of a higher-speed, lower-cost oxidative stabilization process and development of a microwave-assisted plasma process carbonization method.

This ORNL research project seeks to develop a plasma processing technique to rapidly and inexpensively oxidize polyacrylonitrile (PAN) precursor fibers. Conventional oxidation is a slow thermal process that typically consumes more than 80% of the processing time in a conventional CF conversion line. A rapid oxidation process could dramatically increase the conversion line throughput and appreciably lower the fiber cost.

The 1 ton/year plasma oxidation oven.

The oxidation residence time must be greatly reduced to effect fast conversion and match the speed of the advanced carbonization technology. This project is developing an atmospheric plasma oxidation technology that could be used in line with conventional conversion equipment or integrated with other advanced fiber conversion processes to produce low-cost CF with properties suitable for use by the automotive industry. This effort is aimed at further developing technologies to be able to continuously process 12–50K tows of fiber and achieve properties meeting program minimum property requirements with tow-to-tow and along-the-tow property variations within ±15%. The goals also include significantly reducing the time required for oxidative stabilization (conventionally 90–120 min), which will permit greater fiber production rates and improved economics.



Processing of two commodity-grade, 24,000-filament tows of precursor fiber in the large reactor.

The strategy for transitioning this technology to industry is to involve potential industry partners as early in the development process as is practical; this strategy will also reduce investment risk. The advanced oxidation task soon will be mature enough to start involving oxidation oven manufacturers. The new technology must address the diffusion time limitations of the conventional method and scale that technology sufficiently to demonstrate the success of this approach to the carbon fiber industry. ORNL's partner in this project, RMX, is leading commercialization efforts with the automotive industry. At the same time, ORNL is developing plans and specifications for a 25 ton/year plasma oxidation oven for the Carbon Fiber Technology Facility.

Publications/Presentations/Patents

1. F. L. Paulauskas and T. A. Bonds. 2014. "Plasma oxidation commercialization status update," presented at the Carbon Fiber Consortium meeting, Knoxville, Tennessee, March 27.

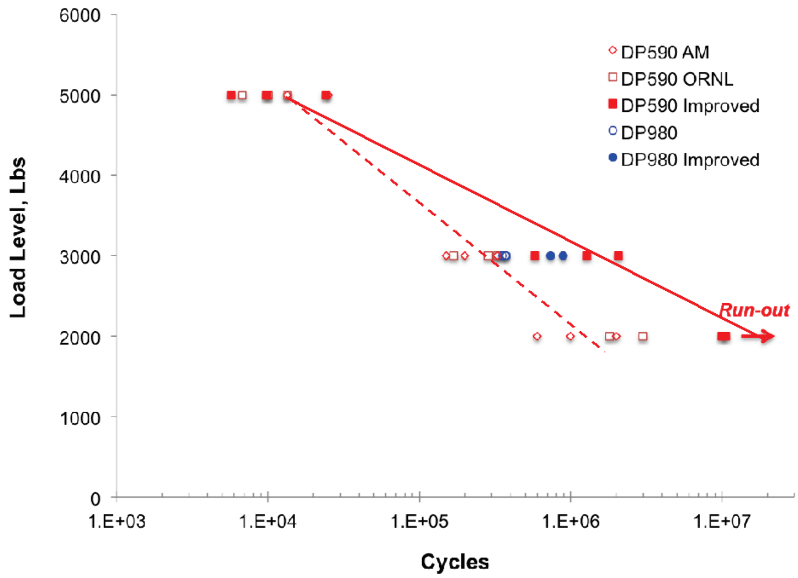
2. T. A. Bonds and F. L. Paulauskas. 2014. "Plasma oxidation commercialization status update," presented at the Carbon Fiber Consortium meeting, Knoxville, Tennessee, October 29.

Improving Fatigue Performance of Welds in Lightweight Materials

Contact: Zhili Feng, fengz@ornl.gov, 865-576-3797

ORNL and its partner have demonstrated that thermomechanical weld stress management can significantly improve the weld fatigue life of automobile body components. To demonstrate the feasibility of the approach, they designed and developed a lap joint weld fatigue test mimicking the weld configuration common in automobile body components.

The tests showed considerable improvement in weld fatigue life at low stress levels critical to the durability of auto-body structural components (i.e., low stress, high number of cycles). At a 2,000 lb load, the cycle-to-failure time of the welds increased by more than an order of magnitude. Weld coupons treated with the residual stress management technique did not fail at 10^7 cycles.



Fatigue test results showing reduction of weld residual stresses by in-process thermomechanical stress management.

Durability is a primary metric in designing and engineering auto body structures. The fatigue performance of welded joints is critical to auto body durability because welds are the likeliest locations for fatigue failure. Weld fatigue life is a key technology barrier to widespread use of lightweight materials (e.g., advanced high-strength steels, aluminum and magnesium alloys) in auto bodies. The technology developed in this project is expected to provide practical, cost-effective solutions to the automotive industry to address this critical issue.

Previous attempts to address residual stresses, although viable at the laboratory scale, proved to be too expensive and/or difficult to apply in production. Therefore, this project focused on developing in-process residual stress modification technologies as part of the welding operation. The goal was to develop effective ways to control and mitigate key factors limiting the fatigue life of advanced high-strength steel welds: weld residual stress, weld profile, and weld microstructure/chemistry.

The researchers used advanced integrated computational welding engineering, neutron/synchrotron, and other advanced stress measurement techniques, and fatigue testing and microstructure analysis capabilities at ORNL and ArcelorMittal. Both technical and economic issues unique to the auto body structural welding environment were identified and addressed.

The researchers designed the weld fatigue test specimens to resemble actual stress-strain conditions in vehicle structures and to retain the residual stresses in the weld region. They conducted an industry survey on the types of welds used in auto bodies and based the weld stress tests on lap joints, the most commonly used weld type. The project determined the dominant role of weld start-and-stop in fatigue failure in short-stitch welds in body-in-white structures, which present unique challenges in managing stress.

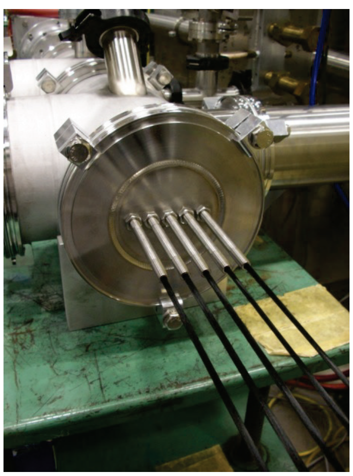
ORNL Pursues Energy-Efficient Advanced Carbonization Technology

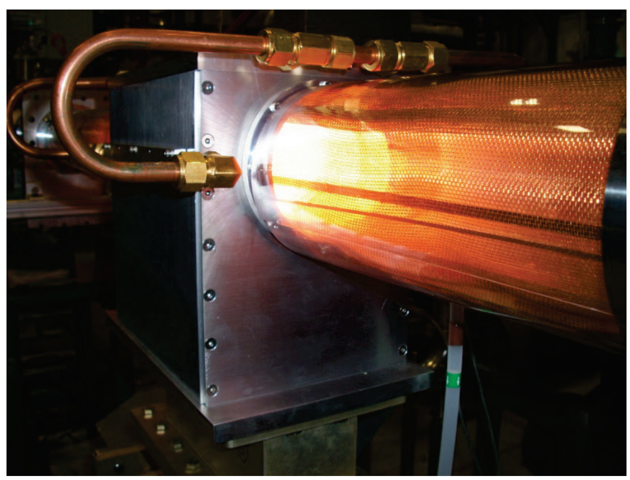
Contact: Felix Paulauskas, paulauskasfl@ornl.gov, 865-576-3785

A project at ORNL'S Carbon Fiber Technology Facility (CFTF) seeks to demonstrate and eventually commercialize a revolutionary energy-efficient advanced conversion technology. Co-funded by VTO and the Advanced Manufacturing Office, this technology enables the manufacturing of carbon fiber that is technically and economically viable in industrial markets. Lower-cost carbon fibers are attractive for many industrial applications critical to efficient energy production and use (e.g., in transportation, wind energy, infrastructure, and oil drilling) that do not require aircraft-grade carbon fiber.

The advanced conversion process is based on previous ORNL work in microwave-assisted plasma (MAP) and related technologies for carbonization. ORNL previously demonstrated that microwave energy combined with plasmas can be used to rapidly convert polyacrylonitrile precursor fibers into finished carbon fibers. The researchers demonstrated a residence time of approximately one-third to one-half of the conventional residence time.

The technology development team recently completed modifications and upgrades to the MAP line that enable it to process five tows continuously and demonstrate a >2-hour stable run. Mechanical properties meeting program requirements (250 KSI strength, 25 MSI modulus) have been achieved, but uniformity limitations and tow-to-tow energy distribution within the chamber resulted in higher property variability than the targets allow.





(Left) MAP line exit feedthroughs are fully strung with five tows in the horizontal configuration. (Right) Improved microwave energy and enhanced plasma hardware, demonstrated here in a single unit, should allow improved energy deposition control for industrial scale-up.

Guided by modeling results, the team implemented significant changes to the fiber-handling equipment, achieving enhanced tensioning control and improved tow-to-tow energy distribution. The changes included horizontal tow spacing with vertical energy introduction and nonlinear tow orientation in the processing chamber. Additionally, the team developed an alternative technique for focusing and controlling microwave energy deposition in the processing chamber. Preliminary results show substantial energy efficiency improvements and indicate that the technique can be deployed easily on a larger scale. It likely will make unnecessary the common industrial practice of separating low- and high-temperature carbonization approaches.

Appropriate tools to assist with hardware development include a system model complemented with dielectric measurement capability as a function of temperature. Optimization of plasma parameters for conversion will continue focusing on improving process economics and uniformity, because the process has been shown capable of meeting performance targets. The team will continue to review energy balance data to refine the data and prioritize remaining projects. Progress continues on improvements to the current hardware transition regions, sealing approaches, and effluent handling.

Understanding Protective Film Formation by Magnesium Alloys

Contact: Michael P. Brady, bradymp@ornl.gov, (865) 574-5153

ORNL scientists used small-angle neutron scattering and secondary ion mass spectroscopy techniques to study the formation of surface films on magnesium alloys.

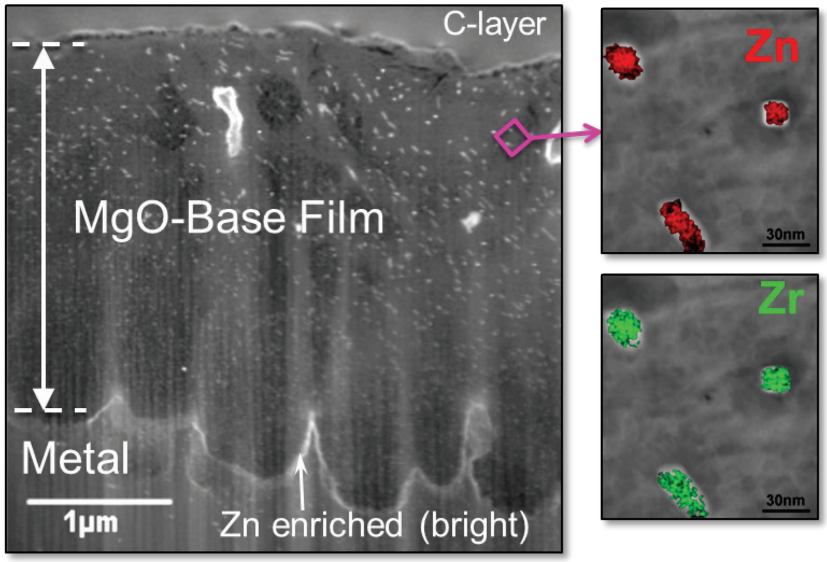
Magnesium alloys are of great interest to reduce vehicle weight because of their low density and good strength, but corrosion susceptibility is a major obstacle to their widespread adoption. Magnesium's inability to establish a continuous and fully protective surface film under many exposure conditions is a key factor underlying this susceptibility to corrosive attack. Alloying and/or conversion coatings have been shown to modify surface film performance; however, a detailed understanding of how and why is currently lacking. Such understanding is needed to develop improved alloys and coatings to permit more widespread adoption of magnesium. Developing an improved understanding of how alloy composition, microstructure, and exposure conditions affect the nature and growth of protective films on magnesium alloys is the purpose of this research project, a collaboration of ORNL, Magnesium Elektron North America, and the University of Manitoba.

The experimental strategy is based on applying advanced characterization techniques not previously widely applied to the study of magnesium corrosion. The project has focused on systematic study of two representative commercial magnesium alloy classes relative to ultrahigh purity (UHP) magnesium as a control. Alloy AZ31B was studied as representative of the Mg-Al-Zn alloy class, and alloy Elektron 717 (also known as ZE10A, but referred to as E717 for simplicity) was studied as representative of the rare earth and zirconium-alloyed class of magnesium alloys. Initial study of these alloys serves as a baseline relative to modified model alloy compositions and surface coatings.

Secondary ion mass spectrometry $D_2{}^{16}O$ and $H_2{}^{18}O$ (^{18}O water) isotopic tracer study techniques have been developed successfully for magnesium and applied to better understand the aqueous and humid air film formation growth mechanism of UHP magnesium, AZ31B, and E717. Small angle neutron scattering was successfully applied to characterization of the formation of nonprotective, nanoporous $Mg(OH)_2$ corrosion products formed by AZ31B and E717 in salt solutions.

To our knowledge, this is the first time such techniques have been applied to the corrosion of magnesium. Both techniques were complemented by transmission electron microscope imaging of magnesium film cross sections.

Future project work will focus on similar characterization studies of coatings formed on AZ31B and E717, with additional collaborations recently initiated with Henkel Corporation and McMaster University.



High angle annular dark field scanning transmission electron microscope image and elemental maps of the cross-section of the film formed on Elektron 717 after exposure for 48 h in ambient water [2]. The fine white precipitates are Zn_2Zr_3.

Publications and Presentations

1. K. A. Unocic, H. H. Elsentriecy, M. P. Brady, H. M. Meyer, G.-L. Song, M. Fayek, R. A. Meisner, and B. Davis. 2014. "Transmission electron microscopy study of aqueous film formation and evolution on magnesium alloys," *Journal of the Electrochemical Society*, **161**(6), C302–C311.

2. M. P. Brady, M. Fayek, H. H. Elsentriecy, K. A. Unocic, L. M. Anovitz, J. R. Keiser, G.-L. Song, and B. Davis. 2014. "Tracer film growth study of hydrogen and oxygen from the corrosion of magnesium in water," *Journal of the Electrochemical Society*, **161**(9), C395–C404.

3. G.-L. Song, M. P. Brady, et al. 2014. "Advanced characterization of Mg alloy surface films," invited presentation at CORROSION 2014, NACE, San Antonio, Texas, March 9–13.

Carbon Fiber Technology Facility

Contact: Ron Ott, ottr@ornl.gov, 865-574-5172

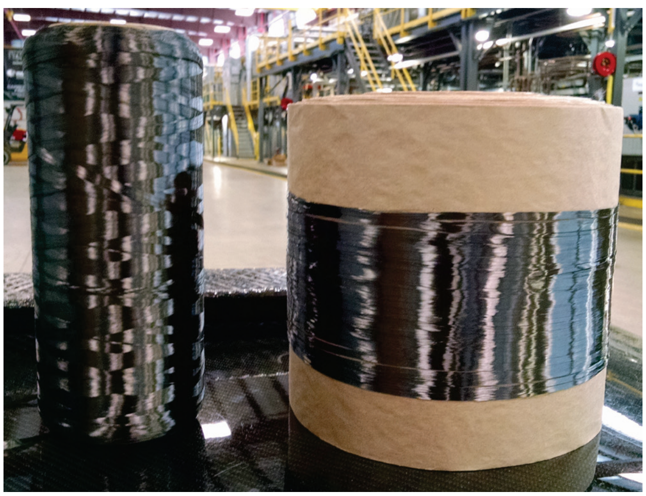
The Carbon Fiber Technology Facility (CFTF) demonstrated during FY 2014 that a low-cost carbon fiber (LCCF) can be produced from a textile-grade acrylic fiber, resulting in many inquiries from industry partners about the use of LCCF and ultimately scaling up the technology. CFTF staff worked aggressively to develop the appropriate process science and scale up the conversion of the textile polyacrylonitrile (T-PAN) fibers to carbon fiber.

The T-PAN precursor was supplied by Kaltex, a producer in northern Mexico. Tests of the fibers made from T-PAN showed tensile strength and tensile modulus values reaching 450 Ksi and 33.6 Msi, respectively (DOE automotive targets are 250 Ksi and 25 Msi). The results indicate that the T-PAN may be a good candidate for full-scale production of LCCF.

Chopped carbon fiber made from the T-PAN was sent to Plastics Analytics Laboratory for comparison with commercially available carbon fiber produced using standard methods. Results show carbon fiber based on T-PAN performed much like the commercial fiber in a bulk molding compound, which would be used in injection molding applications. This will probably be a targeted automotive composite process because the necessary infrastructure is available.

Other sources of textile fiber are also being evaluated, because multiple sources of precursor materials will be needed for industry to truly scale and commercialize LCCFs. High volumes of T-PAN are available at much lower prices than traditional PAN precursors. New entrants into the carbon fiber industry could use T-PAN based carbon fiber for high-volume industrial, transportation, wind, and automotive applications. There are plans to scale up other alternative precursor materials, including lignin-based and polyolefin-based carbon fibers and cellulosic paper carbon materials.

Since target performance metrics were achieved, research turned to the handling aspects of large-tow fibers. Ultra-large tows—up to 600 K filaments—are produced from T-PAN. The large tows could be advantageous in some intermediate and composite processes in the long term; but the composites industry is currently built around lower-tow, i.e., ~24 K, fiber. For use in the existing compositing infrastructure, large-tow fiber must be split into smaller, more manageable tows. This is one of several handling concerns that must be resolved to truly commercialize this LCCF.




(Left) Typical spools of (a) 24 K industrial-grade carbon fiber and (b) 610 K rolls of textile-based carbon fiber. (Right) Carbon fiber produced at CFTF using a textile acrylic fiber.

CFTF operation during FY 2014 primarily focused on converting carbon fibers in a variety of formats in anticipation of supporting projects approved by VTO and the DOE Advanced Manufacturing Office. Approximately 1,275 kg were produced from a variety of traditional PAN and T-PAN precursors in small (12 K), medium (24 K and 48 K), and large tow (610 K) formats.

VTO and the Advanced Manufacturing Office provide operating funds for the CFTF. The facility continues to train technical staff in the production of carbon fiber, and multiple tools have been developed to establish a training program for future carbon fiber production facilities.

Presentations/Publications/Patents

1. L. B. McGetrick. 2014. Presentation to the Aviation and Missile Research, Development, and Engineering Center, Oak Ridge, TN, July 9.

2. L. B. McGetrick. 2014. Presentation to the DOE Vehicle Technologies Program Annual Merit Review, Washington, D.C., June 17.

3. L. B. McGetrick. 2014. Presentation to the USDRIVE Materials Technical Team, Oak Ridge, TN, February 12.

4. L. B. McGetrick. 2013. Presentation to the Electric Power Research Institute Advanced Manufacturing Workshop, Knoxville, TN, November 13.

Spot Joining of Aluminum to Advanced High-Strength Steel

Contact: Zhili Feng, fengz@ornl.gov, 865-576-3797

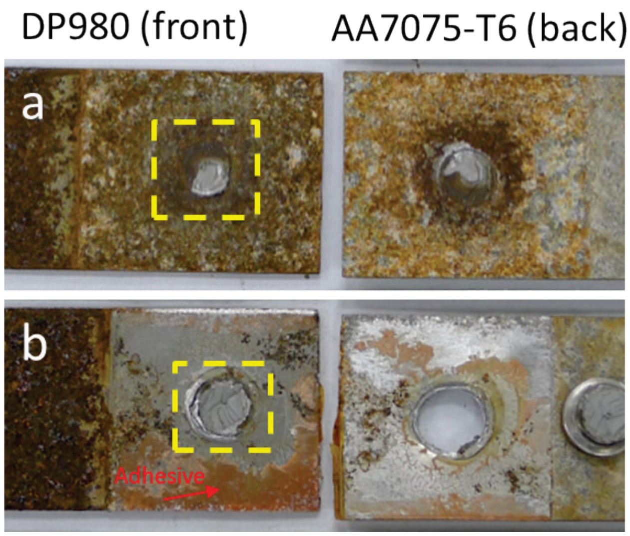
ORNL researchers are seeking to develop, mature, and validate near-production readiness of a solid-state spot joining technology to join prototype-scale auto body-in-white (BIW) subsystems, made of advanced high-strength steel (AHSS) and 7000/6000 series high-strength aluminum alloys, to meet the dissimilar metal joining challenges in high volume mass production.

The project consists of two phases. Phase I involves further development and evaluation of friction bit joining (FBJ) and filling friction stir welding (FSSW) and compares them with self-piecing riveting, the de facto benchmark BIW mechanical fastening method. In Phase II, the “winning” process will be selected for further development for prototype scale BIW assembly level joining.

The hardware of the selected joining process will be integrated with an assembly-line welding robot. Prototypical BIW subsystems will be welded and assembled with the robotic joining system to evaluate and validate production readiness of the joining technology for high-volume mass production assembly. Aluminum–steel joints at both the coupon and prototype scales will be tested and characterized to determine the performance and function of the joints per requirements as well as against a set of industry-relevant process and performance criteria.

A modeling framework will be adopted and applied to (1) refine and optimize the solid-state joining process, (2) understand the microstructure changes in the weld region and their effects on the strength/properties of individual joint, and (3) optimize the joining ability and joint performance at the prototype assembly level.

One of the major challenges in dissimilar metal joining is the galvanic corrosion in the weld region. In this work, the effectiveness of adhesives as a corrosion insulation barrier was systematically studied. Four treatment conditions are being studied: uncoated DP980, galvannealed DP980, adhesive on uncoated DP980, and adhesive on galvannealed DP980. The Dow Betamate 4601 adhesive served as a corrosion insulation layer in the team’s approach. Adhesives were applied only between the aluminum and steel sheets. An accelerated laboratory test procedure followed. The effects of corrosion on the joint strength were determined by lap-shear tests of welded coupons after different exposure cycle time.



Comparison of optical images at fracture surface for (a) FBJ only and (b) weld-bonding (adhesive + FBJ) at 23 corrosion cycles. Note that there is some residual adhesive (orange color) left on both bare DP 980 and AA 7075-T6 surfaces.

The initial corrosion study indicated very good corrosion resistance of FBJ with the application of adhesive. Also, galvannealed DP980 (with and without adhesive) showed adequate corrosion resistance for most cases (remaining more than 80% of the initial joint strength).

Publications

1. Y. C. Lim, L. Squires, M. Miles, Y. Wang, T.-Y. Pan, and Z. Feng. 2014. "Overview of friction bit joining process for dissimilar material joining," presented at 10th TWI Friction Stir Welding Symposium, Beijing, China, May 20–22.

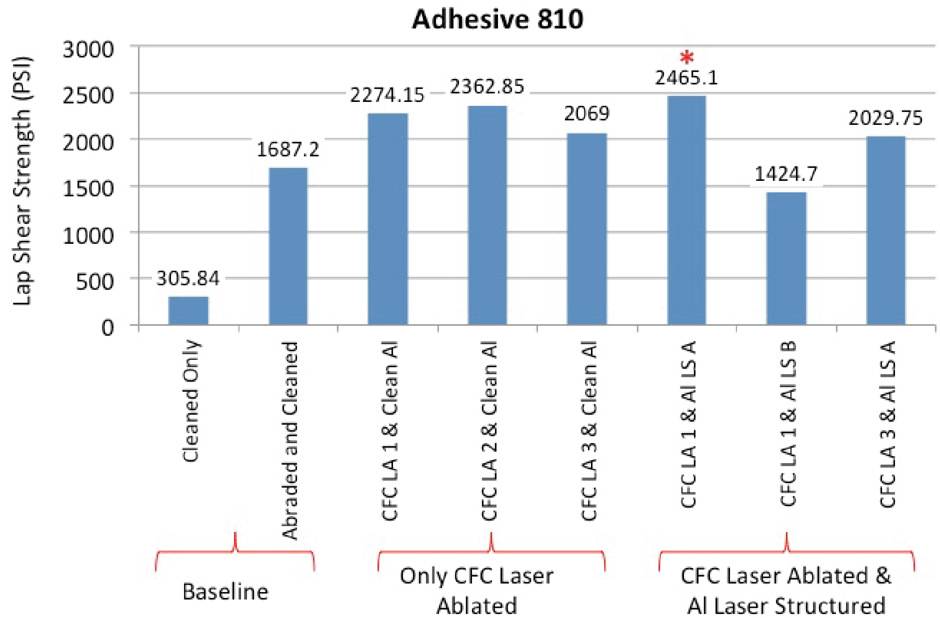
2. Y. C. Lim, L. Squires, T.-Y. Pan, M. Miles, Y. Wang, Z. Feng. 2014. "Mechanical and corrosion performance of aluminum/steel joints spot welded by friction bit joining," presented at Sheet Metal Welding Conference, Livonia, Michigan, October 22–24.

Laser-Assisted Dissimilar Material Joining

Contact: Adrian S. Sabau, sabaua@ornl.gov, 865-574-4357, and C. David Warren, mwarrencd@ornl.gov, 865-574-9693

Researchers at ORNL have demonstrated a breakthrough laser structuring technology for joining carbon fiber polymer composites (CFPCs) and aluminum components. Joining CFPCs and aluminum 5000, 6000, or 7000 series components currently is performed by (1) simply wrapping the CFPC composite over the aluminum or (2) using specially formulated adhesives coupled with extensive surface preparation techniques. In fact, surface preparation is one of the main challenges in both consistent quality and productivity for bonding CFPC with aluminum.

Labor-intensive surface preparation methods are incompatible with the degree of automation required in automotive applications and add significant part-to-part variability to the process. ORNL researchers used a laser structuring technique before the adhesive bonding operation by which the untreated, smooth adherend interface of the CFPC was replaced by a rough fiber-reinforced interface. This was expected to increase the bond strength of the CFPC/adhesive interface. The smooth aluminum interface was replaced by a textured interface, providing surface cleaning, oxide removal, and a greater bonding area. Laser surface treatment of the substrate surface can be optimized to limit necessary surface preparation cleaning processes, thereby increasing industrial acceptance for high-volume applications.



Shear lap strength for CFC–aluminum dissimilar material joints for three different categories: (a) baseline, (b) CFC–as laser structured without cleaning and cleaned aluminum, and (c) CFC–aluminum both as laser structured without cleaning. The 1,424 psi joint was incompletely cured. The CFC LA3 protocol overly damaged the composite surface. (CFC = carbon fiber composite; Al = aluminum; LA = laser ablated; LS = laser structured).

The technology improvement should enhance bonding of aluminum and CFPC to the adhesive for increased joint strength and integrity; eliminate pre-cleaning and surface preparation steps; reduce processing variability in surface preparation because laser surface texturing is a much more controlled process; expand the technology to more structural joints (which are currently limited to panel/sheets for automotive applications); and enable high-volume, automatic, in-line production for the auto industry.

The development of laser ablation to expose the top layer of carbon fibers is important and has resulted in a number of innovations: an increase in surface area, elimination of surface contaminants, removal of mold release, removal of a resin-rich layer, and fiber reinforcement of the interface.

Power Electronics and Electric Motors

All-SiC Inverter Meets Electric Drive Performance Targets

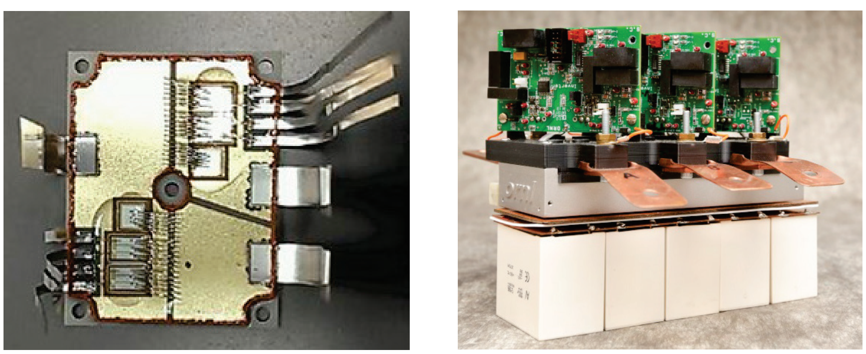
Contact: Burak Ozpineci, burak@ornl.gov, 865-946-1329

ORNL researchers used additive manufacturing to produce a power inverter for use in electric vehicles that is lighter, more efficient, and more rugged against harsh operating conditions.

Power electronics systems in hybrid, plug-in hybrid, and all-electric vehicles impose harsh environmental requirements on the vehicles' electrical components. High operational temperatures, for example, necessitate costly thermal management systems to avoid device failures. Ongoing efforts to reduce vehicle costs are leading to the minimization of hardware, which in turn improves vehicle efficiency through weight reduction.

Emerging wide bandgap (WBG) semiconductor devices are poised to offer significant improvements in power electronics, including opportunities for system-level cost reduction, higher power density, and improvements in efficiency and reliability. The ability of WBG devices to operate at higher efficiencies over higher temperatures and operational frequencies reduces cooling requirements and minimizes passive component requirements, thus providing opportunities for revolutionary strides in electronics.

ORNL researchers developed a 10 kW, all-silicon carbide (SiC) inverter using SiC metal-oxide-semiconductor field-effect (MOSFET) modules (1,200 V, 100 A), also developed at ORNL. The inverter used commercially available gate drivers from Rohm Semiconductor featuring galvanic isolation up to 3,000 V_{rms} and integrated overcurrent protection, undervoltage lockout, and temperature feedback. The modules were mounted on an additively manufactured commercial heat sink with thermal grease as the heat transfer medium from the lower side of the power modules.



(Left) A 1,200 V, 100 A SiC power module.(Right) Layout of the 10 kW SiC inverter prototype.

Test results demonstrated successful operation of the inverter with an efficiency of ~99% at 20 kW operating power. The additive manufacturing process contributed to the specific power increase because less material was used in the innovative metal processing techniques versus what would have been used with traditional techniques. The weight of the additive manufacturing prototype was also reduced by ~25%.

The total volume of the ORNL-developed inverter is ~1.5 L. The total operating power density, based on the test conditions of the inverter, is ~13.3 kW/L (the DOE 2015 target is 12 kW/L), and there is a possibility for higher power. The operating specific power based on the testing conditions is

~11.3 kW/kg. The total weight of the inverter is ~1.76 kg, not including connectors and housing. As higher-power-rating WBG devices become available, the inverter prototype can be scaled for higher power operation. Test results show that an inverter scaled to 30 kW has the potential to meet US DRIVE and DOE 2020 targets.

Presentations

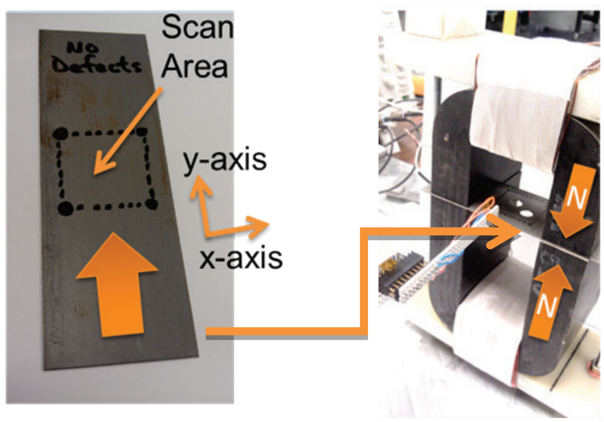
1. M. Chinthavali. 2014. Interview with Lee Teschler, *Design World*, podcast audio, December 1, 2014, powerelectronictips.com/podcast-designing-sic-power-semiconductors/.

New System Improves Characterization of Materials

Contact: Burak Ozpineci, burak@ornl.gov, 865-946-1329

A custom characterization system recently developed at ORNL provides a deeper understanding of magnetization and loss mechanisms in electrical steel and yields information needed for high-fidelity electric motor modeling.

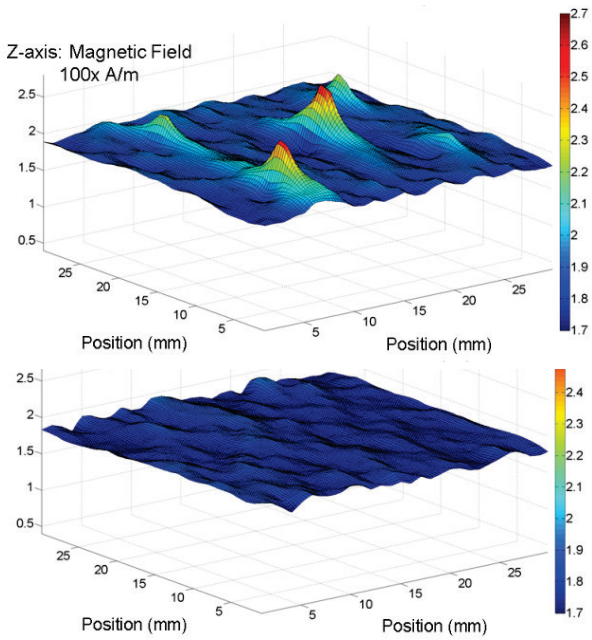
The magnetic characterization tool allows researchers to observe localized properties in electrical steel. The measurement stage of the characterization system includes excitation coils that apply a magnetic field on a single sheet sample while the local magnetic field on the surface of the sample is measured.



Measurement stage of the magnetic material test sample (left) and characterization system (right).

Conventional motor simulation techniques assume that the material properties are homogeneous for the bulk of the material. However, many things can affect magnetic properties, such as residual stress from stamping or laser cutting. Additionally, stamped or laser cut edges are near the air gap, which is a critical location for the magnetic circuit and operation of the motor.

Characterization of the impact of residual stress upon magnetic properties revealed significant degradations near areas that have sustained mechanical deformation. Following a brief application of laser pulses in five different areas of the sample, a resulting magnetic field with a flux density of 1.4 tesla was observed. Although the disturbed areas are barely visible on the physical sample, five distinct areas are visible in the plot of the scanning results, where the magnetic properties are significantly affected.



Magnetic field results before disturbances (top) and after a brief application of five laser pulses (bottom).

Other test results indicate that stamped edges can have magnetic fields up to five times higher at the deformation zone for a given flux density. These results also indicate that a substantial negative impact upon magnetic properties is incurred on the order of millimeters from the site of deformation. These degradations have a significant impact on motor performance and efficiency, and they will be included in advanced motor models to ensure proper optimization.

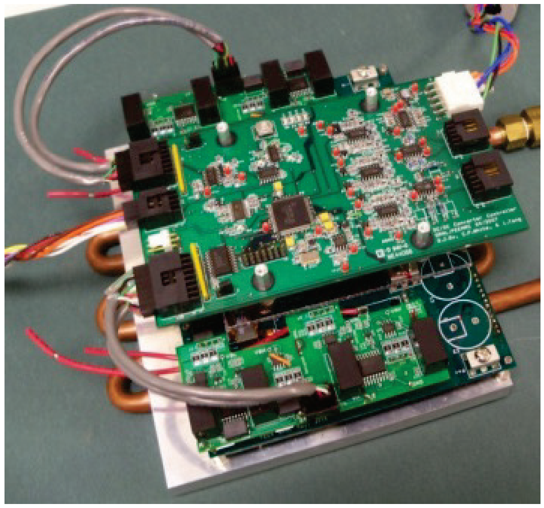
Onboard Charger and dc–dc Converter Offers Double the Power Density at Half the Cost

Contact: Burak Ozpineci, burak@ornl.gov, 865-946-1329

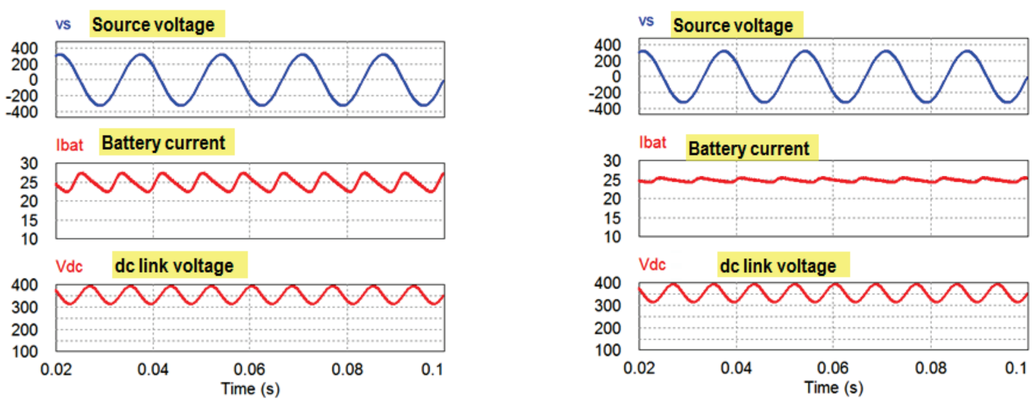
Stand-alone onboard battery chargers (OBC) and 14 V dc–dc converters that currently dominate plug-in electric vehicles and all-electric vehicles are bulky (~0.41 kW/kg, ~0.66 kW/L), are not cost-effective (~$106/kW), and have relatively low efficiency (85–92%) because of the limitations of current semiconductor and magnetic materials. ORNL researchers aim to leapfrog the present silicon-based charger technology to address charger and converter cost, weight, volume, and efficiency by overcoming the limitations of silicon semiconductor and magnetic materials. The project does so by using wide bandgap devices, including silicon carbide (SiC) and gallium nitride (GaN); advanced magnetic materials; and a novel integrated charger architecture and control strategy.

ORNL has developed a new bidirectional integrated OBC and dc–dc converter architecture that significantly reduces the number of components. The design offers a 47% reduction in power circuit components alone, not counting savings in the gate driver and control logic circuits. ORNL built and tested a 6.6 kW bidirectional SiC-based isolation converter prototype that has a built-in 2 kW, 14 V buck (voltage reducing) converter to meet vehicle accessory electrical loads. Test results demonstrated successful soft-switching operation and a peak efficiency of 99%.

ORNL also developed a control strategy for the charger isolation converter to reduce the battery ripple current of twice the ac main frequency that is inherent in single-phase ac–dc converters. Simulation results show the control strategy reduces the ripple current by 60% and thereby enables a corresponding reduction in the size of the bulky dc link capacitor in the ac–dc front-end converter.



A 6.6 kW SiC-based isolation converter with an integrated 2 kW 14 V buck (voltage reducing) converter.



Battery ripple current shown at left without ripple reduction control, and at right with ripple reduction control. Significant reduction of battery ripple current is visible.

Emerging GaN devices fabricated on silicon substrates are poised to offer significant improvements in power converters at costs comparable to those of silicon devices. Because of their enhanced switching speed and reduced switching and conduction losses, these switches offer the opportunity to minimize passive component requirements, a major driver of cost, weight, and volume in charger and dc–dc converters. ORNL has characterized both low (<200 V) and high (600 V) voltage GaN switches and has obtained valuable data for GaN-based OBC and dc–dc converter designs.

Publications

1. G. J. Su and L. Tang. 2014. "A new integrated onboard charger and accessory power converter for plug-in electric vehicles," pp. 4790–4796 in *Energy Conversion Congress and Exposition* (ECCE) 2014, IEEE.

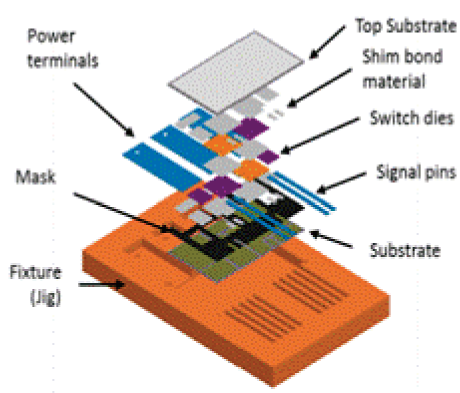
Next-Generation Wide Bandgap Packaging Improves Inverter Efficiency

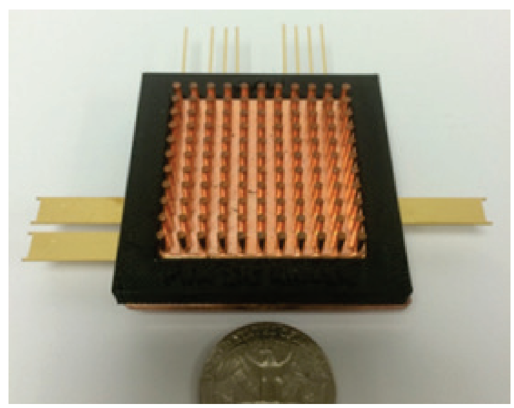
Contact: Burak Ozpineci, burak@ornl.gov, 865-946-1329

ORNL is leveraging its multidisciplinary capabilities, including packaging technology, to develop advanced wide bandgap (WBG) automotive power electronics technologies. A three-dimensional (3D) planar interconnected silicon carbide (SiC) power module developed at ORNL using innovative packaging offers comprehensive improvements in performance, efficiency, density, and cost.

The module's packaging technology employs area bonding instead of wire bonding to build multiple layer/multiple component stacks in a two-step process. A prototype of an SiC 1,200 V, 100 A single-phase-leg power module was fabricated at the ORNL Packaging Laboratory using this technology. The module employs the latest industrial SiC power devices—metal oxide semiconductor field effect transistors and Schottky barrier diodes—as well as an optimized 3D planar interconnection with double-sided direct cooling (both forced air and liquid cooling).

Results of the module evaluation indicated that the electric parasitic parameters of the package were reduced by 70%, and the specific thermal resistivity of the double-sided cooling package was reduced by more than 45% compared with state-of-the-art industrial products, such as modules used in the Nissan LEAF and Toyota Camry. These improvements are represented by a four times larger allowed current density of the SiC device in the module for the same temperature increase. The packaging improvements leading to system operation at high efficiency (half power loss) and frequency that is five times higher result in considerable strides in achieving power density and cost targets for power electronic systems in electric-drive vehicles.





Prototype of the planar-bond-all (PBA) power module integrated with a special coolant manifold. Combining the superior attributes of SiC devices and advancements in packaging, this module allows for greater efficiency and high-density power conversion.

Publications and Presentations

1. Z. Liang. 2014. "A phase-leg power module packaging with optimized planar interconnection and integrated double sided cooling," *IEEE Journal of Emerging and Selected Topics in Power Electronics* **2**(3), 487–495.

2. Z. Liang. 2014. "Power module and cooling system thermal performance evaluation for HEV application," *IEEE Journal of Emerging and Selected Topics in Power Electronics* **2**(3), 443–450.

3. Z. Liang. 2014. "Packaging technology for multifunctional integration of advanced SiC power modules," presented at the fourth International Power Supply on Chip Workshop (PwrSoC2014), Boston, October 6–8.

4. Z. Liang. 2014. "Development of packaging technologies for advanced SiC power modules," presented at the second IEEE Workshop on Wide Bandgap Devices and Applications (WiPDA), Knoxville, Tenn., October 13–15.

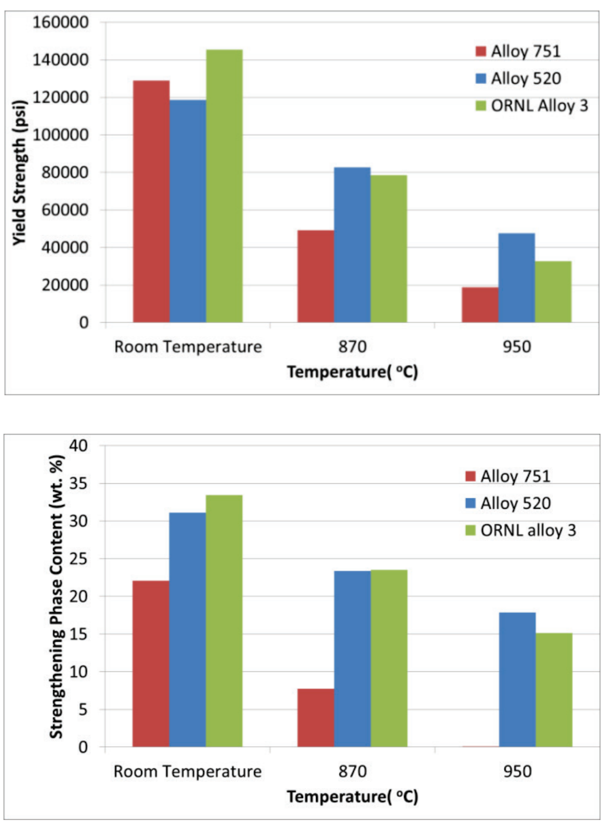
Propulsion Materials

Computational Modeling Assists Development of New Valve Alloys

Contact: Govindarajan Muralidharan, muralidhargn@ornl.gov, 865-574-4281

Several strategies such as lean-burn operation, high levels of exhaust gas recirculation, turbocharging, variable valve actuation, and variable compression ratios are being pursued to improve engine combustion efficiency. Strategies that retain more heat in the exhaust gas to improve efficiency result in increased operational temperatures for components in the exhaust path, such as valves. Exhaust gas temperatures are projected to increase from 760 to at least 870°C (and possibly as high as 1,000°C) as engine efficiencies increase. However, a major barrier to this design route is the availability of affordable materials with adequate high-temperature mechanical properties and oxidation resistance.

ORNL researchers used a “materials-by-design” approach with synergistic computational and experimental aspects to develop cost-effective nickel-based alloys for higher-temperature use. High-temperature fatigue strength was identified as critical in determining the performance of these alloys in valve applications. Understanding of the strengthening mechanisms in existing commercial alloys was required to enable computational modeling to develop materials with improved properties and lower cost. A range of nickel-based alloys with potentially varying fractions of the γ’ strengthening phase were identified to correlate fatigue properties with the alloy microstructures.



(Left) Comparisons of ORNL alloy 3 and commercial alloys 751 and 520. (Right) Yield strengths of alloys 751 and 520 and ORNL alloy 3 as a function of temperature.

Nine commercial nickel-based alloys, including Alloy 751 (currently used for valve applications), with Ni+Co contents ranging from 66 to 76 wt % were selected to understand which microstructures result in the best fatigue properties. The results of the thermodynamic calculations showed that all the alloys have a matrix of γ with a major strengthening phase as γ’. One or more carbide phases, such as $M_{23}C_6$, MC, and M_7C_3, may also be present. The primary differences among the microstructures were the weight percent of the γ’ phase at a given temperature and the highest temperature at which the γ’ phase is stable.

With these alloy microstructures as a target, researchers used computational thermodynamics to design new alloys with microstructures yielding high-temperature tensile and fatigue properties similar or superior to those of the commercial alloy currently used in exhaust valves. In contrast to commercially available alloys, with Ni+Co contents above 66 wt %, these newly identified candidate alloys have Ni+Co content lower than 50 wt %, which will reduce materials costs. These new alloys will enable the development of exhaust valves that can operate at much higher temperatures at potentially lower cost, facilitating the deployment of more efficient vehicles.

Enabling Materials for High-Temperature Power Electronics

Contact: Andrew Wereszczak, wereszczakaa@ornl.gov, 865-576-1169

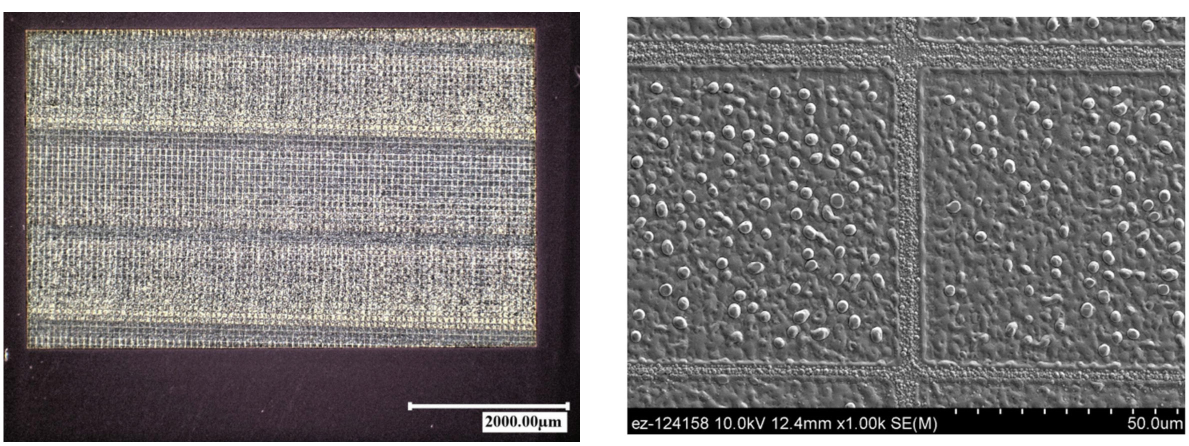
ORNL research is helping develop power electronic modules (PEMs) that can perform reliably at high temperatures over a sustained lifetime while meeting DOE size, weight and cost goals. PEMs are subject to high operating temperatures that require effective thermal management strategies. The use of wide bandgap (WBG) semiconductors that can operate at higher temperatures than conventional devices also is pushing PEM operating temperatures higher.

VTO is emphasizing research that meets technical cost-effectiveness challenges. These include high-temperature components, packaging, and reliability for long-term transformation technologies, and thermal management technologies to reduce PEM volume and enhance thermal reliability.

ORNL is addressing four aspects of the problem in parallel:

- *Increase strain tolerance among and between PEM constituents* by increasing the inter-bonding strain tolerance, or strength.
- *Reduce imposed strain on PEM constituents* by using thermally conductive materials and simpler architectural designs that position the semiconductor closer to the heat sink.
- *Increase the temperature capability of constituents* by developing polymers capable of operating at higher temperatures.
- *While meeting the other requirements, control cost* via innovative material science, including the use of materials now used in non-electrical applications.

ORNL researchers successfully bonded WBG silicon carbide semiconductor diodes and metal-oxide-semiconductor field-effect transistors (MOSFETs) onto silver-plated, copper–clad substrates using a sinterable silver paste. A commercially available sinterable paste was used to bond integrated gate bipolar transducers and diodes at elevated temperatures with pressure assistance. Polished cross-sections of the bonded joint showed that a consistently good joint was produced.



Low-magnification (left) and high-magnification (right) images of the WBG silicon carbide MOSFET surface interconnected with a copper-clad substrate.

A perfluoropolymer matrix material combined with an MgO filler was tested as a thermally conductive molding compound. Perfluoropolymer was chosen for its high-temperature capability and the MgO filler was chosen because it had been demonstrated to increase the thermal conductivity of epoxy. The MgO did increase the thermal conductivity, but processing complications developed that were associated with the bonding between the perfluoropolymer and the MgO. This system will need further development to exploit its potential.

A study of plating materials and printing methods (screen and stencil printing) on interconnect shear strength is under way. Processing of the test coupons has neared completion.

Publications, Presentations, and Patents

1. Wereszczak. 2014. "Improved sintered silver joints via controlled topography of electronic packaging subcomponents," US Patent 8,822,036 B1, September 2.

2. Wereszczak, Z. Liang, M. K. Ferber, and L. D. Marlino. 2014. "Uniqueness and challenges of sintered silver as a bonded interface material," *Journal of Microelectronics and Electronic Packaging* **11**(4), 158–165.

3. Wereszczak, T. G. Morrissey, C. Volante, P. Farris, Jr., R. Groele, R. H. Wiles, and H. Wang. 2013. "Thermally conductive MgO-filled epoxy molding compounds," *IEEE Transactions on Components, Packaging and Manufacturing Technology* **12**(3), 1994–2005.

4. Wereszczak, Z. Liang, M. K. Ferber, and L. D. Marlino. 2014. "Uniqueness and challenges of sintered silver as a bonded interface material," Paper WA23, pp. 178–187 in *Proceedings of the IMAPS HiTEC 2014*, Albuquerque, NM.

5. D. Devoto, P. P. Paret, and A. A. Wereszczak. 2014. "Stress intensity of delamination in a sintered-silver interconnection, Paper WA26, pp. 190–197 in *Proceedings of the IMAPS HiTEC 2014*, Albuquerque, NM.

Reducing Friction Through Surface Modification

Contact: Jun Qu, 865-574-5377, qujn@ornl.gov

A heavy-duty diesel engine loses 10–15% of the power produced by its engine to parasitic friction. Research aimed at reducing parasitic engine and drivetrain losses is part of DOE's push to achieve 50% higher freight efficiency (ton miles per gallon) for heavy vehicles.

ORNL researchers are working to improve the fuel efficiency of diesel vehicles by reducing the friction between contacting surfaces in the engine via a combination of surface texturing and coating technologies. ORNL has identified a texturing process and a wear-resistant thin coating for textured bronze bearing surfaces that reduce friction by more than 20%.

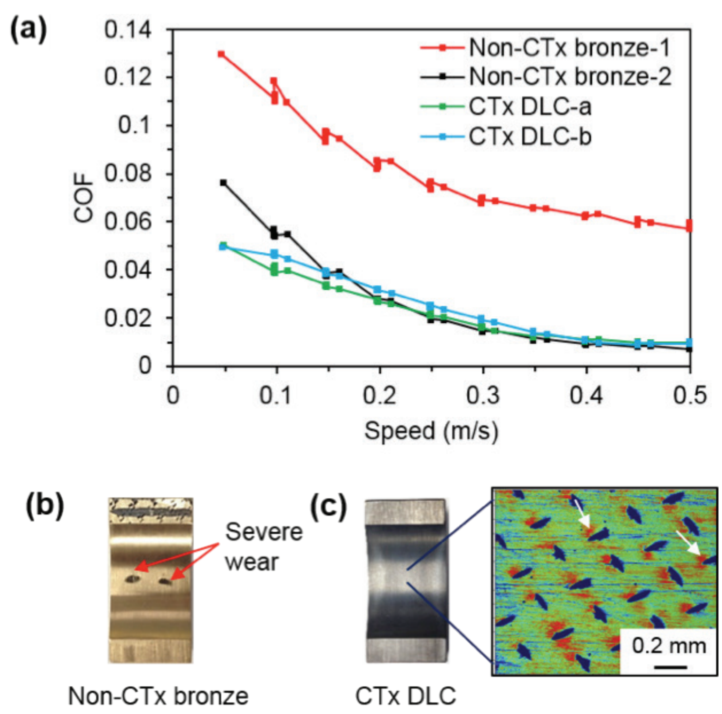
The research goals are to reduce boundary and mixed friction, allow the use of lower-viscosity engine oils to reduce hydrodynamic drag, and mitigate thinner oil films induced by higher peak-cylinder pressures. Proper surface texturing/dimpling may alter the flow and film thickness of lubricating fluids locally and across the contact region, change the bearing pressure distribution, provide channels to supply lubricant to surfaces, and trap debris that might otherwise become embedded or abrade the surfaces. The study focused on surface engineering techniques for connecting-rod bronze end bearings.

After testing methods of creating textures on bronze bearing surfaces, ORNL identified wire mesh compression as a feasible texturing process and demonstrated 20–40% friction reduction in bench tests. Finer textures showed more favorable results. Since the surface texture created by a 50×50 mesh outperformed a 20×20 mesh texture, even finer meshes—100×100 and 140×140—were acquired and used to produce textures in FY 2014. Multiple compressions were applied for higher dimple densities: 90 and 45° for 100×100 mesh and 90, 45, and 0° for 140×140 mesh. All compressed surfaces were re-polished using 600 grit silicon carbide abrasive paper to remove the rims of dimples.

Because wear and sometimes scuffing failure is inevitable for a relatively soft bronze surface in mixed and boundary lubrication, a wear-resistant diamond-like-carbon (DLC) coating was identified and applied to the wire-mesh-compressed surface to prevent excessive wear. A DLC coating was superimposed on the compression-textured bronze surface by Northeast Coating Technologies.

Nontextured, textured, coated, and textured+coated surfaces were tested against a steel counterface in a low-viscosity SAE 0W-30 engine oil. Stribeck curve friction tests were carried out on the variable-load/speed bearing tester (VLBT) and on a pin-on-disc (POD) system under a series of loads and speeds. VLBT tests were carried out under a 100 N load and POD tests under 10 N. In every case, the DLC coating exhibited strong binding to the substrate and excellent wear resistance, and consistently lower friction was observed for the textured+coated surface.

Future work, if funding is available, will combine advanced surface engineering and lubrication technologies for synergistic effects on friction reduction and wear control.



(a) Friction behavior of uncoated bronze vs. a compression textured + DLC surface. (b) Post-testing image shows worn spots on uncoated bronze; (c) no detectable wear and well-preserved texture on DLC-coated surface.

Publications and Presentations

1. P. J. Blau, J. Qu, Y. Zhou, K. M. Cooley, D. L. Erdman III, and S. M. Hsu. 2014. *Friction Reduction through Surface Modification—Texturing of Lubricated Sliding Surfaces*, ORNL/ TM-2014/599.

2. P. J. Blau, K. M. Cooley, and D. L. Erdman. 2014. "Effects of indentation and compression texturing on the lubricated friction of non-ferrous surfaces under spectrum loading," presented at the Society of Tribologists and Lubrication Engineers 69th Annual Meeting and Exhibition, Orlando, Florida, May 18–22.

3. P. J. Blau, K. M. Cooley, and J. Qu. 2014. "Friction reduction through surface modification," presented at the 2014 DOE Vehicle Technologies Program Annual Merit Review, Washington, D.C., June 19.

Integrated Computational Materials Engineering of New Propulsion Materials

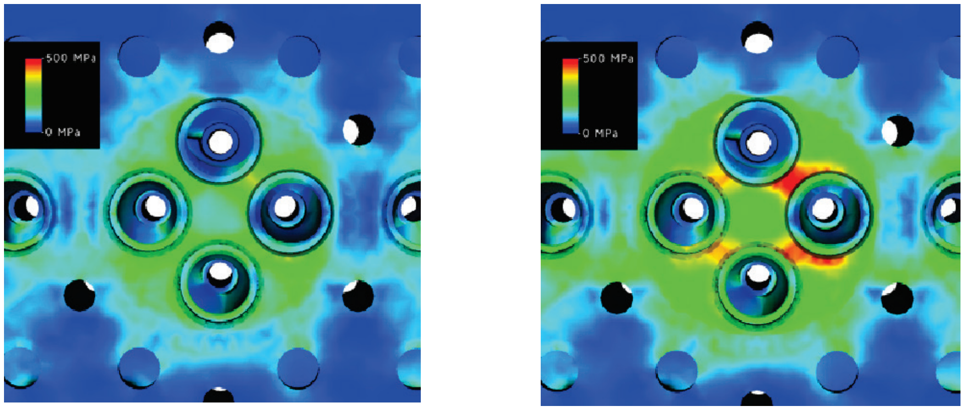
ORNL is using Integrated Computational Materials Engineering, involving close feedback between theory and experiment, to develop improved propulsion materials for applications such as high-performance engines, piezoelectric materials for fuel injector actuators, low-light-off temperature catalysts, and permanent magnets to enable electric drive propulsion systems. The studies make important findings in several different research areas, which are described below.

Modeling of High-Performance Engines

Contact: Charles Finney, finneyc@ornl.gov, 865-946-1243

Heavy-duty internal combustion engines are operating at increasingly high peak cylinder pressures to achieve required increases in brake thermal efficiency. Materials used now, such as gray cast iron, are inadequate for the high pressures and temperatures that will characterize future higher-efficiency engines.

Heat-flux calculations from computational fluid dynamics simulations were used in finite element analysis simulations at baseline (192 bar) and elevated (300 bar) pressures. The calculations showed calculated materials stresses in the engine head for the baseline and elevated-pressure cases. Of particular concern were results showing the bridges between the exhaust ports, which showed unacceptable stresses at elevated-pressure operation. Based on the yield stresses in the first-pass analysis, the current generation of materials will not be sufficient for future generations of heavy-duty internal combustion engines.



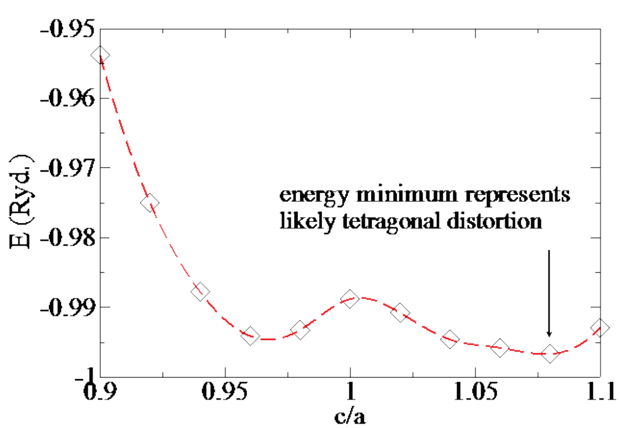
(Left). Materials stresses in engine head at baseline pressure (192 bar). The four circular areas represent intake and exhaust gas ports. (Right) Materials stresses in engine head at elevated pressure (300 bar). Red areas indicate high stresses in the bridges between the exhaust ports, which current-generation engine materials cannot withstand.

New Piezoelectric Materials

Contact: David S. Parker, parkerds@ornl.gov, 865-574-7128

High-performance engines require improved fuel injection control to maintain fuel efficiency and emissions control. Currently, most high-performance fuel injectors use piezoelectric actuators such as $PbZr_{0.5}Ti_{0.5}O_3$ (PZT). However, PZT does not perform well enough for engines under development. In particular, its tetragonality is only 1.025, limiting its performance. Therefore, a PZT-based compound with larger tetragonality is sought.

ORNL's primary theoretical results found that the energy of the oxide composition $(PbZr_{0.5}Ti_{0.5}O_3)_{0.75}(BiZn_{0.5}Ti_{0.5}O_3)_{0.25}$ shows minima near the two c/a ratios 0.97 and 1.08 with the c/a=1.08 ratio an absolute minimum. This c/a ratio of 1.08 greatly exceeds the 1.025 value of PZT. The larger c/a ratio means that larger ferroelectric polarizations, and associated piezoelectric coefficients, will be associated with this composition.



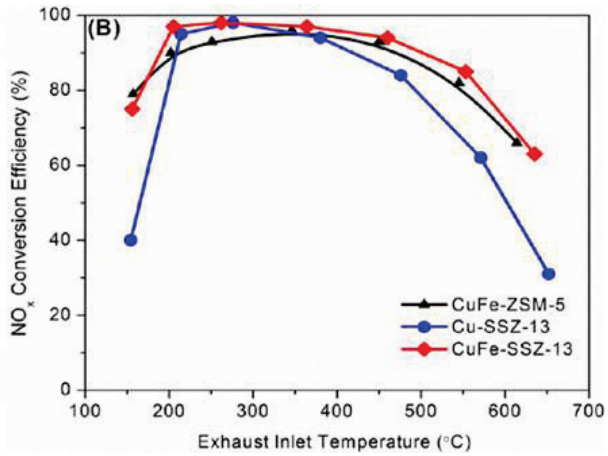
The variation of energy with c/a ratio for the oxide composition $(PbZr_{0.5}Ti_{0.5}O_3)_{0.75}(BiZn_{0.5}Ti_{0.5}O_3)_{0.25}$.

Catalysis Materials

Contact: Chaitanya Narula, narulack@ornl.gov, 865-574-8445

Increasingly high-efficiency engines require the development of new catalytic materials that achieve high conversion efficiency for nitrogen oxides (NOx) at lower exhaust temperatures.

A comparison of NOx reduction from laboratory measurements shows that the catalyst CuFe-SSZ-13 and CuFe-ZSM-5 have much higher NOx conversion than the commercially available Cu-SSZ-13.



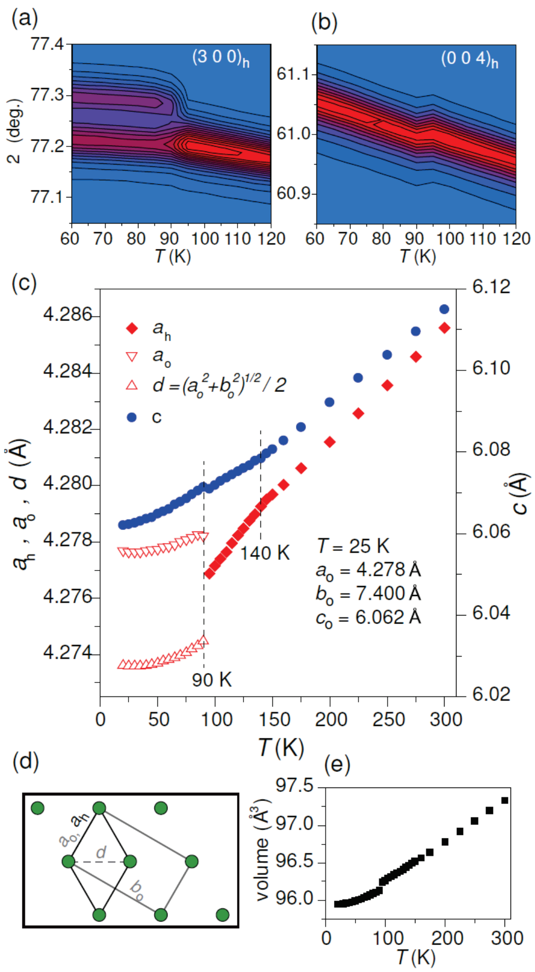
CuFe-SSZ-13 and CuFe-ZSM-5 show remarkable low-temperature reactivity compared with commercial Cu-SSZ-13.

Permanent Magnets

Contact: Michael McGuire, mcguirema@ornl.gov, 865-574-5496

Strong permanent magnets, such as $Nd_2Fe_{14}B$ and $Sm_2Co_{17}/SmCo_5$, are used in a number of clean energy applications such as hybrid and battery electric vehicles and wind turbines. However, the key rare earth elements in these magnets, such as neodymium and samarium, are subject to supply disruptions.

ORNL discovered new structural information on rare-earth free MnBi from a single-crystal neutron diffraction measurement. The data show anisotropic vibrations of the bismuth atoms which increase at high temperature. In addition, crystal structure distortion was found to occur below about 90 K, the temperature at which the magnetic moments are known to reorient.



From the top: Neutron diffraction intensity patterns of the ferromagnet MnBi showing the hexagonal to orthorhombic transition, at which the moments re-orient.

The bottom plot shows the relationship of the hexagonal and orthorhombic unit cells and the volume with temperature.

Publications

1. M. Moses-DeBusk, M. Yoon, L. Allard, L., D. Mullins, Z. Wu, X. Yang, G. Veith, G. M. Stocks, and C. K. Narula. 2013. "CO oxidation on supported single Pt atoms—Experimental and ab initio density functional studies of CO interaction with Pt atom on θ-Al_2O_3(010) surface," *J. Am. Chem. Soc.* **135**, 12634.

2. C. K. Narula, L. F. Allard, G. M. Stocks, and M. Moses-DeBusk. 2014. "Remarkable NO oxidation on single supported platinum atoms." *Sci. Rep.* **4**, 7238.

3. M.A. McGuire, H. Cao, B. C. Chakoumakos, and B. C. Sales. 2014. "Symmetry-lowering lattice distortion at the spin reorientation in MnBi single crystals." *Phys. Rev. B* **90**, 174425.

Vehicle Systems

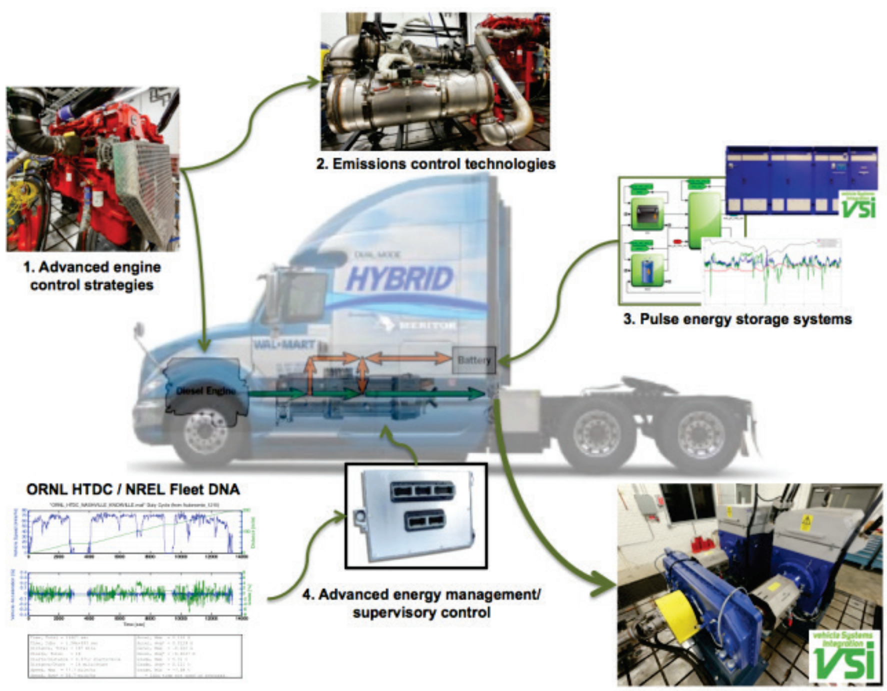
Optimization of Powertrain Controls for Hybrid Trucks

Contact: David E. Smith, smithde@ornl.gov, 865-946-1324

Hybrid medium and heavy-duty (MD and HD) powertrains offer large potential reductions in fuel consumption, criteria pollutants, and greenhouse gases. In addition to powertrain electrification, advanced combustion regimes could further reduce the fuel consumption of these vehicles. However, to maximize the benefits of powertrain electrification and advanced combustion, coordination of engine operation and emissions control is essential to fully realize the compound benefits of all the candidate technologies being investigated in the project.

Using advanced hybrid technologies and control systems, researchers at ORNL are taking a multi-faceted approach to developing an advanced heavy-duty powertrain system that will decrease energy consumption and criteria emissions in Class 8 line haul vehicles. The project focuses on advanced combustion regimes and engine control strategies, emissions control technologies, pulsed energy storage systems, and advanced energy management. It involves analytical modeling and supervisory controls development, as well as experimental verification and validation at the component, powertrain, and full vehicle system level.

A first-generation energy management strategy involving a hybrid energy storage system and emissions control for optimizing powertrain controls for hybrid line haul trucks has been completed. Using a hybrid Class 8 powertrain designed for line haul applications that can be operated as a series hybrid, parallel hybrid, or all electric vehicle, ORNL scientists have leveraged powertrain supervisory controls software from a previous program and past transient engine modeling experience to build a baseline dual energy storage system model. Also, a, transient model of a Cummins ISX-450 15 L engine has been developed and installed in the ORNL Vehicle Systems Integration (VSI) Laboratory.



Project focus areas.

Perhaps the greatest opportunity for powertrain efficiency improvement is the implementation of new approaches for increased regenerative braking energy collection for Class 8 line haul hybrid trucks. Previous R&D to support hybrid energy storage systems for light-duty passenger car applications has been extended to the MD and HD sector, where current battery technology, which is reasonably mature for light duty applications, is not capable of absorbing the large amounts of energy required to slow trucks down. However, the proposed dual energy storage system model offers substantial gains in overall vehicle efficiency. This actively controlled model builds on previous work conducted at Argonne National Laboratory and uses a framework available in the release of the Autonomie model.

Progress on this project includes establishing reference supervisory controls based upon experimental powertrain results from the ORNL VSI Laboratory, a completed literature review of various approaches to hybrid energy storage systems, development of a transient model of a Cummins engine and a full aftertreatment suite of models, and a baseline dual energy storage system model.

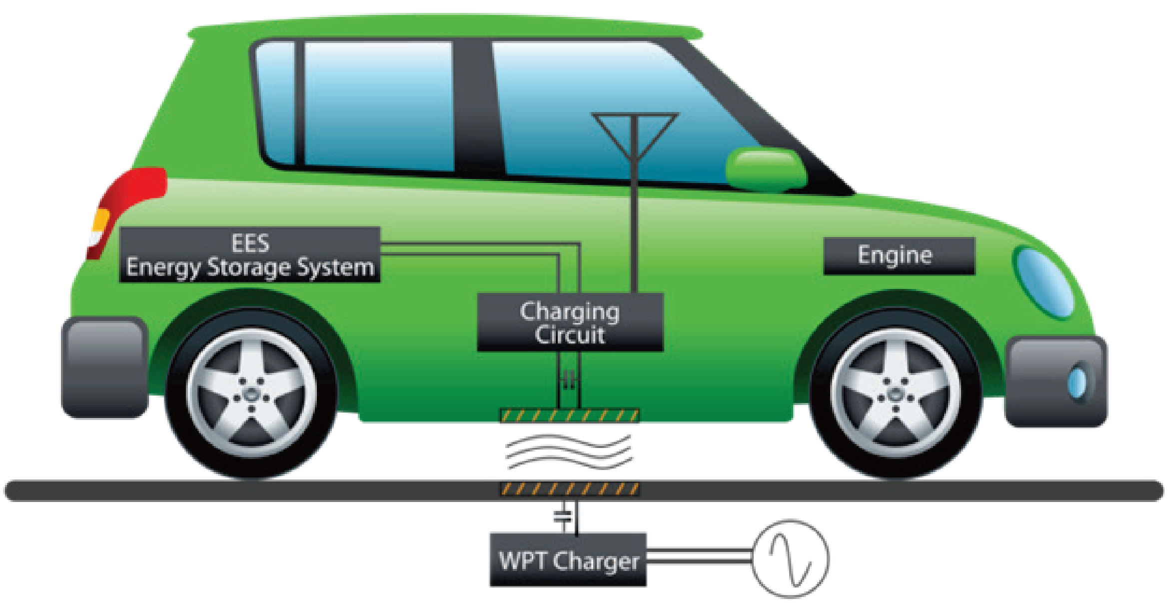
Wireless Charging for Electric Vehicles

Contact: Omer Onar, onaroc@ornl.gov, 865-946-1351

Thanks to ORNL and its partners, hybrid and electric vehicle owners may soon be able to cut the cord. A team led by ORNL has developed and demonstrated a stationary wireless charging system that operates at the same efficiency as plug-in charging.

ORNL and its partners have improved wireless changing technology with transformational innovations. Working with ORNL are commercialization partner Evatran (which developed the first commercially available wireless vehicle charging system for vehicle charging), the Clemson University Integrated Center for Automotive Research (ICAR), and Toyota.

Wireless power transfer (WPT) systems use inductive charging, in which a coil in a charging pad sends power in the form of a high-frequency electromagnetic field to a receiving coil in the vehicle. It eliminates the need for power cables and plugs to charge the vehicle batteries.



How a wireless power transfer system works.

ORNL researchers designed new WPT transmitting and receiving coils that are more efficient and have a higher tolerance for misalignment. The new coils can handle power transfer at greater than 20 kW levels. The ORNL system can interact with multiple vehicles and charging architectures. It is now capable of charging through a J1772 standard charging system, a CHEdeMO system, or directly to a custom high-voltage energy storage system.

In addition, ORNL and Evatran have developed cost reduction recommendations that could shave $8,000—9,000 in costs per grid-side unit.

Evatran is integrating the coils and vehicle-side electronics into a Toyota Prius plug-in vehicle and Toyota Rav4 and Scion IQ electric vehicles in collaboration with ORNL. Under a cooperative research and development agreement between ORNL and Toyota, a small fleet of Toyota vehicles will be outfitted with the new systems. Clemson has outfitted its ICAR facility with the infrastructure necessary to deploy and test the vehicle fleet.

Once the integration of the charging systems into the vehicles is complete, ICAR will begin evaluating each of the charging scenarios. Eventually, under ORNL guidance and direction, ICAR will evaluate the vehicles under both stationary charging scenarios and dynamic operation, in which vehicles are charged in motion on specially designed roadways.

The goals of the project are to integrate WPT power electronics and coils into demonstration vehicles, validate them in an independent testing laboratory, and provide a facility for field testing to assist in the development of standards for wireless charging.

Publications, Presentations, and Patents

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Simulating the Effects of Integrated Advanced Vehicle Technologies

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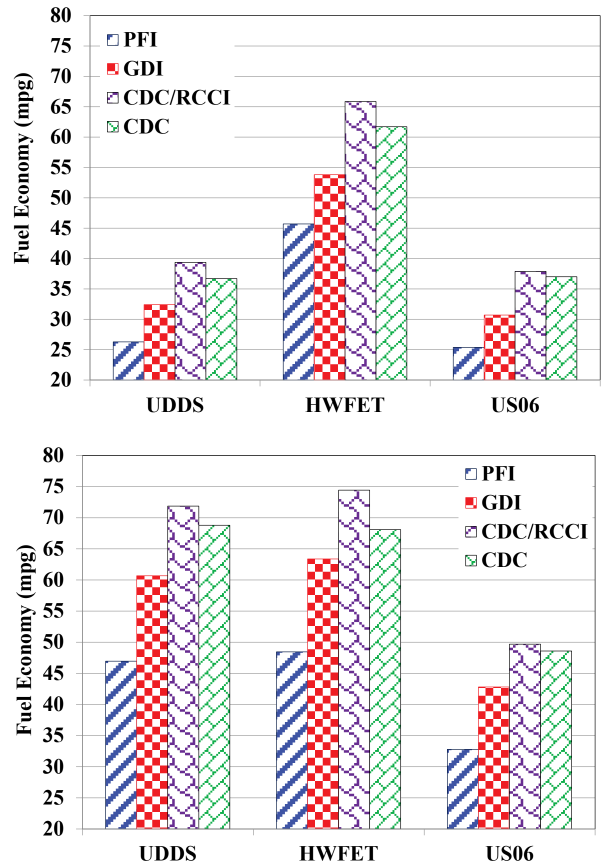
A combination of vehicle technologies—including high-efficiency clean-combustion engines, improved catalysts, and renewable fuels—will be necessary to satisfy coming standards for fuel economy, emissions, and renewable fuel blending. ORNL is providing experimental data and using them to conduct substantial computer simulations for evaluating the technologies that help US automakers meet regulations and produce cleaner, more efficient vehicles.

Advanced combustion regimes such as reactivity-controlled compression ignition (RCCI) and renewable fuels such as ethanol blends dramatically improve engine efficiency while reducing engine-out NOx and particulate matter emissions. However, they also result in lower exhaust temperatures that diminish the performance of conventional catalytic aftertreatment systems, resulting in increases in CO and hydrocarbon emissions. Thus innovative aftertreatment devices are needed that can perform in cooler exhaust streams. Moreover, to avoid mechanical damage to engines, vehicles must be able to switch between conventional and high-efficiency combustion cycles. And as hybrid electric vehicles (HEVs) become more prevalent, it is essential to understand how to integrate new engines, exhaust systems, and fuel mixtures to achieve vehicle energy efficiency and emissions control.

In FY 2014, ORNL researchers assessed the impacts of RCCI operation on fuel economy and emissions in both hybrid and non-hybrid vehicles using detailed vehicle systems simulations. Their work resulted in the following accomplishments:

- Developed new engine maps capable of mixed-mode operation, including RCCI and conventional diesel combustion, using data from dynamometer measurements at ORNL.
- Updated and refined an engine model to evaluate fuel consumption and exhaust properties associated with various aftertreatment control strategies during cold start and the transition to mixed-mode operation.
- Developed hybrid and non-hybrid powertrain models and used them to evaluate the performance of RCCI and other advanced combustion strategies in various powertrain configurations.
- Calibrated and refined hybrid and non-hybrid powertrain models to improve the simulation of cold starts and better predict the effects of HEV control systems on fuel consumption and emissions.
- Simulated fuel economy and exhaust properties of different engine technologies in conventional and hybrid light-duty vehicles over multiple city and highway driving cycles.
- Quantified the fuel economy benefit, based on passenger vehicle simulations, of an RCCI-enabled engine relative to a 2009 port fuel injection gasoline engine.
- Completed preliminary simulations of tailpipe emissions for a light-duty power-split HEV equipped with an RCCI-enabled engine and a full aftertreatment train of diesel oxidation catalyst, lean NOx trap, and diesel particulate filter devices.

The simulation results indicate that an RCCI-enabled engine significantly improves fuel economy for all hybrid and non-hybrid drive cycles, and hybridization increases the opportunity for RCCI operation and dramatically reduces NOx emissions from the engine. However, the simulations also show that RCCI lowers exhaust temperatures for significant periods below the 200°C threshold at which conventional catalysts can reduce CO, hydrocarbons, and NOx emissions effectively. The simulations for the HEV show that implementing RCCI in HEVs could cut NOx emissions with a reduced fuel penalty.



Fuel economies in simulated vehicles powered by different combustion engine technologies over various city and highway drive cycles.

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Improving Efficiency with Connected Vehicles

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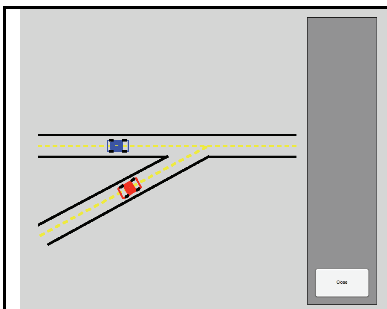
Researchers at ORNL have developed an optimization framework and decentralized control algorithms for vehicle coordination in intersections and merging roadways, aimed at avoiding stop-and-go driving and thus improving traffic flow and efficiency.

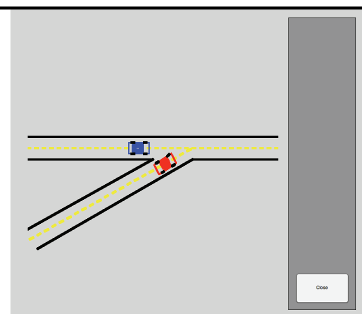
The increasing numbers of vehicles on roadways pose significant challenges related to traffic congestion and accidents. Driver responses to various disturbances can cause congestion. Intersections and merging roadways are the primary sources of bottlenecks, further contributing to traffic congestion. In the United States, 5.5 billion hours are wasted each year on average as a result of vehicular congestion, which translates to about $121 billion dollars. In 2012, around 1.7 billion metric tons of CO_2 were released to the environment by vehicles as a result of congestion. Moreover, traffic congestion results in driver discomfort, distraction, and frustration.

ORNL research efforts hinge on the idea that in the "new world" of massive amounts of available data from vehicles and infrastructure, what once was modeled as uncertainty becomes additional input or extra state information in a much higher-dimensional vector. Given this new environment, the overarching goal of this project is to develop a framework and decentralized algorithms for real time coordination of vehicles that are wirelessly connected to one another and to an infrastructure.

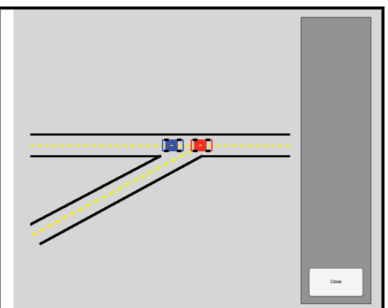
To visualize this process, consider an example: two vehicles (one red, one blue) arrive at an intersection at the same time. The blue vehicle is approaching a "yield" sign; hence, its driver ordinarily must come to a full stop and let the red vehicle proceed. In this case, however, the control algorithm promotes an optimal outcome: the blue vehicle decelerates precisely enough to allow the red vehicle to reach the intersection first and proceed without braking. The blue vehicle will not have to come to a full stop, thereby conserving momentum and fuel while also improving travel time.



Two vehicles with V2V communication approach an intersection at the same time.



The blue vehicle reduces speed through decentralized control to avoid a full stop.



Both vehicles pass through the intersection without stopping.

Although designing such outcomes may seem obvious and simple on the surface, decentralized control algorithms that are scalable to large fleets are non-trivial, and significant research is necessary to ensure they achieve operational objectives.

Several simulation case studies contacted so far using this framework have shown that fuel consumption can be reduced by up to 49%, and there are significant implications for improving travel time as well.

Vehicle Technologies Office Communications

ORNL Publications Support VTO Outreach Efforts and Data Needs

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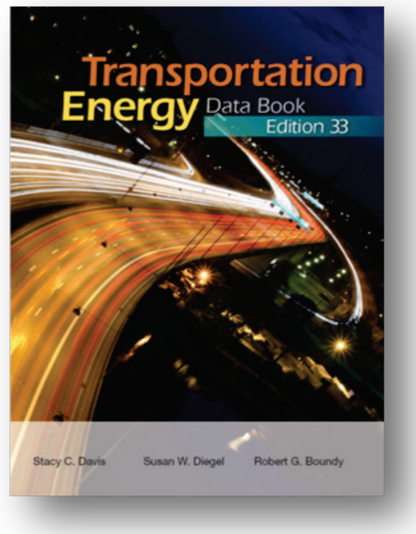
ORNL continued to support VTO's public communication efforts in 2014 with publication of the 2014 *Transportation Energy Data Book*, the *Vehicle Technologies Market Report*, and the "Fact of the Week" for the VTO home page.



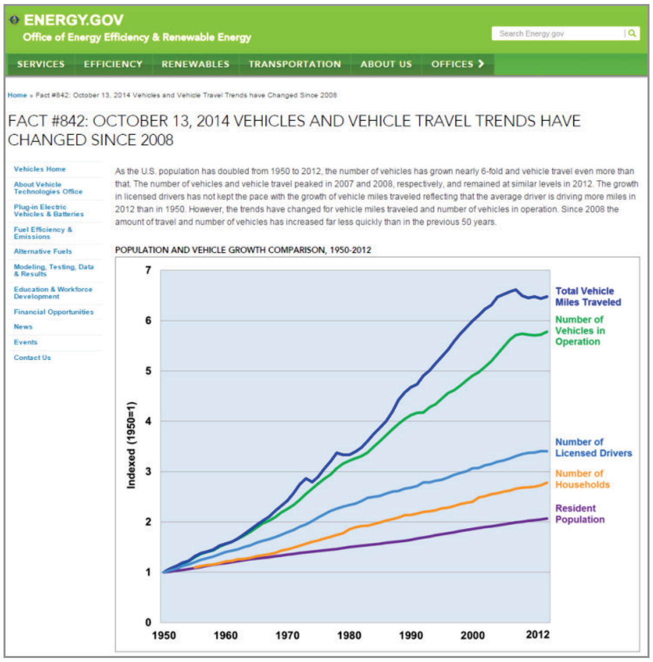
The ***Transportation Energy Data Book***, published in July, is the 33rd edition of the data collection that ORNL has published for VTO. This long-running project has been active at ORNL since 1975; the first *Data Book* was published in 1976. The Transportation Energy Data Book website allows visitors to download the *Data Book* in pdf format, download any of the Excel spreadsheets in the book individually, or request a hard copy of the report free of charge. Users log between 6,000 and 8,000 monthly visits to the website. In 2014, 1,400 copies of the *Data Book* were printed and distributed to a nationwide mailing list.

The document supports VTO public outreach, allowing VTO staff and the EERE Public Affairs Office to provide quick responses to internal and external queries on transportation energy use. Its purpose is to draw together, in one publication, transportation data from diverse sources, to resolve data conflicts and inconsistencies, and to produce a comprehensive document.

Its historical data tables provide a foundation for the analysis performed by VTO staff and other transportation analysts in pursuit of energy-efficient and environmentally friendly technologies. Policymakers, transportation analysts, and VTO staff require quality historical data and information on the transportation sector to make decisions for the future. Data from the book feed into many VTO products as well as into other federal agency projects.

The ***Vehicle Technologies Market Report*** was the fifth edition published by ORNL. It supports VTO public outreach by providing information on vehicle research to the public and meets internal VTO needs for data. The colorful, graphics-based report details major trends in US light-duty vehicle and medium/heavy truck markets and provides data on an individual manufacturer level. Special attention is given to the progress of high-efficiency and alternative fuel technologies, in accordance with

VTO's mission. The associated website (http://cta.ornl.gov/vtmarketreport) allows users access to data in both Excel and pdf format and hosts about 3,500 visitors sessions each month.



ORNL began developing the VTO **Fact of the Week** in April 2001 and continues to be responsible for the content each week. Every Monday morning, ORNL's Sustainable Transportation Program provides a new Fact of the Week for the VTO home page (http://energy.gov/eere/vehicles/transportation-fact-week). The topics align with the VTO mission, mainly concentrating on energy use and energy efficiency in highway driving mode. Transportation stakeholders and the general public benefit from VTO's data expertise through these readily accessible bits of information. More than 60% of visitors to the VTO website come through the Fact of the Week web page, and most of those are new visitors.