Sustainable Transportation Program

2015 Annual Report

OAK RIDGE
National Laboratory

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ORNL/SR-2016/402

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2016-G00496/cae

ORNL/SR-2016/402

Sustainable Transportation Program 2015 Annual Report

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Date Published: August 2016

Prepared by
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managed by
UT-BATTELLE, LLC
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

Table of Contents

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 (R&D) portfolio includes vehicle systems integration, fuel and lubricant technologies, advanced combustion engines, innovative materials, intelligent transportation systems, 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 other branches of government. Policy makers, 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 the Vehicle Technologies Office (VTO), Bioenergy Technologies Office (BETO), and Fuel Cell Technologies Office (FCTO). Support also comes from the Department of Transportation (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.

STP 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 powertrain technologies;
- enabling widespread use of cleaner fuels such as biofuels and natural gas; and
- 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; and
- 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 27% of US greenhouse gas emissions and about 58% of US petroleum consumption. 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—commercial light-duty trucks and heavy trucks are projected to use 21% more energy in 2040 than in 2015.

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 2015, ORNL led a multilaboratory effort focused on high-octane fuels, which found that mid-level ethanol blends used in engines that are optimized for the fuel can achieve vehicle performance benefits, realize better fuel economy, and lower greenhouse gas emissions. In another BETO-funded project, researchers explained the mechanism behind a technology that converts bio-based ethanol into hydrocarbon blend-stocks for use as fossil fuels. They found that the underlying reaction unfolds in a different manner than previously thought, with potential positive implications for the energy efficiency and cost of catalytic upgrading technologies proposed for use in biorefineries. A key compatibility study conducted by ORNL on ethanol and infrastructure materials was cited in the *Federal Register* in reference to regulations for underground storage tanks. Research on the safe storage of feedstocks determined how factors such as feedstock type and bale size, shape, and spacing affect the speed at which a biomass fire can spread. These experimental results have informed multiple changes to the *International Building Code*.

In research supporting DOT, ORNL and its industry partners completed the pilot test phase for an onboard monitoring system for fuel trucks to prevent fuel tax evasion. The system tracks the movements of fuel tankers from bulk storage to final destination in real time to prevent blending of taxable and nontaxable fuels and other tax evasion attempts. Researchers also worked with DOT to examine security and privacy issues associated with vehicle-to-vehicle and vehicle-to-infrastructure connectivity. One project assessed the feasibility of building a vehicle-based credential verification system to ensure the validity of communications for connected vehicles. Another project focused on preserving privacy through developing algorithms for vehicle trajectory information that remove identifying characteristics from data while retaining the usefulness of the data.

ORNL research sponsored by FCTO included advanced characterization of catalysts and thin ionomer layers for fuel cells. One study focused on the effects of atomic-level changes to the structure and chemistry of Ir-Ru oxygen evolution reaction catalysts, identifying which catalyst pairs improved long-term durability through repeated cycles of starting up and shutting down. Another study determined optimized conditions for imaging and spectroscopic analysis of perfluorosulfonic acid ionomer thin films within fuel cell electrodes, defining best practices and enabling new insights that could lead to higher-performance fuel cells. ORNL also worked with Virginia Tech to produce melt-spun carbon fibers of up to 25 Msi modulus and 250 ksi strength. The melt-spinning approach could save 25% of the costs associated with producing carbon fiber for high-pressure hydrogen storage systems.

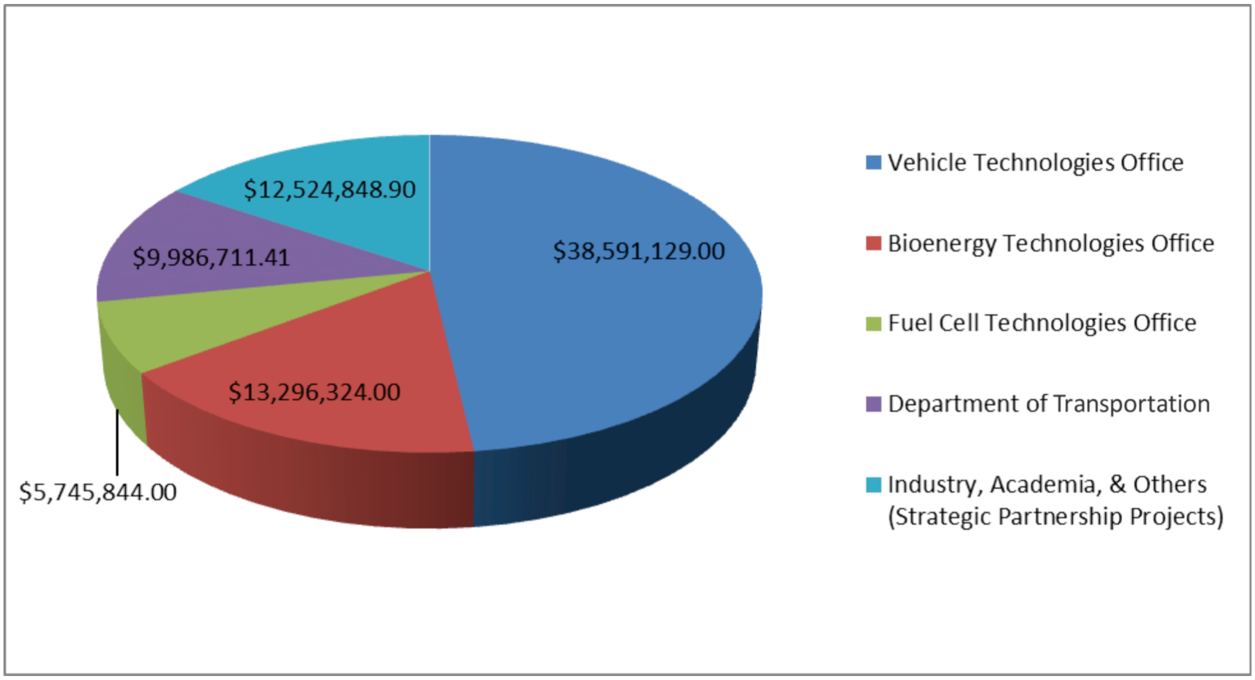
With funding from VTO, researchers assisted Delphi in developing power electronics packaging for an improved traction drive inverter used in the second-generation Chevrolet Volt EV. ORNL also worked with industry to develop a novel device for in situ atomic microscopy at up to 1 atm of pressure, enabling new research avenues for catalysts and other applications. In another VTO project, researchers developed and demonstrated the world's first bidirectional wireless power transfer system for level 2 (10 kW) charging. The bidirectional wireless charging system enabled a vehicle to power a building and vice versa as part of an integrated energy system. Projects focused on internal combustion, energy storage, and new alloys used high-performance computing to accelerate knowledge discovery and technology development. Neutron imaging captured cavitation events inside the nozzle of fuel injectors, informing injector design for greater fuel efficiency. Researchers conducted experiments to validate new models for the design of lightweight automotive structural components made with carbon fiber-reinforced injection-molded thermoplastics. Using infrared thermography, researchers are developing an evaluation process for battery electrodes and other roll-to-roll manufactured products that allows examination of materials on the production line to ensure quality without destroying the integrity of the examined material. Researchers also continued a multifaceted approach to developing optimized controls for an advanced hybrid heavy-duty powertrain that could decrease energy consumption and pollutant emissions in Class 8 line haul vehicles.

Highlights of these and other STP R&D efforts begin on page 12.

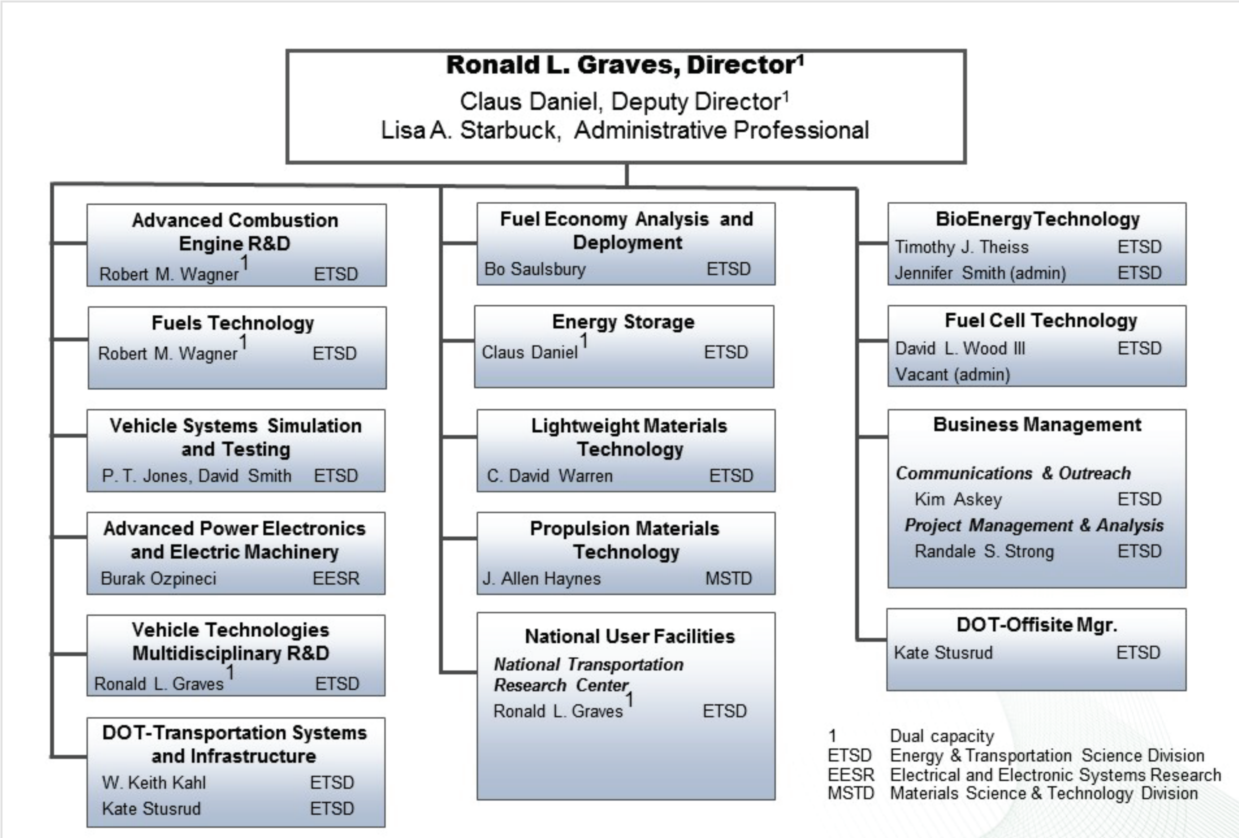
Program Metrics

Funding

STP received $80.1 million in new budget funding in FY 2015. Approximately $12.5 million or 16% is awarded competitively 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 2015 compared with the previous year.



Program funding provided significant support for 154 scientific and technical staff in 10 technical divisions, reflecting the multidisciplinary character of the ORNL program. STP team leaders are shown in the following organization 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), Strategic Partnership Project agreements, technology licensing, User Facility Agreements, and informal collaborations and information exchanges at technical conferences and workshops.

CRADAS

STP researchers supported 19 CRADAs in FY 2015 with 16 different companies, developing an array of transportation-related technologies. Industry partners contributed about $4.2 million in materials and services to those efforts.

Strategic Partnership Projects

ORNL worked with 60 industrial companies, 22 federal and state government entities, 9 nonprofit organizations, and 14 universities under 121 separate Strategic Partnership Project agreements in FY 2015. Those agreements were valued at about $12.5 million in total.

Laboratory-Directed Research and Development

ORNL's Laboratory-Directed Research and Development (LDRD) initiative supports cutting-edge research with the objective of maintaining the vitality of the laboratory, enhancing the laboratory's ability to address future DOE missions, and stimulating exploration at the forefront of science and technology. The transportation-related projects listed in Table 1 received LDRD awards in FY 2015.

Table 1. FY 2015 LDRD awards

Principal Investigator	Project Type/ID No.	Title	Type of Research	FY15 Funding
Todd Toops	6814	Dynamic Neutron Imaging of Intra-nozzle Fluid Dynamics of Fuel Injectors	Basic Research	$475,000.00
Nance Ericson	6923	Complementary Silicon Carbide Wide Bandgap Integrated Circuits for Bidirectional Electric Vehicle Chargers	Applied Research	$320,000.00
Mircea Podar	6944	Transformative Process for Coupling Solar Energy to Biofuel Production in Yeast for Steady State Bioconversion Reactors	Basic Research	$310,000.00
Balasubram Radhakrishnan	7238	Fundamental Understanding of Banded Structure Formation during Laser Additive Manufacturing of a Titanium Alloy using Massively Parallel Phase Field Simulations	Basic Research	$51,185.00
Xiao-Guang Sun	7315	Developing Hydroxide Fuel Cells Based on Novel Polymers with Improved Stability and Higher Ionic Conductivity	Applied Research	$170,000.00
Andreas Malikopoulos	7396	Scalable Data and Informatics for Connected Vehicles Leveraged to Enhance Efficiency	Basic Research	$385,000.00
Gerald Tuskan	7428	Increasing Advanced Biofuels Production from Terpenes in Eucalyptus Leaves	Basic Research	$325,000.00
Joseph Raetano	7340	Transportation Security: Trustworthy Vehicle Computing System	Applied Research	$385,000.00
Daniel Close	7570	Characterization of Inulinase-Expressing *Saccharomyces cerevisiae* Strains for the Consolidated Bioprocessing of Agave Feedstocks	Biosciences Division	$190,000.00
Burak Ozpineci	6928	Next Generation Compact and Reliable WBG-Based Inverter Breakthrough with Additive Manufacturing and High Performance Computing	Applied Research	$340,000.00

Patents

Table 2. Patents awarded during FY 2015

Inventor	Patent Number	Title
Chengdu Liang, Nancy J. Dudney, and Jane Y. Howe	9,023,528	Sulfur-Carbon Nanocomposites and Their Application as Cathode Materials in Lithium-Sulfur Batteries
Chengdu Liang, Zengcai Liu, Wujun Fu, Zhan Lin, Nancy J. Dudney, Jane Y. Howe, and Adam J. Rondinone	8,871,391	Lithium Sulfide Compositions for Battery Electrolyte and Battery Electrode Coatings
Zhenxian Liang, Laura D. Marlino, Puqi Ning, and Fei Wang	9,041,183	Power Module Packaging with Double Sided Planar Interconnection and Heat Exchangers
John Miller and Perry T. Jones	9,035,790	Wireless Power Transfer Electric Vehicle Supply Equipment Installation and Validation Tool
William P. Partridge, Jr.; James E. Parks, II; and Ji Hyung Yoo	9,068,933	EGR Distribution and Fluctuation Probe Based on Co_2 Measurements
William Partridge Jr.; James E. Parks, II; and Ji Hyung Yoo	9,000,374	EGR Distribution and Fluctuation Probe Based on CO_2 Measurements
Chaitanya Narula and Xiaofan Yang	8,987,161	Zeolite Based SCR Catalysts and Their Use in Diesel Engine Emission Treatment
Chaitanya Narula and Xiaofan Yang	8,987,162	Hydrothermally Stable, Low-Temperature NOx Reduction NH_3-SCR Catalyst
Amit Naskar, Marcus A. Hunt, and Tomonori Saito	9,096,955	Method for the Preparation of Carbon Fiber from Polyolefin Fiber Precursor, and Carbon Fibers Made Thereby
Claus Daniel, Jianlin Li, Beth L. Armstrong, and David L. Wood, III	8,956,688	Aqueous Processing of Composite Lithium Ion Electrode Material
Claus Daniel	9,012,803	Method of Varying a Physical Property of a Material Through its Depth
Amit Naskar	9,096,959	Method for Production of Carbon Nanofiber Mat or Carbon Paper
Jae-Soon Choi, Beth Armstrong, and Vivian Schwartz	9,012,349	Method of Synthesizing Bulk Transition Metal Carbide, Nitride, and Phosphide Catalysts

Table 3. Patent applications filed during FY 2015

Inventor	Patent Docket Number	Title
Chengdu Liang	201403349	Electrochemically Stable $Li_7P_2S_8I$ Superionic Conductor
Chengdu Liang	201403404	Polyarene Mediators for Mediated Redox Flow Battery
Chengdu Liang	201303224	All-Solid-State Lithium Carbon Monofluoride Batteries
Sheng Dai and Xiao-Guang Sun	201503486	Nanoconfined Electrolytes and Their Use in Batteries
Mariappan Paranthaman and Amit Naskar	201503528	Carbon-Metal Oxide Composite Materials and Their Use in Anodes of Lithium and Sodium Ion Batteries

Table 3. (continued)

Inventor	Patent Docket Number	Title
Omer Onar and John Miller	201202956	Buffering Energy Storage Systems for Reduced Grid and Vehicle Battery Stress for In-Motion Wireless Power Transfer Systems
William Partridge Jr., James Parks II, and Gurneesh Jatana	201303118	Diagnostic System for Measuring Temperature, Pressure, CO_2 Concentration and H2O Concentration in a Fluid Stream
Clifford White, John Miller, Omer Onar, Paul Chambon, Lixin Tang, and Perry T. Jones	201303196	Overvoltage Protection System for Wireless Power Transfer Systems
Charles Warren, Claus Daniel, Adrian Sabau, Jian Chen, and Donald Erdman III	201403405	Nanostructured Surface Preparation for Joining Dissimilar Materials
Felix Paulauskas and Amit Naskar	200902241	Advanced Oxidation Method for Producing High-Density Oxidized Polyacrylonitrile Fibers
Soydan Ozcan and Amit Naskar	201303091	Method of Manufacturing Tin-Doped Indium Oxide Nanofibers
Zhili Feng and Stan David	201403240	Welding Method for Hydrogen Embrittlement Control
Govindarajan Muralidharan and Bruce Pint	201403395	Alumina-Forming, High Temperature Creep Resistant Ni-Based Alloys
Amit Naskar and Chau Tran	201403426	High Performance Lignin-Acrylonitrile Polymer Blend Materials
Mariappan Paranthaman and Amit Naskar	201503527	Highly Flexible and Low-Cost Conductive Carbon/Polymer Composite Paper as Ultra-Long Cycle Life Pseudocapacitive Electrode

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
Curt Ayers, Steven Campbell, Madhu Chinthavali, Burak Ozpineci, and Randy Wiles	Distinguished Achievement Award for 3D printed electric drive inverter, DOE Vehicle Technologies Office
Robert Bowman	Award for Outstanding Achievement, DOE Fuel Cell Technologies Office
Michael Brady	2015 Brimacombe Medalist Award, The Minerals, Metals, and Materials Society
Tim Burress	Appointed chair for Institute of Electrical and Electronics Engineers Standard 11, "IEEE Standard for Rotating Electric Machinery for Rail and Road Vehicles"
Madhu Chinthavali	Tech-to-market Excellence, Special Recognition from DOE Assistant Secretary for Energy Efficiency and Renewable Energy
Scott Curran	Forest R. McFarland Award, SAE International
	Stefan Pischinger Young Industry Leadership Award, SAE Foundation
Sujit Das	Forest R. McFarland Award, SAE International
	Appointed to the Transportation Research Board Committees on Transportation Economics and Alternative Transportation Fuels and Technologies
Nancy Dudney	Corporate Fellow, ORNL
Zhili Feng	Tech-to-market Excellence, Special Recognition from DOE Assistant Secretary for Energy Efficiency and Renewable Energy
Michael Kass	Appointed to serve on the UL Renewable Energy Council
Jan-Mou Li	Appointed to the Transportation Research Board Urban Transportation Data and Information Systems Committee
Changzheng Liu	Best Presentation at the 28th International Electric Vehicle Symposium and Exhibition
Andreas Malikopoulos	Appointed Secretary, Model Identification and Intelligent Systems Technical Committee, ASME Dynamic Systems and Control Division
James Parks, II	Associate Editor, *Frontiers in Engine and Automotive Engineering*
William Partridge Jr.,	Tech-to-market Excellence, Special Recognition from DOE Assistant Secretary for Energy Efficiency and Renewable Energy
Jun Qu	Associate Editor, *Frontiers in Engine and Automotive Engineering*
Scott Sluder	Lloyd L. Withrow, Distinguished Speaker Award, SAE International
	Editorial Board, *Journal of Fuels and Lubricants*
	Appointed to Government/Industry Meeting General Committee, SAE International
Derek Splitter	Forest R. McFarland Award, SAE International
	2014 Myers Award, SAE International
Gui-Jia Su	Tech-to-market Excellence, Special Recognition from DOE Assistant Secretary for Energy Efficiency and Renewable Energy
James Szybist	Harry L. Horning Award, SAE International
John Thomas	Editorial Board, *Journal of Fuels and Lubricants*

Table 4. (continued)

ORNL Awardee Name(s)	Name/Type of Award
Robert Wagner	Associate Editor, *Frontiers in Engine and Automotive Engineering*
	Co-Editor, *International Journal of Engine Research*
	Appointed to Executive Committee, SAE International Powertrain Fuels and Lubricants Technical Committee
Brian West	Harry L. Horning Award, SAE International
	Appointed to Fellows Selection Committee, SAE International
Martin Wissink	2014 Myers Award, SAE International
Thomas Zawodzinski	Fellow, American Chemical Society
	Royal Academy of Engineering Distinguished Visiting Fellowship

Infrastructure and Facility Investments

New Laboratory for Vehicle Cyber Security R&D. A new laboratory focused on vehicle cyber security has been installed at ORNL's National Transportation Research Center. The Vehicle Cyber Security Laboratory offers a suite of capabilities to assess cyber vulnerabilities while vehicles are in operation. It includes a full vehicle dynamometer with specialized scanning equipment (controller area network communications analysis and calibration tools for electronic control units) in a space with signal isolation, ensuring data integrity. The lab has been established, and major equipment has been installed. C commissioning is scheduled for early FY16.

The new laboratory is part of ORNL's Vehicle Security Center (VSC), which brings together expertise and facilities from across the laboratory to address the emerging national transportation challenge presented by modern vehicles that are increasingly computerized and connected. The VSC assesses potential threat vectors for cyber attack in automotive systems and partners with industry to engineer secure solutions for new vehicles before they hit the road. The main focus of the VSC is predictive assessment.

VSC capabilities include

- prototyping,
- malware discovery,
- large-scale data analysis,
- vehicle security assessment for current and future vehicles,
- anti-tamper and encryption devices,
- authentication and privacy protections,
- reverse engineering of embedded systems, and
- vehicle-based credential generation.

New magnetic properties observation system implemented. A new observation system that provides high-resolution analysis of localized magnetic properties was implemented in the Power Electronics and Electric Machinery Laboratory. The system was designed primarily to investigate properties of soft magnetic materials such as silicon steel laminations that are used in electric motors, but it can also be used on many other types of magnetic materials. This system complements the custom characterization system previously developed by providing higher resolution and therefore increased insight into the fundamental phenomena of electrical steel. The previously developed system is more advantageous for high-level observations.

Dithering flow reactor: new capability in the Fuels, Engines, and Emissions Research Center. Researchers designed, constructed, and commissioned a new automated flow reactor system with fast transient flow control and instrumentation capabilities that enable rapid oscillations in gas composition similar to those seen in exhaust from stoichiometric combustion in gasoline and natural gas engines. Capturing these oscillations, known as dithering, is a key capability for evaluating three-way catalyst materials that will play a critical role in achieving emissions compliance with future high-efficiency engine technologies, such as highly dilute stoichiometric or lean gasoline engines.

ORNL installs new demonstration line in Battery Manufacturing Facility. Scientists completed the installation and trial run of the new battery electrode ultraviolet (UV) curing system with assistance from Conquip and Miltec engineers. Required system modifications are ongoing. The UV curing process promises substantial gains in production efficiency and cost savings of more than 50% vs. conventional solvent-drying systems.

State-of-the-art dynamometer to advance engine research. ORNL is upgrading Engine Cell 5 in the Fuels, Engines, and Emissions Research Center with a state-of-the-art dynamometer to support current and next-generation advanced engine development, including hardware-in-the-loop capability for advanced controls development.

Key Findings Show Benefits of High-Octane Fuels

Contact: Timothy J. Theiss, theisstj@ornl.gov, 865-946-1348

Scientists at ORNL have been working with colleagues at Argonne National Laboratory, the National Renewable Energy Laboratory (NREL), and automakers to assess the benefits of high-octane midlevel (E25 to E40) ethanol blends, barriers to their adoption, and strategies for introducing them. Automakers have long known that boosting the octane level of fuels can translate to performance benefits such as faster acceleration, improved fuel economy, or greater towing capacity. Ethanol, which has a higher octane rating and higher heat of vaporization than gasoline, is an effective octane booster. It has the added benefit of reducing use of petroleum-based fuels and greenhouse gas emissions. Through a series of studies, ORNL, Argonne, and NREL researchers have demonstrated that multiple benefits can be garnered when high-octane midlevel ethanol blends are used in vehicles designed for these fuels with innovations such as direct injection, higher compression ratio, downspeeding, downsizing, and turbocharging.

The following are among the most significant findings and outcomes from the 2-year Bioenergy Technologies Office study, which will end in early 2016.

- Fuel efficiency gains of up to 10% over E10 were demonstrated with high-octane E30 in a vehicle with a turbocharged direct injection engine. Such efficiency gains can offset the lower energy density of high-octane ethanol blends compared to gasoline or E10.

- High-octane midlevel ethanol blends offer a performance benefit (improved acceleration) compared to E10 for most legacy flexible-fuel vehicles, with no engine modifications. This finding could help establish consumer demand for these fuels and ease the transition to a new fueling infrastructure and new vehicles designed for high-octane fuels.

- Using a gasoline blend containing 40% ethanol (E40) generated from cellulosic feedstocks such as corn stover or other nonedible sources of biomass could reduce greenhouse gas (GHG) emissions by 30%. E25 and other ethanol blends were also analyzed, and all lowered GHG emissions compared to fuel with no ethanol, although smaller benefits were realized for lower concentrations of ethanol.

- Compatibility studies confirm that currently available materials are viable for use in the fueling infrastructure with midlevel ethanol fuel blends.

Using models, including ORNL's MA3T (Market Acceptance of Advanced Automotive Technologies), researchers have evaluated the market conditions and potential consumer acceptance for high-octane-fuel vehicles. The studies show these vehicles can be market competitive. They are attractive in part because the fuel they require is projected to cost no more than E10.

Complementary work is continuing under the Bioenergy Technologies Office and Vehicle Technologies Office Co-Optimization of Fuels and Engines Initiative (http://energy.gov/eere/bioenergy/co-optimization-fuels-engines), looking not only at high-octane fuels for advanced spark-ignition engines, but also at exploring new bio-derived fuels for advanced compression-ignition engines.

Publications, Presentations, and Patents

(Note: Where authors were from multiple organizations, ORNL author names have been bolded.)

1. J. F. Thomas, B. H. West, and S. P. Huff. 2015. *Effects of High Octane Ethanol Blends on Four Legacy Flex-Fuel Vehicles and a Turbocharged GDI Vehicle*. ORNL/TM-2015/116, Oak Ridge

National Laboratory, Oak Ridge, Tennessee; available at http://info.ornl.gov/sites/publications/Files/Pub54888.pdf.

2. **T. J. Theiss,** T. Alleman, A. Brooker, A. Elgowainy, G. Fioroni, J.Han, **S. Huff**, C. Johnson, **M. Kass, P. Leiby**, **R. Martinez**, R. McCormick, K. Moriarty, E. Newes, **G. Oladosu, J. Szybist, J. Thomas**, M. Wang, and **B. West.** 2016. *Summary of High-Octane Mid-Level Ethanol Blends Study*. ORNL/TM-2016/42, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3. K. Moriarty, **M. Kass, and T. Theiss**. 2014. *Increasing Biofuel Deployment and Utilization through Development of Renewable Super Premium: Infrastructure Assessment*. NREL/TP-5400-61684, National Renewable Energy Laboratory, Golden, Colorado.

4. B. H. West. 2015. "Higher Ethanol Blends for Improved Efficiency." presented at the National Ethanol Conference, February 20, 2015, Grapevine, Texas.

5. **T. J. Theiss,** R. McCormick, and M. Wang. 2015. "Increasing Biofuel Deployment through Renewable Super Premium." presented at the Energy Future Coalition, March 24, 2015.

6. R. McCormick, **B. West**, M. Wang, and **T. Theiss**. 2015. "Increasing Biofuel Deployment through Use of High Octane Fuels." 25x'25 Webinar, June 18, 2015.

Researchers at the National Transportation Research Center evaluate engine technologies with high-octane fuels using this modified Cadillac ATS.

Groundbreaking ORNL Compatibility Work Used by Industry and Government

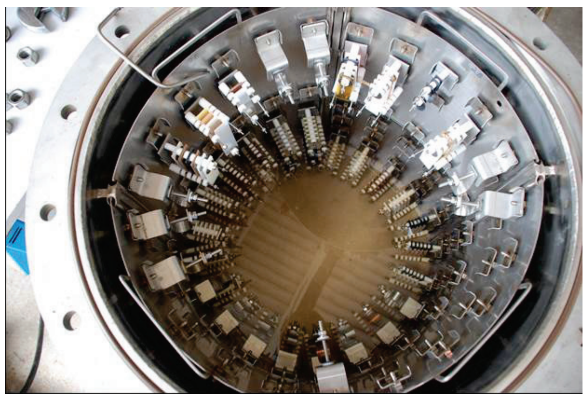
Contact: Mike Kass, kassmd@ornl.gov, 865-946-1241

A key ORNL compatibility study, *Intermediate Ethanol Blends Infrastructure Materials Compatibility Study: Elastomers, Metals, and Sealants* (ORNL/TM-2010/326, 2011), was cited in the July 15, 2015, *Federal Register* [**80**(135): 41566–41683; https://www.gpo.gov/fdsys/pkg/FR-2015-07-15/pdf/2015-15914.pdf] under "Revising Underground Storage Tank Regulations—Revisions to Existing Requirements and New Requirements for Secondary Containment and Operator Training; Final Rule."

ORNL has been conducting fuel compatibility studies over the past 7 years to determine the compatibility of new fuel types (especially biofuels) with existing fuel storage and delivery system infrastructure components. These studies have focused on common elastomers, metals, plastics, and sealants. Properties used to assess compatibility were primarily volume and hardness change, but dynamic mechanical analysis was also performed on selected materials. The results show that oxygenated biofuels such as ethanol and butanol behave similarly. Both alcohol types show heightened solubility to elastomer and plastic seal and hose materials when added to gasoline at intermediate levels (15% to 50%). Bio-oil is also being evaluated as a distillate (i.e., diesel) substitute. Unlike the alcohols, it is not compatible with high-performance elastomers, such as fluorocarbons. It does, however, show good compatibility to lower-cost silicone rubber.

ORNL compatibility work is of great interest to the petroleum and biofuels industries, where compatibility of biofuels with the existing infrastructure is a concern. Industry stakeholders such as the Petroleum Equipment Institute and the American Petroleum Institute have been consulted by ORNL researchers and provided input to the cited ethanol blends report (ORNL/TM-2010/326) and ongoing compatibility studies.

A key outcome of this ORNL work has been the establishment of a large database of compatibility properties that has been used by UL LLC (formerly Underwriters Laboratories Inc.) in developing new listing protocols for dispenser materials.



ORNL conducts studies to determine the compatibility of new fuel types with various materials using specially designed exposure chambers such as this one.

Publications, Presentations, and Patents

1. M. Kass, C. Janke, and T. Theiss, et al. 2015. “Compatibility Assessment of Plastic Infrastructure Materials with Test Fuels Representing E10 and iBu16.” *SAE Int. J. Fuels Lubr.* **8**(1): 95–110; doi: 10:4271/2015-01-0894.

2. M. Kass, C. Janke, and R. Connatser, et al. 2015. “Compatibility Assessment of Elastomeric Infrastructure Materials with Neat Diesel and a Diesel Blend Containing 20 Percent Fast Pyrolysis Bio-Oil.” *SAE Int. J. Fuels Lubr.* **8**(1): 50–61; doi: 10.4271/2015-01-0888.

3. M. Kass, C. Janke, and R. Connatser, et al. 2015. “Compatibility Assessment of Plastic Infrastructure Materials with Neat Diesel and a Diesel Blend Containing 20 Percent Fast Pyrolysis Bio-Oil.” *SAE Int. J. Fuels Lubr.* **8**(1): 80–94; doi: 10.4271/2015-01-0893.

4. M. Kass. 2015. “Compatibility Assessment of Elastomeric Infrastructure Materials with Neat Diesel and a Diesel Blend Containing 20 Percent Fast Pyrolysis Bio-Oil.” presented at the SAE 2015 World Congress, Detroit, Michigan, April 22, 2015.

5. M. Kass. 2015. "Compatibility Assessment of Plastic Infrastructure Materials with Off-Highway Diesel and a Diesel Blend Containing 20 Percent Fast Pyrolysis Bio-Oil." presented at the SAE 2015 World Congress, Detroit, Michigan, April 22, 2015.

ORNL Develops International Fire Codes for the Bioenergy Industry

Contact: Erin Webb, webbeg@ornl.gov, 865-576-4814

Reducing the risk of biomass fires through science-based codes and standards was the focus of a multimember project led by ORNL in collaboration with the American Society of Agricultural and Biological Engineers; Idaho National Laboratory; and industry leaders Abengoa, DuPont, POET, Antares, and Genera Energy.

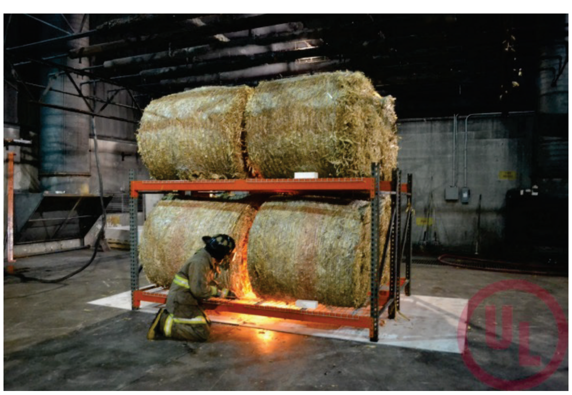
Collectively known as the Biomass Industry Panel for Codes and Standards (BIPCS), the committee has actively influenced the development of international fire codes for the bioenergy industry. Fire risks, both real and perceived, have emerged as a potential barrier to the developing bioenergy industry. Feedstock volumes processed by commercial biorefineries have necessitated new standards that proactively address and ameliorate risks and promote improved safety strategies for the industry.

As part of the BIPCS effort, ORNL conducted experiments at UL LLC (formerly Underwriters Laboratories Inc.) to determine how factors such as feedstock type and bale size, shape, and spacing affect the speed at which a biomass fire can spread. Results showed, for instance, that round bales burn more quickly than square bales.

These studies informed the development of future standards and codes on the safe handling and storage of biomass. The science-based codes and standards reduce risk to people and assets while improving the insurability of biomass facilities.

With support from the DOE Bioenergy Technologies Office, the BIPCS effort has accomplished five code changes to the *International Building Code* to date. The new code changes better reflect current knowledge of biomass properties and conventional and emerging storage, handling, and preprocessing technologies. Changes to the codes include clarifying that biomass is not a hazardous material, adding bioenergy feedstocks to wood chapters, revising design of biomass storage piles, and adjusting the category for sprinkler design.

In addition to code changes, BIPCS also developed training and reference materials for engineers and code reviewers.



ORNL is working with UL to evaluate how feedstock type, bale shape, and bale spacing affect fire intensity under controlled conditions. (Images courtesy of UL.)

Publications, Presentations, and Patents

1. E. Webb. "Addressing Fire Risk in Biomass Handling and Storage." presented at the 2015 ASABE Annual International Meeting, New Orleans, Louisiana, July 27, 2015.

ORNL-Led Consortium Leverages DOE Resources to Advance Biofuels Production; Impacts Feedstock Variations on Carbon Yield, Composition in Pyrolysis Oil

Contact: Stuart Daw, dawcs@ornl.gov, 865-946-1341

ORNL coordinated the Computational Pyrolysis Consortium (CPC), a joint collaboration among the National Renewable Energy Laboratory (NREL), Pacific Northwest National Laboratory, Argonne National Laboratory, Idaho National Laboratory, and several universities to improve the yield and efficiency of catalytic bio-oil upgrading for biofuels production. ORNL coordinated the CPC's public website (http://cpcbiomass.org/), which shared models, data, and simulation results and facilitated collaboration with outside research groups.

Among the results highlighted by the CPC were two low-order modeling methods developed by ORNL to facilitate improved estimation of the impact of different biomass feedstock species and preprocessing levels on the carbon yield and oxygen content of raw bio-oil used for catalytic upgrading. The first method was developed in collaboration with NREL and focused on particle-scale transport and kinetic effects that impact biomass conversion and oil yield during fast pyrolysis. The second method was developed in collaboration with one of the CPC industrial advisors and addressed how to predict the impact of pyrolysis mixing processes on overall conversion and yield. Taken together, the new modeling methods provided a direct computational link between the DOE Bioenergy Technologies Office biomass feedstock interface and the three targeted pathways for pyrolysis-derived biofuels. Open publications describing the modeling methods are listed on the CPC website.

Preliminary analysis of catalytic upgrading of fast pyrolysis bio-oils indicated that this process has the potential to produce significant quantities of bio-derived diesel and gasoline fuels at costs approaching $3.00/gal. However, significant uncertainties remained concerning the costs and performance of the upgrading catalysts, the impact of biomass feedstock variations, and the ability of key reaction steps in the process to be scaled up to commercially relevant sizes. The computational facilities and expertise available across multiple national labs provided unique analytical and predictive capabilities harnessed to address remaining uncertainties, increasing the efficiency and value of ongoing pilot-scale demonstrations at the labs.

The level of lab-to-lab collaboration and coordination on this project set a new standard for minimizing duplication, maximizing efficient use of DOE lab resources, and leveraging capabilities and data across DOE programmatic boundaries. The DOE Bioenergy Technologies Office was the primary supporter of this work with high-performance computing time contributed by the Office of Science and computational tools developed with support from the DOE Fossil Energy Program and the DOE Vehicle Technologies Office.

Acting collectively, the CPC team identified four key areas in bio-oil technology for focusing its efforts: (1) feedstock impact, (2) reactor analysis and scale-up, (3) vapor-phase catalysis, and (4) liquid phase catalysis.

In addition, a special team of industry advisors was established to review progress and ensure that the lab activities maintained their commercial relevance. The CPC provided a model for future multilab and multiprogram contributions to strategic DOE objectives, public information transfer, and direct collaboration among lab, industry, and university partners.

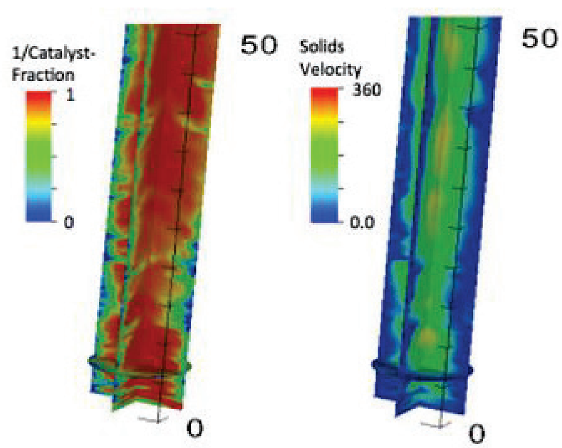
Publications, Presentations, and Patents

1. T. R. Braun, A. Dutta, and J. Ziegler. 2014. "One Dimensional Steady-State Circulating Fluidized-Bed Reactor Model for Biomass Fast Pyrolysis." *Fuel* **133**: 253–262.

2. E. Ramirez, C. S. Daw, S. Pannala, J. Halow, C. E. A. Finney, and J. Galvin. 2014. "Computational Analysis of Biomass Particles in a Bubbling Bed." presented at the 2014 AIChE Annual Meeting, Atlanta, Georgia, November 16–21, 2014.

3. G. Wiggins, C. S. Daw, and J. Halow. 2014. "Low-Order Modeling of Biomass Particle Mixing and Reaction in a Bubbling-Bed Fast Pyrolysis Reactor." presented at the 2014 AIChE Annual Meeting, Atlanta, Georgia, November 16–21, 2014

4. J. L. Ziegler, S. Pannala, D. J. Robichaud, and M. R. Nimlos. 2015. "3D Multiphase Gas/Particle Flow Modeling for Reactor-Scale Biomass Conversion and Upgrading Simulations: Heat Transfer, Mixing, and Basic Deactivation Modeling in Fixed, Bubbling, and Fluidized Bed Reactors." presented at the 2014 NETL Workshop on Multiphase Flow Science, Morgantown, West Virginia, August 12–13, 2015.



Maps of instantaneous void fraction (inverse of catalyst fraction) and catalyst velocity in a lower riser section from 3D computational fluid dynamics simulations.

Study Explains Underlying Process Behind Biofuel-to-Hydrocarbon Conversion Technology

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

ORNL researchers have explained the mechanism behind a technology that converts bio-based ethanol into hydrocarbon blend-stocks for use as fossil fuel alternatives.

Scientists have experimented for decades with a class of catalysts known as zeolites that transform alcohols such as ethanol into higher-grade hydrocarbons. As ORNL researchers were developing a new type of zeolite-based conversion technology, they found that the underlying reaction unfolds in a different manner than previously thought.

It has been long thought that these types of reactions must first go from ethanol to ethylene, and then on to form longer chains. ORNL's research showed that this energy-consuming intermediary step is not necessary for the conversion to happen. Instead, a “hydrocarbon pool” type mechanism allows the zeolite catalysts to directly produce longer hydrocarbon chains from the original alcohols.

ORNL researchers tracked the molecular transition in labeling experiments with deuterium, a hydrogen isotope, to confirm the hydrocarbon pool mechanism.

The research, supported by DOE’s Bioenergy Technologies Office, has implications for the energy efficiency and cost of catalytic upgrading technologies proposed for use in biorefineries. Uncovering the mechanism behind the reaction helps support the potential economic viability of ORNL’s direct biofuel-to-hydrocarbon conversion approach. The ORNL technology is a new pathway to biomass-derived renewable fuels, lowering greenhouse gas emissions, and decreasing US reliance on foreign sources of oil.

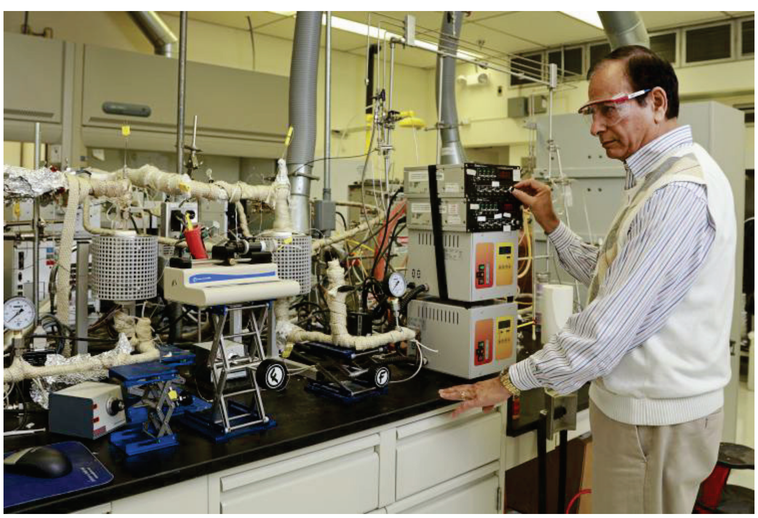
The ORNL-developed catalyst and conversion process were licensed in 2014 to Vertimass, a startup company based in Irvine, California. ORNL researchers are working with Vertimass through a separate DOE-funded project to scale the technology to the commercial level.

In addition, ORNL analysis in collaboration with the National Renewable Energy Laboratory shows the catalytic technology could be retrofitted into existing bio-alcohol refineries at various stages of ethanol purification. The direct conversion process produced minimal amounts of ethylene by-product, making the technology more cost-effective than previous approaches. The ORNL team’s lab-scale tests also indicated that the catalyst can operate at relatively low temperatures and pressures and can be regenerated under mild conditions, helping the technology withstand long periods of operation without significant degradation.

The technology uses an inexpensive zeolite catalyst to transform ethanol into hydrocarbon blend-stock. The resulting liquid is blended at various concentrations into gasoline, diesel, and jet fuels without negatively affecting engine performance. After being mixed with petroleum-derived fuels, the blend-stock does not require modifications to the existing distribution infrastructure. This technology is a pathway to overcoming the ethanol blend wall.

Publications, Presentations, and Patents

1. C. Narula, Z. Li, E. Casbeer, R. Geiger, M. Moses-Debusk, M. Keller, M. Buchanan, and B. Davison. 2015. “Heterometallic Zeolite, InV-ZSM-5, Enables Efficient Conversion of Biomass Derived Ethanol to Renewable Hydrocarbons” *Scientific Reports* **5**: 16039 [Highlighted in *Science*, 2015, 350, 1329].



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

ORNL Completes Pilot Phase of System to Thwart Fuel Tax Evaders

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

Researchers at ORNL, working with partners from private industry, have completed the pilot phase of testing an integrated monitoring system that can track the movement of fuel tankers in real time and flag suspicious activity. The goal of the research was to provide a proof-of-concept system to identify illegal blending of nontaxable petrochemical products with taxable fuel products and cross-jurisdictional fuel tax evasion (FTE).

Revenues from motor fuel and other highway use taxes are the primary source of funding for the US transportation system, and ensuring that all of these taxes are collected, remitted, and credited to the Highway Trust Fund remains a priority for the DOT Federal Highway Administration (FHWA). While the exact figure is not known, more than $1 billion of revenue is estimated by FHWA to be lost each year to FTE.

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. About half of the states in the United States have the same point of taxation. For the remaining states, the point of taxation is at the wholesaler/distributor level or below. This has caused additional challenges in tracking untaxed fuel after it leaves bulk storage. Approaches to preventing FTE are time-consuming, along with attempts 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 late 2014. Data from the systems were processed daily. In 2015, data collections were completed. The pilot demonstration was performed for FHWA, state auditors, and enforcement personnel. More than 1,000 loads were monitored over the 8-month period. The system logged 374,453 miles and 7.5 million gallons of transported fuel.

The results of the pilot are expected to inform possible FHWA rulemaking on tracking and monitoring equipment. This system could also be used to track other kinds of goods as it is good for real-time tracking where suspicious or unusual activity needs to be flagged.

Overall, 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, and a query tool was developed for use by state and federal auditors.

ORNL researchers developed a supply-chain-based system that tracks fueling stops, loading, and unloading, providing near-real-time notification of any variation in standard delivery processes from the tanker's point of origin to its final destination.

Publications, Presentations, and Patents

None to report this period.

Private and Secure Connected Vehicle Communications Leads to Safer Transportation

Contact: Jason Carter, carterjm@ornl.gov, 865-574-1480

Connected vehicle technology has the potential to reduce accidents by 81% according to a study by the DOT. With the potential to save lives, save money, and even save fuel, connected vehicle technology is a "game changer" according to the ORNL Cyber and Information Security Research Group (CISR).

CISR has assisted DOT on connected vehicle research since 2012. ORNL's work was cited in DOT's 2014 proposed rulemaking announcement regarding the potential regulation of vehicle-to-vehicle and vehicle-to-infrastructure connectivity.

The project was supported by the National Highway Transportation Safety Administration, the Federal Highway Administration, and the Intelligent Transportation Systems Joint Program Office.

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

Before this can happen, however, several challenges associated with the technology must be addressed, and ORNL has worked with DOT to be proactive in examining security and privacy.

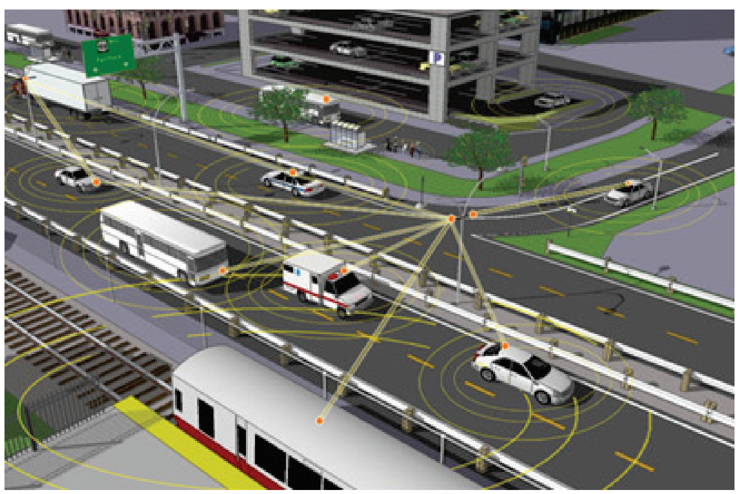
ORNL worked with DOT on the security side to research the means of ensuring the validity or trustworthiness of the messages exchanged between vehicles without revealing identifying information. Authenticating message broadcasts is a complex problem made more complicated by the size of the proposed deployment. After implementation, the credential management system will be the largest system of its kind, dwarfing a similar DOD system for information exchange.

ORNL's role was to assess the feasibility of building this type of system with the trust/validation function delegated to the vehicles, including investigating the various technical solutions to make the approach feasible. The ORNL team delivered a concept of operations for the vehicle-based system.

ORNL also researched how this technology can best preserve privacy while meeting the promise of improved safety and security. Privacy-preserving data publishing strategies were developed to remove or modify certain identifying characteristics within data streams and sets that will be used for future research and development, so the likelihood of the data being associated with a particular individual is reduced while the usefulness of the data is retained. The ORNL team developed an algorithm to successfully automate this process for vehicle trajectory data collected from pilot studies. They also examined how additional designed-in privacy techniques can be integrated into future operational connected vehicle technology.

Publications, Presentations, and Patents

1. J. M. Carter, N. Paul, and J. Zhang. 2015. "Analysis of Vehicle-Based Security Operations." in Proceedings of the 24th International Technical Conference on the Enhanced Safety of Vehicles (ESV), June 8–11, 2015, Gothenburg, Sweden, Paper 15-0457 (PTS #55304); http://www-esv.nhtsa.dot.gov/Proceedings/24/files/24ESV-000457.PDF.



ORNL assisted DOT with the development of a vehicle-based credential management system that can increase safety and security while maintaining privacy in vehicle-to-vehicle and vehicle-to-infrastructure communications. Image courtesy of Department of Transportation.

Wireless Roadside Inspection Project Improves Safety and Efficiency for Trucks and Buses

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

Safety inspections of commercial motor vehicles (CMVs) are critical to promoting safety on the roadways. Currently, safety inspectors in the United States perform about 3.4 million CMV inspections per year. The use of a wireless inspection method could dramatically increase the number of safety inspections without the need for additional enforcement personnel or new roadside infrastructure. Key data such as driver licensing and medical card, carrier and load information, and on-road hours are collected remotely through the Wireless Roadside Inspection (WRI) system developed by ORNL in partnership with industry. WRI allows this virtual inspection to occur without requiring the driver to stop. Routine inspections at weigh stations could supplement wireless inspections by further investigating trucks with questionable WRI data and trucks randomly selected for hands-on inspection.

ORNL developed a system to collect and evaluate CMV safety data, working with a producer of onboard electronic recorder technology to develop software compatible with in-cab devices routinely used by the trucking industry.

WRI is similar to weigh station bypass in that it uses red/yellow/green light in the cab to indicate whether the driver can continue driving, pass through a station, or stop to see an inspector. The WRI system differs because it gathers safety and compliance data from all participants in addition to managing which trucks receive a hands-on inspection.

Overall, the WRI system is expected to increase the number of inspections and decrease the number of unsafe CMVs on the road. WRI speeds up the inspection process, enabling more inspections to occur, minimizing wait times, and reducing fleet costs. Since WRI is triggered when CMVs pass by designated geographic coordinates along the roadways, the system would make it far more unlikely that drivers could avoid inspection.

The WRI team has completed the first two phases of the project: (1) evaluation of commercially available off-the-shelf or near-off-the-shelf technology to validate the wireless inspection concept; and (2) pilot testing, safety technology maturation, and back office system integration. The project is now entering Phase 3, the field operational test with a group of vehicles travelling a multiple-state instrumented corridor.

Publications, Presentations, and Patents

1. G. J. Capps, O. Franzese, H. Knee, R. Plate, and M. B. Lascurain. 2009. *Wireless Roadside Inspection Proof of Concept Test Final Report*. ORNL/TM-2008/128. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

2. G. J. Capps, 2013. “Wireless Roadside Inspection Field Test.” Tennessee Trucking Association Quarterly Meeting.

The Wireless Roadside Inspection system remotely evaluates safety records of vehicles moving on the highways and flags trucks that are unsafe.

Analysis of Hydrogen Fuel Cell Onboard Storage Pressure

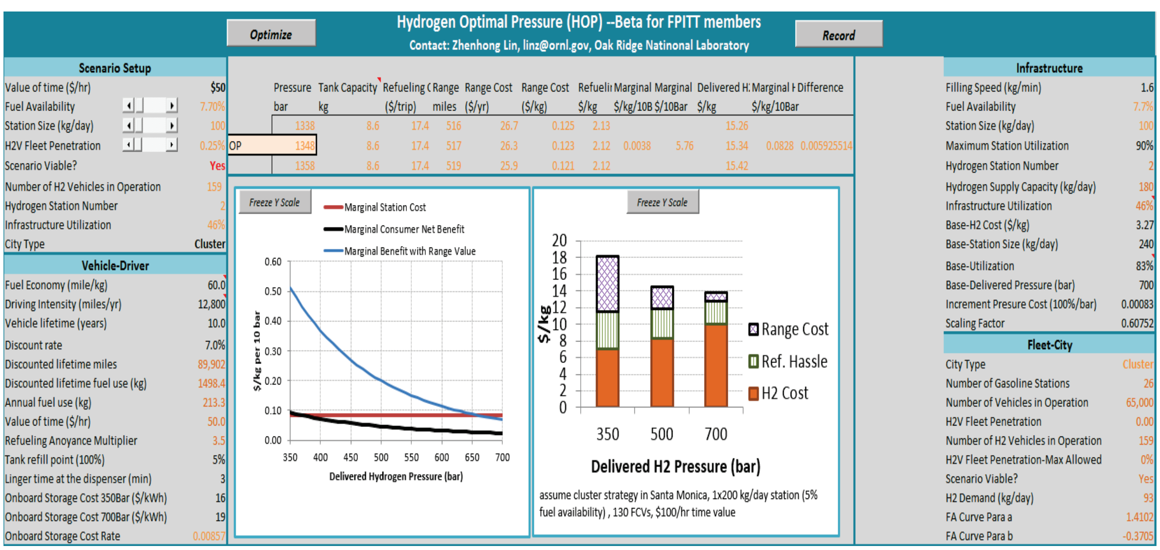
Contact: Zhenhong Lin, linz@ornl.gov, 865-946-1308

Fuel cell electric vehicles (FCEVs) are among the transportation options DOE is exploring to reduce greenhouse gas emissions and dependence on fossil fuels. Many issues have to be resolved before FCEVs can compete with traditional internal combustion engines or even battery electric vehicles. One of these relates to the onboard storage pressure of the hydrogen.

Higher hydrogen storage pressure allows more hydrogen to be stored on board, enabling a longer driving range between hydrogen refills, but the cost of the hydrogen supply infrastructure, and therefore the delivered cost of hydrogen, will be higher. Lower hydrogen storage pressure shortens the driving range and results in higher refueling frequency, and the range limitation cost can be higher. However, the lower capital cost of low-pressure stations (the infrastructure) may encourage investment in developing more stations, resulting in better refueling convenience for consumers and lower delivered hydrogen cost.

The purpose of this project is to develop an optimization model to identify the delivered pressure of hydrogen that best reflects the tradeoff among hydrogen cost, infrastructure capital cost requirements, onboard storage cost, driving range, refueling frequency, and refueling convenience in such a way as to maximize consumer acceptance of hydrogen vehicles and then analyze the results and recommend delivered hydrogen pressure as a function of technology cost, regional geography, hydrogen demand, driver types, and driving patterns. The model and findings can inform decisions affecting storage and market transformation barriers.

Based on the method developed for the hydrogen pressure analysis, a hydrogen optimal pressure (HOP) model with a user-friendly interface was implemented in Microsoft Excel. Model inputs are organized into three groups: Vehicle-Driver, Infrastructure, and Fleet-City. HOP model users can use the interface to examine in real time how the marginal cost curves shift up and down and how cost components of 350 bar (about 5,000 lb/in.^{2}), 500 bar (about 7,252 lb/in.^{2}), and 700 bar (about 10,000 lb/in.^{2}) vary with changes of any input parameter.



Beta version of the interface for the HOP model. Left chart: marginal cost curves. Right chart: variations in cost components with changes of input parameters.

Over the 3 years of the project, the optimal pressure has varied due to different parameters and contexts. For example, FY 2013 results found 700 bar (about 10,000 lb/in.^{2}) to be more desirable in many region-strategy scenarios. FY 2014 results demonstrated that 350 bar or 500 bar can be more competitive in reducing system cost in certain cluster strategy scenarios. FY 2015 results show strong preferences for 700 bar over 350 bar or 500 bar because 700 bar is the only one among the three pressure levels to enable the greater than 300-mile range required for maximum ZEV (California Air Resources Board zero emission vehicle) credits. The ZEV credit, based on available credit trading information, is so valuable that the ZEV credit value becomes a dominating factor in the optimization, regardless of driver types. In addition, the longer driving range of 700-bar tanks (360 miles vs. 200–300 miles for 350- and 500-bar tanks) can be valuable to consumers with frequent long-distance and away-from-station-cluster trips.

More research is needed on identifying the optimal pressure for early adopters of FCEVs, for maximizing FCEV market acceptance, and for standardization concerns. In 2016, the study will systematically investigate the optimal delivered hydrogen pressure with respect to how it is affected by parameters from the driver, vehicle, and hydrogen-refueling station categories. The interface for the HOP model will be further improved and will be used for analysis of the uncertainty of key parameters such as fuel economy, pressure incremental station cost, and driving intensity.

Publications, Presentations, and Patents

1. Z. Lin and C. Liu. 2015. "Analysis of Optimal Onboard Storage Pressure for Hydrogen Fuel Cell Vehicles." presented at the 2015 DOE H^2 Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting, Washington, DC, June 8–12, 2015.

Imaging and Microanalysis of Thin Ionomer Layers Using Advanced Microscopy Techniques

Contact: David A. Cullen, cullenda@ornl.gov, 865-356-3400

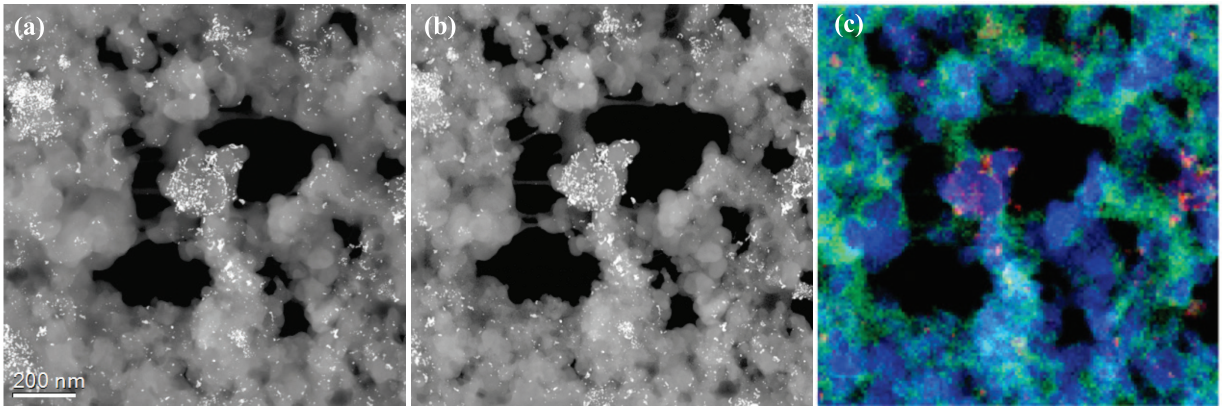
Many features of fuel cells make them attractive as power sources for vehicles, but currently they are too expensive to be viable commercial replacements for internal combustion engines. Among the strategies for making them more cost-competitive is improving catalyst performance to decrease the amount of the expensive platinum-group metals needed in the catalysts.

It is known that the percolating ionomer phase within a fuel cell electrode plays a critical role in mass transport and electrochemical kinetics within the catalyst layer. Distribution of the ionomer (thickness, morphology, contact with carbon and platinum) determines the electrochemical surface area and therefore the high-voltage and high-power performance of the fuel cell. Understanding ionomer dispersions within catalyst layers as a result of processing methods is thus important for achieving high-performing catalysts.

ORNL staff and colleagues at the General Motors R&D Center; the University of Georgia; North Carolina State University; and CEA [the (French) Alternative Energies and Atomic Energy Commission], Grenoble, France, undertook a study using high-resolution scanning transmission electron microscope (STEM) imaging combined with compositional mapping to visualize and quantify the ionomer distributions within catalyst layers. To perform such studies, proper imaging protocols (temperature, voltage, and electron dose) were established to minimize beam damage during STEM.

To date, optimized conditions for imaging and spectroscopic analysis of perfluorosulfonic acid ionomer thin films within fuel cell electrodes have been investigated. Model systems comprising thin ionomer films of varying thickness applied to platinum surfaces were used to establish the proper STEM conditions for analysis. These conditions were then applied to quantitatively assess the through-thickness ionomer loadings of actual catalyst electrode layers prepared via different synthesis methods.

Additionally, high-resolution compositional mapping has been performed to show nonhomogeneous ionomer distributions within electrode structures.



STEM images acquired from a fuel cell electrode (a) before and (b) after acquisition of an energy-dispersive spectroscopy (EDS) image and (c) principal component analysis of the EDS image showing the different components in the image (catalyst support = blue, ionomer = green, platinum = red).

Publications, Presentations, and Patents

1. D. A. Cullen, R. Koestner, R. S. Kukreja, Z. Y. Liu, S. Minko, O.Trotsenko, A. Tokarev, L. Guetaz, H. M. Meyer, C. M. Parish, and K. L. More. 2014. "Imaging and Microanalysis of Thin Ionomer Layers by Scanning Transmission Electron Microscopy." *Journal of the Electrochemical Society* **161**: F111–F1117; doi: 10.1149/2.1091410jes.

Impact of Iridium-Ruthenium Oxygen Evolution Reaction Catalysts on PEMFC Electrode Catalysts

Contact: David A. Cullen, cullenda@ornl.gov, 865-356-3400

Polymer electrolyte membrane fuel cells (PEMFCs) have numerous applications, but they are particularly attractive for transportation applications because of their high power density and low weight. PEMFCs are more efficient than internal combustion engines, and their only emissions are water and heat, making them very environmentally friendly. However, because they typically use platinum group metal (PGM) catalysts, their costs are too high for market acceptability. Attempts to lower the PGM content and thus cost have run into durability problems, particularly under transient conditions such as start-up or shutdown (SU/SD)

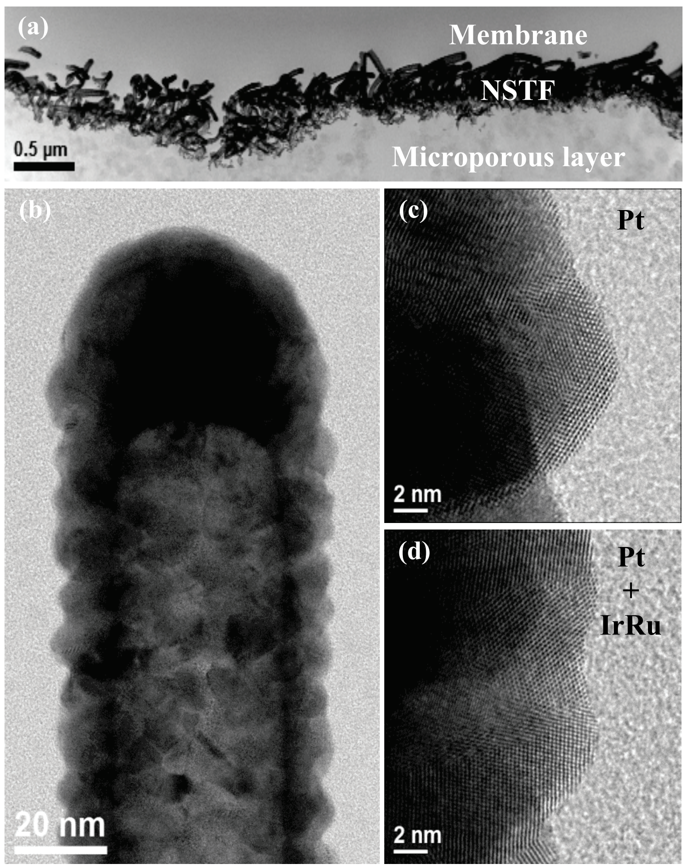
ORNL is working with a team that includes 3M, Argonne National Laboratory, and Los Alamos National Laboratory to address these issues.

In 2015, the team used advanced analytical electron microscopy techniques to study the effects of using oxygen evolution reaction (OER) catalysts to modify PEMFC anode and cathode catalysts to lower the overpotential for oxidation of water during transient conditions such as SU/SD. Keeping the electrode potential as close as possible to the thermodynamic potential of the OER leads to greater robustness and durability (i.e., increased catalyst stability and reduced degradation of the components of the fuel cell).

Different loadings of ruthenium and iridium OER catalysts were incorporated onto 3M's unique platinum nanostructured thin film (NSTF) catalyst. Aberration-corrected scanning transmission electron microscopy (STEM) was used to investigate the chemistry and structure of the iridium and ruthenium catalysts and the platinum NSTF (Pt-NSTF) catalysts before and after SU/SD testing. The results demonstrated that OER catalysts greatly improve the durability of Pt-NSTF catalysts by limiting platinum dissolution and that an OER catalyst loading of 2 μgcm^{-2} provided the optimal balance between performance, durability, and cost. Results of the atomic-scale investigations could provide new insights regarding fuel cell degradation mechanisms such as catalyst particle coalescence, platinum dissolution, and alloying.

Publications, Presentations, and Patents

1. D. A. Cullen, K. L. More, L. L. Atanasoska, and R. T. Atanasoski. 2014. "Impact of IrRu Oxygen Evolution Reaction Catalysts on Pt Nanostructured Thin Films under Start-up/Shutdown Cycling." *Journal of Power Sources* **269**: 671–681; doi: 10.1016/j.jpowsour.2014.06.153.



Bright field STEM images of (a) Pt-NSTF cathode layer in a membrane electrode assembly, (b) an individual Pt-NSTF whisker, (c) platinum surface without iridium-ruthenium catalyst modified by the oxygen evolution reaction (OER), and (d) platinum surface with epitaxially grown Ir-Ru OER catalyst.

Melt-Spun Polyacrylonitrile for High-Strength Compressed Hydrogen Storage Systems

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

High-strength carbon fiber (CF) enables the manufacture of durable, lightweight compressed hydrogen storage vessels for use in high-pressure storage and other clean energy applications. Unfortunately, current high-strength CF products are too expensive to meet DOE cost objectives—that is, too expensive for automotive applications. Melt-spun precursor has the potential to make a significant impact not only on the cost of the CFs used in hydrogen storage, but also on the cost of CFs used in the high-performance composites industry, including CF composites for vehicle body parts.

The technology typically employed for producing CF, known as "wet or solution spinning," uses expensive, highly corrosive solvents and requires costly, time-consuming solvent recovery. Melt spinning avoids the significant costs entailed in handling and recovering the solvents used in solution spinning; it also eliminates a significant bottleneck in production caused by the time, space, and energy needed for the solvent recovery steps. Because of this, it is anticipated that the melt-spinning approach could save 25% of the costs associated with producing CF for high-pressure gas storage systems and that additional savings may be possible in combination with ORNL-developed advanced conversion approaches. It is also projected that the melt-spinning process would be more attractive for polyacrylonitrile (PAN) fiber production in the United States, possibly helping to revitalize some of the acrylic fiber business lost due to environmental concerns.

However, melt processing of a PAN precursor is a difficult issue because PAN degrades, even without main-chain scission or weight loss, and this essentially precludes melt processing with existing technology. ORNL and its partner, Virginia Tech, are addressing this in a strategy that builds on past patents and publications, ORNL's decades-long CF R&D experience, and the capabilities of the Carbon Fiber Technology Facility.

A major milestone was achieved in 2015 with demonstration of CF properties exceeding the DOE go/no-go point of 15 Msi modulus and 150 ksi strength. Properties meeting follow-on milestone levels up to 25 Msi modulus and 250 ksi strength were also achieved. These properties were achieved with melt-spun PAN produced at Virginia Tech and using a conversion protocol developed by ORNL in previous work. 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. Currently this work is being scaled up to continuous processes that are projected to meet project technical and economic targets for producing significantly lower cost CF for high-pressure storage of hydrogen.

Publications, Presentations, and Patents

None to report this period.

Carbon Fiber Technology Facility pilot line being upgraded for automated operation and production of high-strength CF.

Analysis

MA^{3}T Model Continues to Grow in Richness and Use

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

Understanding the diverse purchasing behaviors of individuals is key for designing efficient and effective policies for promoting advanced vehicle technologies. To address this need, ORNL developed Market Acceptance of Advanced Automotive Technologies (MA^{3}T), a market simulation model for the DOE Vehicle Technologies Program. Implemented using Microsoft Excel and cored with the nested multinomial logit model, MA^{3}T simulates market demand for advanced vehicle technologies by representing relevant attributes of technologies and consumer behavior such as technological learning by doing, range anxiety, access to recharging points, daily driving patterns, and willingness to accept technological innovation. Much remains to be learned about how consumers will evaluate novel vehicle technologies and how these technologies are likely to be accepted and used. Because of this, the approach taken in developing the MA^{3}T model was to create a framework for integrating data and behavioral models at an appropriate level of detail, whether all data were available or the behaviors were fully understood. MA^{3}T projections currently cover the period from 2005 to 2050 and capture the temporal interaction between market penetrations and product diversity and risk.

Programmed with Visual Basic for Applications in Microsoft Excel, the model can run on computers with Microsoft Excel 2010 or newer versions. As more is learned about advanced vehicle technologies and consumer preferences toward them, the model is being updated and improved.

During FY 2015 the following updates/improvements were made.

- The representation of natural gas vehicles and state policies in MA^{3}T was improved.
- Technical documentation was updated.
- An updated version of MA^{3}T was released with the latest energy price and vehicle data.

In addition, a number of tasks to make MA^{3}T more useful and user friendly were completed, including establishing systematic calibration and validation processes and completing major structure upgrades and interface improvements.

MA^{3}T has been used in a wide variety of studies over the years, including, in 2015, the multilaboratory BaSce evaluation of the benefits of DOE Vehicle Technologies Office technologies and programs; the University of California, Davis, energy modeling project for the California Energy Commission; multiple ORNL studies; the International Institute for Applied Systems Analysis MESSAGE modeling framework; and the Tsinghua University Beijing, energy-vehicle market analysis for Honda.

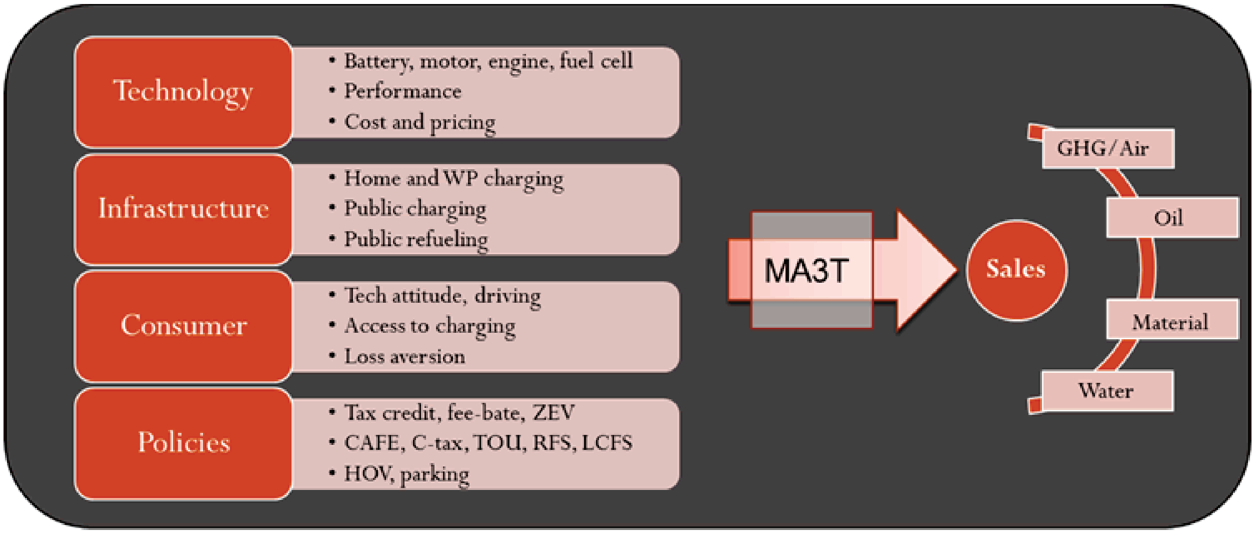
The MA^{3}T team started development of an MA^{3}T “MiniTool” in 2015. Scheduled for release in 2016, the MiniTool will be a lighter, web-based version with a more user-friendly interface for both technical and nontechnical users. With the MiniTool, users will be able to efficiently check and download MA^{3}T outputs and learn about major functions of MA^{3}T online.

The current version of the model can be requested by contacting Zhenhong Lin (linz@ornl.gov).

Publications, Presentations, and Patents

1. E. Kontou, Y. Yin, and Z. Lin. 2015. "Socially Optimal Electric Driving Range of Plug-In Hybrid Electric Vehicles." *Transportation Research Part D: Transport and Environment* **39**: 114–125; doi: http://dx.doi.org/10.1016/j.trd.2015.07.002.

2. X. Wu, M. Aviquzzaman, and Z. Lin. 2015. "Analysis of Plug-In Hybrid Electric Vehicles' Utility Factors using GPS-Based Longitudinal Travel Data." *Transportation Research Part C: Emerging Technologies* **57**: 1–12; doi: http://dx.doi.org/10.1016/j.trc.2015.05.008.



MA^{3}T model framework.

ORNL Fuel Economy Information Project Accomplishments

Contact: Bo Saulsbury, saulsburyjw@ornl.gov, (865) 574-4694

The Fuel Economy Information (FEI) team developed and deployed "Selecting the Right Octane Fuel" on www.fueleconomy.gov. As part of creating these tips for the public, ORNL researchers evaluated the Ford Fiesta 1.0 turbocharged GDI with both regular and high-octane fuel. The research results provided a data source for the fueleconomy.gov octane tips and were published in a report along with companion results from a high-octane study supported by the DOE Bioenergy Technology Office. Researchers also presented the research data at the National Ethanol Conference.

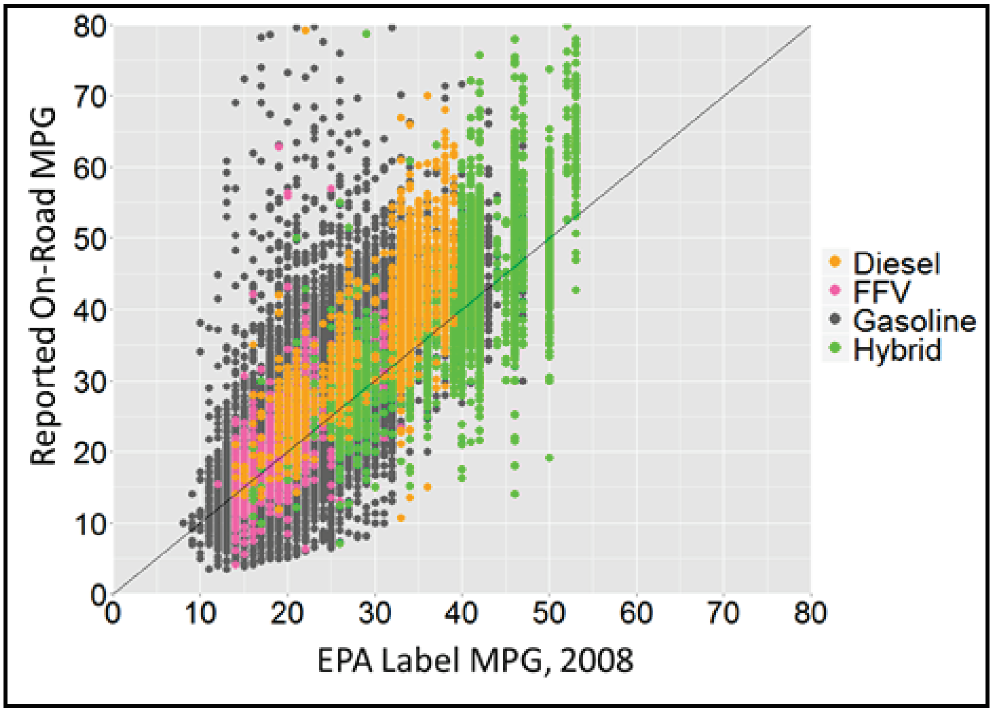
FEI project team members worked with the University of Tennessee and the Virginia Department of Transportation to conduct and publish the study *How Do Motorists' Own Fuel Economy Estimates Compare with Official Government Ratings? A Statistical Analysis*. The study used data from www.fueleconomy.gov "My MPG" database and was a follow-up to the 2011 study *Predicting Individual On-Road Fuel Economy Using Simple Consumer and Vehicle Attributes*.

The FEI project also released seasonal fuel economy tips to media contacts. "Cold Weather Fuel Economy Tips" was featured in several national and local media outlets, including *The Detroit Free Press* and Bankrate.com, while "Save Money on Summer Driving" received coverage from *USA Today, The Detroit Free Press, CBS News,* and numerous local media outlets.

Publications, Presentations, and Patents

1. B. West, 2015. "Higher Ethanol Blends for Improved Efficiency." Presented at the National Ethanol Conference, *Road to Higher Blends Panel*. Grapevine, Texas. February 20.

2. J. Thomas, B. West, and S. Huff. 2015. *Effects of High-Octane Ethanol Blends on Four Legacy Flex-Fuel Vehicles and a Turbocharged GDI Vehicle*. ORNL/TM-2015/116. March.



My MPG on-road estimates vs. EPA label estimates of miles per gallon for all vehicle types.

Combustion, Engines, and Fuels

Advanced Control Strategies Key to Extending Dilution Limits in Light-Duty Vehicles

Contact: Brian Kaul, kaulbc@ornl.gov, 865-946-1299

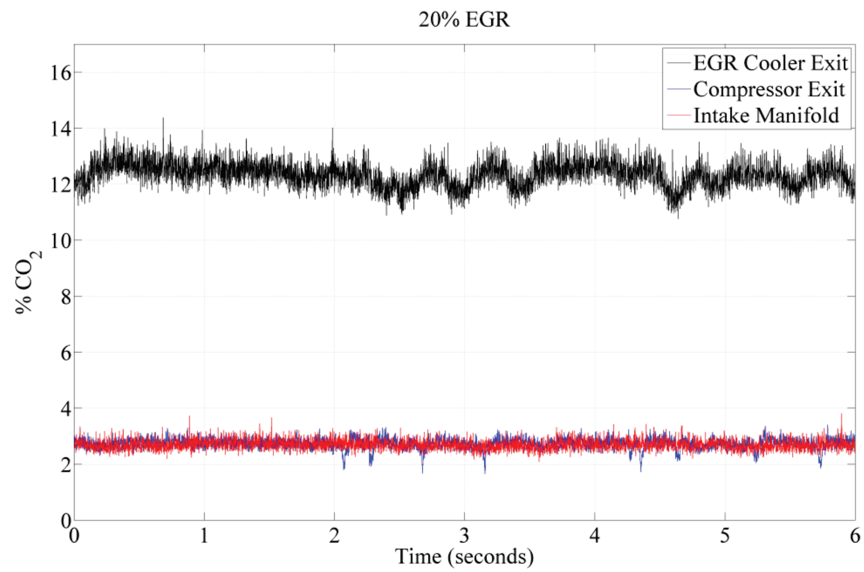
ORNL is working with industry partners to improve light-duty vehicle fuel economy and to reduce emissions through control strategies that enable high-efficiency, high-dilution gasoline direct injection engine operation. An ancillary goal is to extend the exhaust gas recirculation (EGR) dilution limit for even greater gains.

Operating spark ignition engines with high levels of charge dilution through EGR achieves significant fuel efficiency gains and emissions improvements, but dilution is limited by cyclic variability. The closer you get to the theoretical limit of dilution (the so-called “edge of stability”), the greater the cyclic variability/instability, including misfires. This is especially true at the low engine loads typical of standard light-duty drive cycles. As a result, most engines are operated well away from the edge of stability to avoid these consequences, thus failing to achieve the full benefits of charge dilution.

ORNL researchers have determined that the cyclic variability encountered at the dilution limit is not random and that it is influenced by prior engine cycles. Using tools derived from chaos theory, the dynamics of systems using cooled EGR loops have been elucidated for the first time, and recurring patterns in cycle-to-cycle variations have been identified. This knowledge is being used to stabilize combustion near the dilution limit through control strategies based on the events of previous cycles.

In related studies it was found that for high EGR levels, significant changes in the recirculated exhaust gas CO_2 composition are carried through to the intake manifold and influence the events of future engine cycles. However, at lower EGR levels variations in composition are “damped out” before reaching the intake manifold and hence do not have the same impact on future cycles. Based on these findings, a strategy for predicting next-cycle effects has been devised and implemented on a test engine with good results at very high EGR levels, and alternate strategies were tested, with success, for moderate EGR levels. In addition, experiments have been conducted to gain further understanding of the impacts of other factors such as spark timing and spark restrike.

To achieve further improvement, more advanced, model-based control strategies will be pursued in the future, including collaboration in FY 2016 with an existing high-performance computing–based effort to develop control-oriented models (see “Using High-Performance Computing to Accelerate Engine Development” elsewhere in this report).



Carbon dioxide concentration measurements for 20% exhaust gas recirculation.

Publications, Presentations, and Patents

1. T. Wallner, J. M. Sevik, Jr., R. Scarcelli, B. C. Kaul, and R. M. Wagner. 2015. "Effects of Ignition and Injection Perturbation Under Lean and Dilute GDI Engine Operation." SAE Technical Paper 2015-01-1871, 2015, doi:10.4271/2015-01-1871.

2. C. S. Daw, C. E. A. Finney, B. C. Kaul, K. D. Edwards, and R. M. Wagner. 2015. "Characterizing Dilute Combustion Instabilities in a Multi-Cylinder Spark-Ignited Engine Using Symbolic Analysis." *Phil. Trans. R. Soc. A*. **373**(2034), doi: 10.1098/rsta.2014.0088.

3. C. E. A. Finney, B. C. Kaul, C. S. Daw, R. M. Wagner, K. D. Edwards, and J. B. Green, Jr. 2015. "A Review of Deterministic Effects in Cyclic Variability of Internal Combustion Engines." *International J. of Engine Research* **16(**3): 366-378; doi: 10.1177/1468087415572033.

4. B. C. Kaul, B. J. Lawler, C. E. A. Finney, M. L. Edwards, et al. 2014. "Effects of Data Quality Reduction on Feedback Metrics for Advanced Combustion Control." SAE Technical Paper 2014-01-2707, doi: 10.4271/2014-01-2707.

Cross-Cut Lean Exhaust Emissions Reduction Simulations Analysis and Coordination

Contact: C. Stuart Daw, dawcs@ornl.gov, 865-946-1341; Josh A. Pihl, pihlja@ornl.gov, 865-946-1524

As a result of advanced combustion research, in recent years there have been some amazing increases in internal combustion engine efficiencies and reductions in harmful greenhouse gas emissions. However, meeting the more stringent emissions regulations will require a combination of advanced emissions control devices and the computational tools needed to understand and predict their function. Recognizing this need, the DOE Advanced Engine Cross-Cut Team initiated the Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) activity to support the development of improved computational tools and data for high efficiency engines and associated emissions control systems. DOE provides funding to ORNL to perform two complementary roles that support this goal: (1) administrative coordination of

CLEERS collaborations among national laboratories, industry, and academia and (2) focused measurement, analysis, and modeling aimed at developing the strategies, data sets, and device parameters needed to address the most critical technological barriers faced by advanced emissions control systems.

In its administrative role, ORNL serves as the primary interface with a planning committee composed of experts from national laboratories, industry, and academia; facilitates monthly technical teleconferences for an industry-academia focus group; organizes annual public workshops; conducts a biannual industry survey; and maintains a website for exchanging public data and information related to emissions controls (http://www.cleers.org). ORNL also acts as a clearinghouse for pre-proprietary information and reports, provides oral and written status reports to the Crosscut Team, and responds to public requests and inquiries.

Measurement, analysis, and modeling activities are conducted in close collaboration with the Pacific Northwest National Laboratory and include identification of rate-controlling reaction mechanisms in catalytic devices under realistic operating conditions, development of modeling strategies that simulate the rate-controlling mechanisms with high computational efficiency, generation of benchmark data sets for model calibration and validation, and measurement of critical device parameters needed for model development. The results of these activities are disseminated through publications, presentations, and the CLEERS website. Research directions are guided by the Crosscut Team and by regular CLEERS industry participant priority surveys. ORNL's CLEERS research activities have historically focused on approaches to NO_X reduction in lean exhaust but have recently shifted to include low-temperature aftertreatment technologies such as passive adsorbers for NO_X and hydrocarbons.

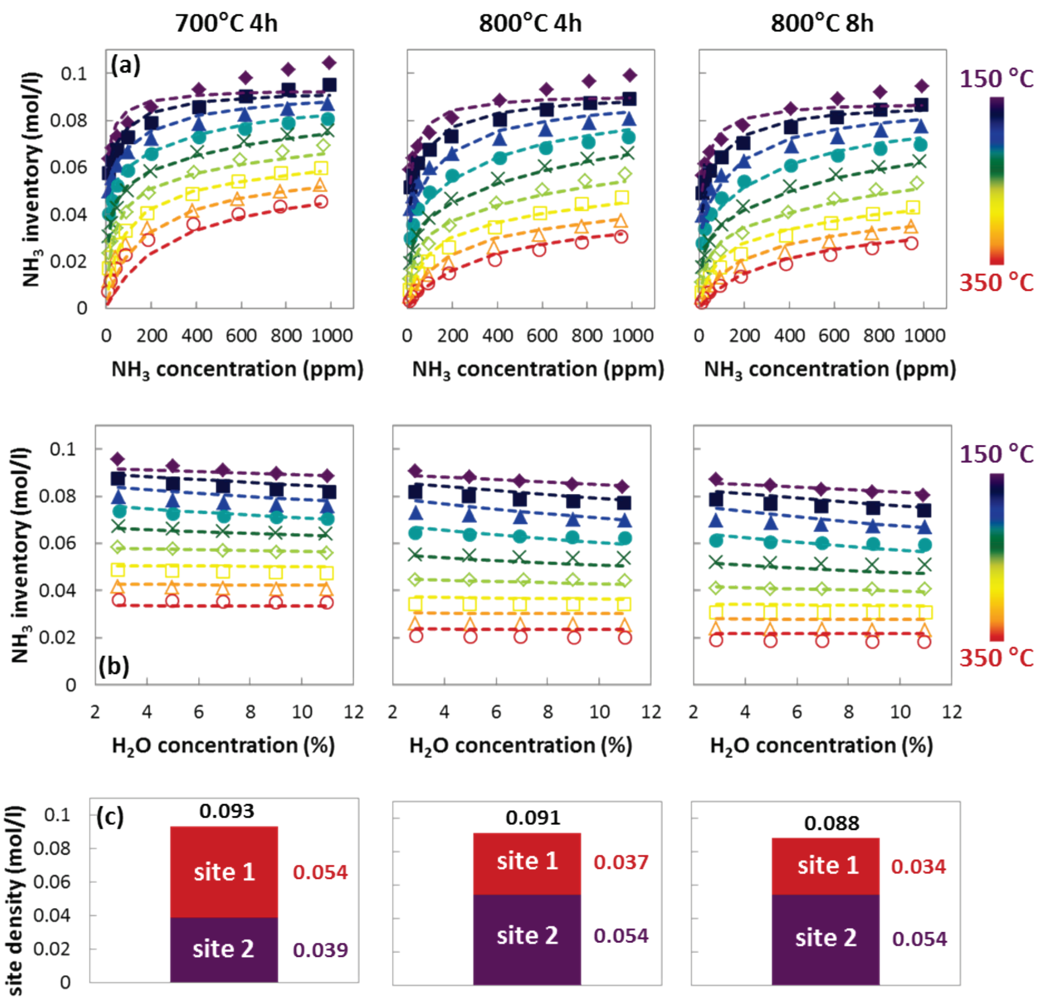
Noteworthy FY 2015 CLEERS activities included the following.

- Supporting the USDRIVE Advanced Combustion & Emissions Control (ACEC) Tech Team Low Temperature Aftertreatment Working Group in the development of new laboratory evaluation protocols that are accelerating the discovery of new catalysts.

- Conducting the biennial CLEERS Industry Priority Survey, collating the results, and issuing recommendations on the most pressing R&D needs to the Crosscut and ACEC Teams and DOE (http://www.cleers.org/reports/2015_CLEERS_Industry_Priorities%20Survey_Final_Report.pdf). This has helped improve the focus and industrial relevance of national laboratory emissions control projects supported by DOE.

- Conducting detailed measurements of N_2O formation during lean NO_X trap regeneration. As a result of this research, the chemical pathways leading to N_2O formation were identified, allowing development of more accurate simulation tools and improved operating strategies with the potential to significantly mitigate N_2O emissions.

- Developing measurement and modeling strategies that accurately replicate the NH_3 stored on commercial small-pore copper zeolite selective catalytic reduction (SCR) catalysts under dynamic driving conditions. The resulting model can now be incorporated into SCR device models to provide better predictions of NOx emissions control performance for these catalysts in proposed advanced vehicle powertrains, which will enable the development of system architectures and control strategies that meet increasingly stringent emissions regulations while reducing petroleum consumption.



NH_3 storage properties of a commercial Cu-SSZ-13 urea selective catalytic reduction catalyst hydrothermally aged under 10% O_2, 5% H_2O, balance N_2 for 4 h at 700°C (left), 4 h at 800°C (center), or 8 h at 800°C (right). Top and middle panels show measured (points) and modeled (dashed lines) steady state NH_3 inventories as a function of temperature and (a) NH_3 concentration under 0.2% O_2, 5% H_2O, balance N_2 or (b) H_2O concentration under 0.2% O_2, 400 ppm NH_3, balance N_2. Bottom panels show estimated storage site densities after hydrothermal aging for site 1 and site 2 based on the model fits shown in (a) and (b). All measurements were conducted on an automated flow reactor at a gas hourly space velocity of 30,000 h^{-1}.

Publications, Presentations, and Patents

1. D. Mráček, P. Kočí, M. Marek, J.-S. Choi, J. A. Pihl, and W. P. Partridge. 2015. "Dynamics of N_2 and N_2O Peaks During and After the Regeneration of Lean NO_X Trap." *Applied Catalysis B: Environmental* **166–167**: 509–517.

2. Š. Bártová, D. Mráček, P. Kočí, M. Marek, and J.-S. Choi. 2015. "Ammonia Reactions with the Stored Oxygen in a Commercial Lean NO_X Trap Catalyst." *Chemical Engineering Journal* **278**: 199–206.

3. D. Mráček, P. Kočí, J.-S. Choi, and W. P. Partridge. 2016. "New Operation Strategy for Driving the Selectivity of NO_X Reduction to N_2, NH_3 or N_2O During Lean/Rich Cycling of a Lean NO_X Trap Catalyst." *Applied Catalysis B: Environmental* **182**: 109–114.

4. J. A. Pihl and C. S. Daw. 2015. "Measuring the Impacts of Catalyst State on NH_3 Adsorption in Copper Zeolite SCR Catalysts." presented at the 2015 DOE Cross-Cut Lean/Low-Temperature Exhaust Emissions Reduction Simulations (CLEERS) Workshop, Dearborn, Michigan, April 27–29, 2015.

5. J. A. Pihl and C. S. Daw. 2015. "NH_3 Storage Isotherms: A Path Toward Better Models of NH_3 Storage on Zeolite SCR Catalysts." poster presented at the 24th North American Catalysis Society Meeting, Pittsburg, Pennsylvania, June 14–19, 2015.

6. T. J. Toops. 2015. "The Measured and Proposed Chemistry of the Selective Catalytic Reduction of NO_X." invited plenary presentation at the 4th International Symposium on Modeling of Exhaust-Gas After-Treatment (MODEGAT IV), Bad Herrenalb, Germany, September 14, 2015.

Improving Vehicle Fuel Economy through Increasing Fuel Octane Ratings

Contact: Scott Sluder, sluders@ornl.gov, 865-946-1235

One of the ways to increase fuel efficiency while maintaining performance is to increase fuel octane, allowing higher compression ratios and greater thermal efficiency. Blending ethanol and other biofuels with conventional petroleum-based fuels can be an effective octane booster. Ethanol has a higher heat of vaporization (HoV) than gasoline, which may provide additional engine efficiency benefits. And it has the added advantage of increasing biofuel use and decreasing petroleum use. However, more data and better predictive tools are needed to adequately determine fuel property effects on combustion and engine efficiency optimization.

ORNL, with partners at other national labs, universities, and industry, is focusing on quantifying the fuel efficiency benefits of increasing the fuel research octane number (RON) by various methods as well as determining ancillary benefits from factors such as increasing the HoV. Currently fuels in the RON range of 90–100 are being investigated to characterize the amount of improvement that is possible using near-term engine hardware and fuel octane levels. Later stages of this project will investigate more aggressive use of octane increases, which are likely to require improved engine boosting, compression ratio increases, and other hardware changes.

In 2015 ORNL researchers evaluated potential fuel economy differences for two different ethanol blends. E10 fuel (10% ethanol, 90% gasoline) was selected as the baseline at the suggestion of research partner Ford Motor Company. It was used to prepare an engine performance map using the Ford EcoBoost 1.6 L engine with the original pistons and a geometric compression ratio of 10.1 (Figure 1). An E30 fuel (30% ethanol, 70% gasoline) was used to examine the potential for increasing the compression ratio, replacing the original EcoBoost pistons with custom-manufactured pistons that produced a geometric compression ratio of about 13 (Figure 2). The impact of the fuel and the compression ratio on fuel economy was evaluated in vehicle system simulations using Autonomie. The results confirmed that use of high-octane fuels as enablers for increasing the compression ratio can produce significant improvements in vehicle fuel economy (4%–13%), but further research is needed to develop a robust estimate of the potential gains available through increasing fuel octane ratings.

Researchers also analyzed three fuels with well-matched RONs and motor octane numbers (similar to RONs but determined under more rigorous driving conditions) to examine the potential of HoV to provide additional antiknock benefits. The three fuels were formulated with ethanol, isobutanol, and toluene to provide differing HoV values. The results indicate that engine performance trends with fuel RON rating, which reinforces the concept that HoV antiknock effects can be viewed as a contributor to octane sensitivity.

Further modeling improvements, along with expanding the vehicle system modeling effort to provide fuel economy for various powertrain configurations, are planned for FY 2016.

Publications, Presentations, and Patents

1. C. S. Sluder, J. P. Szybist, and B. C. Kaul. 2015. "Preliminary Investigation of Heat of Vaporization Effects in High-Octane Fuel Experiments at ORNL." presented to the USDRIVE Advanced Combustion & Emissions Control Technical Team, July 16, 2015.
2. C. S. Sluder and D. A. Splitter. 2014. "Potential for Increasing Fuel Economy through Raising Octane Ratings." presented to the staff of the DOE Vehicle Technologies Office and Biomass Energy Technology Office, US Department of Energy, December 15, 2014.
3. C. S. Sluder. 2015. "An Overview of High-Octane Fuel Projects at ORNL." presented to the USDRIVE Fuels Working Group, February 18, 2015.
4. J. P. Szybist, S. Curran, C. S. Sluder, D. A. Splitter, A. B. Dempsey, and R. M. Wagner. 2015. "Gasoline-Like Fuel Effects on Advanced Combustion Regimes." presented at the 2015 DOE Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting, Washington, DC, June 11, 2015.

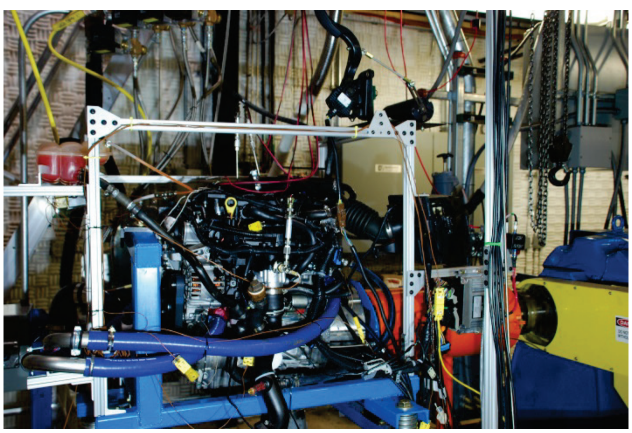


Figure 1. The Ford EcoBoost 1.6 L engine installed at the ORNL National Transportation Research Center.

Figure 2. The pistons used in the tests for (left to right) compression ratios of 10.1, 12, and 13.

Low-Temperature Emissions Control

Contact: Todd J. Toops, toopstj@ornl.gov, 865-946-1207

Advanced, higher-efficiency combustion engines have lower exhaust temperatures, which is problematic for emissions control as most catalysts work better in the 200°C to 350°C range. DOE's low-temperature emissions control program has set a goal of a 90% reduction in pollutant emissions at temperatures at or below 150°C. ORNL researchers are focused on meeting this goal through nontraditional catalysts and materials in three areas: mixed metal oxides that are free of platinum-group metals (PGMs), PGM support modification for enhanced activity, and materials that trap hydrocarbons (HCs).

In 2015 work continued on ORNL's copper-cerium-cobalt oxide (CCC) catalyst, a PGM-free ternary mixed oxide that has shown good activity for CO oxidation at low temperatures in a simulated exhaust stream and exceptional tolerance for C_3H_6 (propylene or propene) and other hydrocarbon species. In thermal-aging investigations, the CCC catalyst has shown stability up to 800°C.

In other investigations, the CCC catalyst was tested in combination with Pt/Al_2O_3, a catalyst known to have good HC activity, to find the lowest combined CO and HC catalyst operating temperatures through synergistic chemistry. A 50-50 mixture of the two was found to have high CO and C_3H_6 oxidation using half as much total platinum as Pt/Al_2O_3 alone (Figure 1).

Efforts to modify PGM supports are focused on enhancing PGM catalyst activity/durability through modifications to the metal-oxide supports. Palladium on ZrO_2 or ZrO_2-modified supports has proven to be a stable catalyst. This year, working with palladium on ZrO_2-modified silica, researchers were able to successfully synthesize a silica core with a ZrO_2 shell with a more uniform ZrO_2 coating than in the past, resulting in improved sulfur tolerance and HC oxidation. Initial results for hydrothermal aging are also good.

ORNL researchers also initiated research on capturing HCs during low temperature operation this past year. The method under investigation could be used to capture HCs under cold-start and other low-temperature exhaust conditions for later release at higher temperatures, when the HCs could be oxidized by conventional catalysts. Zeolite Socony Mobil-5 (ZSM-5) and Beta zeolites were selected for evaluation based on industry feedback and on a literature survey, which indicated their thermal stability and thermodynamic affinity for HCs. Results indicate that both have the ability to adsorb C_3H_6, with Beta zeolites offering superior trapping capacity. Adding silver improves both trapping and desorption of C_3H_6 for both zeolites, with Beta zeolites again showing the most pronounced effects (Figure 2); this metal addition is essential for good trapping efficiency in the presence of water vapor.

Future work on all three approaches will focus on working with the challenges of the full exhaust mixture, aging, and sulfur resistance.

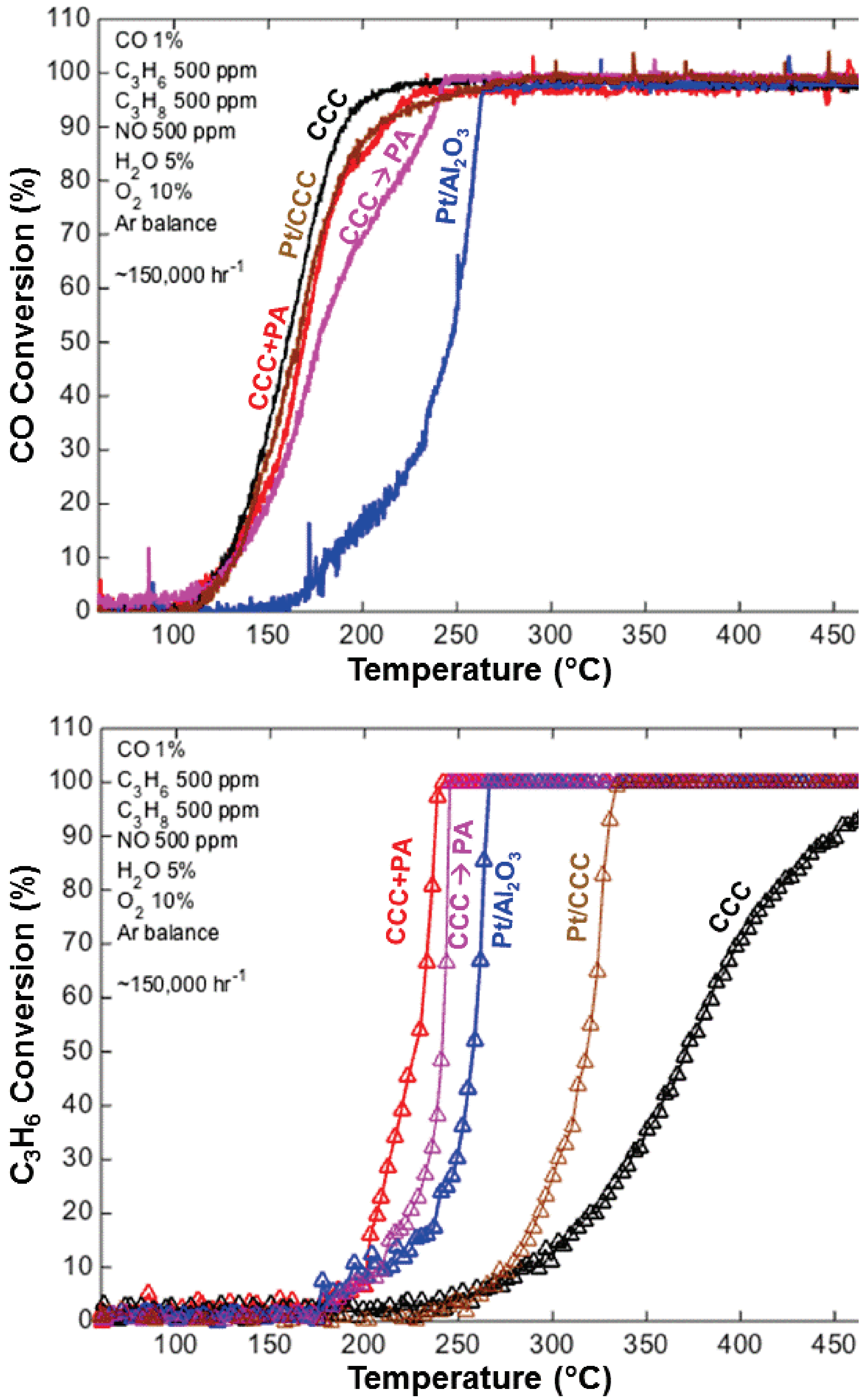


Figure 1. CO and C_3H_6 conversion of mixed bed (CCC+PA), split bed (CCC   PA), and deposited nanoparticle (Pt/CCC) catalysts compared with conversions on single catalyst beds (CCC, Pt/Al_2O_3).

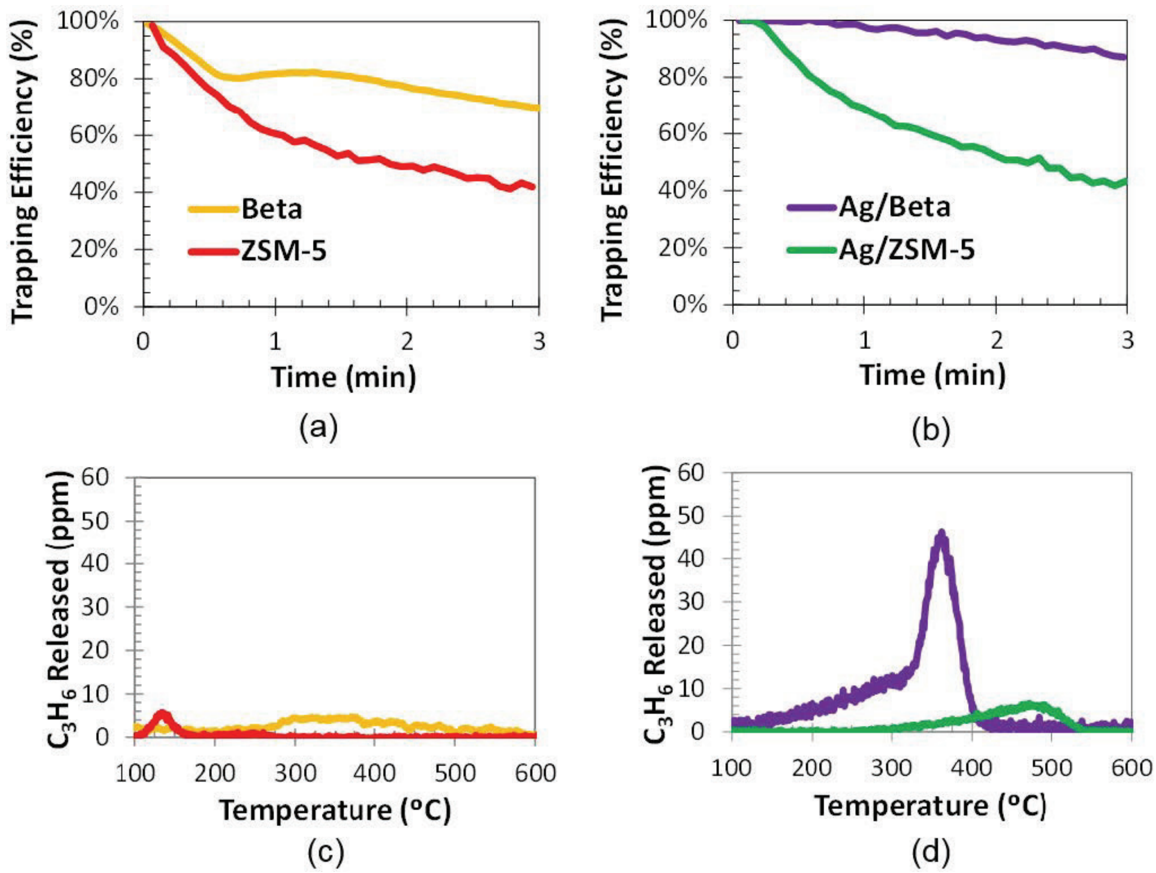


Figure 2. Comparison of C_3H_6 concentration at the catalyst outlet during (a,b) adsorption as a function of time and (c,d) desorption of C_3H_6 as a function of temperature for (a,c) unexchanged and (b,d) silver-exchanged ZSM-5 and Beta zeolites.

Publications, Presentations, and Patents

1. A. J. Binder, T. J. Toops, R. R. Unocic, J. E. Parks II, and S. Dai. 2015. "Low Temperature CO Oxidation over a Ternary Oxide Catalyst with High Resistance to Hydrocarbon Inhibition." *Angew. Chem. Int. Ed.* **54**(45): 13263-13267; doi: 10.1002/ange.201506093.

2. M. Kim, E. A. Kyriakidou, J. Choi, T. J. Toops, A. J. Binder, C. Thomas, J. E Parks II, V. Schwartz, J. Chen, and D. K. Hensley. 2016. "Enhancing Low-Temperature Activity and Durability of Pd-based Diesel Oxidation Catalysts Using ZrO_2 Supports." *Applied Catalysis B: Environmental* **187**: 181–194; doi: 10.1016/j.apcatb.2016.01.023.

3. A. P. Wong, E. A. Kyriakidou, T. J. Toops, and J. R. Regalbuto. 2016. "The Catalytic Behavior of Pt-Pd Bimetallic Catalysts for Use as Diesel Oxidation Catalysts." *Catalysis Today* **267**: 145-156; doi:10.1016/j.cattod.2016.02.011.

4. A. J. Binder, T. J. Toops, R. R. Unocic, J. E. Parks II, and S. Dai. 2015. "Inhibition-Resistant Ternary Oxide Catalyst for Low Temperature CO Oxidation in Automotive Exhaust." presented at the 14th Annual Fall Symposium of the Southeastern Catalysis Society, Clemson, South Carolina, September 27–28, 2015.

5. E A. Kyriakidou, J. Choi, M. Kim, T. J. Toops, and J. E. Parks II. 2015. "A Comparative Study of ZSM-5 and Beta-Zeolites for Hydrocarbon Trap Applications under 'Cold-Start' Condition."

presented at the 14th Annual Fall Symposium of the Southeastern Catalysis Society, Clemson, South Carolina, September 27–28, 2015.

6. T. J. Toops. 2015. “Approaches to the Challenges of Treating Emissions at Low Temperatures.” presented at the Karlsruhe Institute of Technology, Karlsruhe, Germany, September 17, 2015 (invited).

Neutron Imaging of Advanced Vehicle Technologies

Contact: Todd J. Toops, toopstj@ornl.gov, 865-946-1207

Neutrons can penetrate many commonly used metals, can be used to image many light elements such as hydrogen, and are highly sensitive to water and hydrocarbons (fuels), which makes neutron imaging well suited to probe engine parts, fluids, and oil and related residues. Researchers at ORNL are developing high-fidelity nondestructive, noninvasive neutron imaging techniques to improve understanding of advanced vehicle technologies using the unique capabilities of the ORNL High Flux Isotope Reactor and Spallation Neutron Source. To improve upon the results, internal ORNL funds have been invested in the hardware and experimental effort, which will enable dynamic neutron imaging of advanced vehicle technologies, improved resolution, and stroboscopic imaging capability. Once fully developed, the techniques will be used to aid improved design and control of complex advanced combustion systems and to guide model validation and input.

Initial efforts have been focused on two important components of advanced vehicle systems, in-cylinder fuel injectors and particulate filters (PFs).

In-cylinder fuel injectors are among the innovations bringing internal combustion engines into the 21st century; however, they are not without their drawbacks, including fouling or deposit formation, which can affect engine performance. During 2015, the ability of neutron imaging to measure fuel injector fouling has been fully demonstrated in work with research partner Continental Automotive. Use of this technique to measure carbonaceous deposits without cutting the injectors open will be important in the future for understanding fouling under a variety of conditions. Neutron imaging of fuel injection in a dynamic capacity was also demonstrated, with the technique proving capable of visualizing the rate of evaporation in the internal injector sac as a function of injector or chamber conditions. In the future, ORNL researchers will be teaming with injector suppliers on broader studies.

PFs are key components of the emissions control systems of modern diesel engines, and possibly gasoline engines in the future, yet there remain significant questions about the basic behavior of the filters. Regeneration processes, specifically, are not well understood, including how ash (nonregenerable metal-oxide-based particulate) fills a PF and interacts with the wall. Neutron imaging of PFs in collaboration with the Massachusetts Institute of Technology (MIT) is helping to clarify some of these issues. During 2015 ash profiles and densities for different soot regeneration strategies were identified, revealing a series of deposits that greatly compromise the full functionality of PFs. Work with MIT will continue, and if possible, the technique will be used to provide detailed understanding of soot and ash distribution.

Publications, Presentations, and Patents

1. T. J. Toops, J. A. Pihl, C. E. A. Finney, J. Gregor, and H. Bilheux. 2015. “Progression of Soot Cake Layer Properties during the Systematic Regeneration of Diesel Particulate Filters Measured with Neutron Tomography.” *Emission Control Science and Technology* **1**(1): 24–31, doi: 10.1007/s40825-014-0008-1.

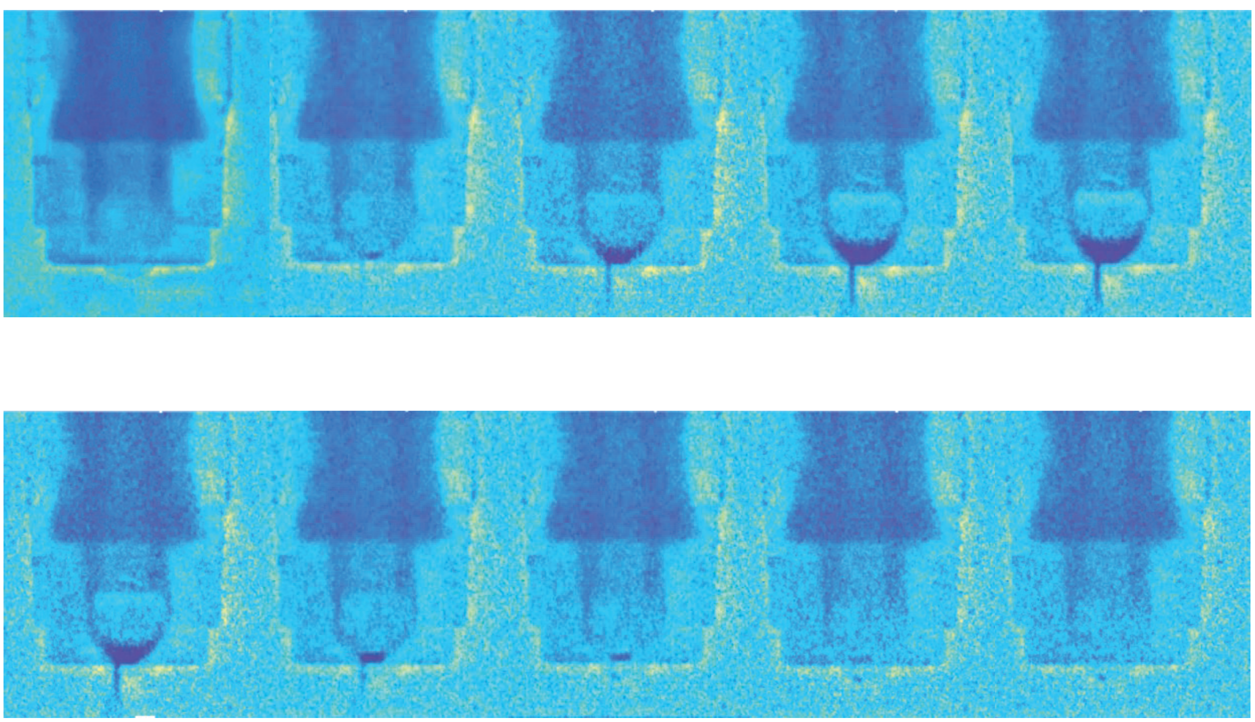
2. T. J. Toops, E. Nafziger, C. E. A. Finney, H. Bilheux, and J. Bilheux. 2015. "Effect of Regeneration Strategy on the Ash Distribution and Packing Density Measured with Neutron and X-Ray Radiography." 2015 SAE World Congress, Detroit, Michigan, April 23, 2015.

3. T. J. Toops, E. Nafziger, C. E. A. Finney, H. Bilheux, and J. Bilheux. 2015. "Effect of Regeneration Strategy on the Ash Distribution and Packing Density Measured with Neutron and X-Ray Radiography." Massachusetts Institute of Technology Consortium to Optimize Lubricant and Diesel Engines for Robust Aftertreatment Systems, Spring Review Meeting, Cambridge, Massachusetts, May 13, 2015.

4. H. Z. Bilheux, C. E. A. Finney, A. E. Pawlowski, D. A. Splitter, T. J. Toops, E. J. Nafziger, and L. J. Santodonato. 2015. "Neutron Imaging of Advanced Transportation Technologies." presented at the Workshop on Needs and Requirements for Future Research Reactors, Oak Ridge National Laboratory, May 12, 2015.

5. T. J. Toops, C. E. A. Finney, E. J. Nafziger, D. Splitter, M. DeBusk, and A. Pawlowski. 2015. "Neutron Imaging of Advanced Transportation Technologies." presented at the US Department of Energy Vehicle Technologies Office 2015 Annual Merit Review and Peer Evaluation Meeting, Washington, DC, June 10, 2015.

6. T. J. Toops, D. A. Splitter, L. J. Santodonato, A. E. Pawlowski, E. J. Nafziger, C. E. A. Finney, and H. Z. Bilheux, "Dynamic Neutron Imaging of GDI-Based Fuel Injection." presented at the US Department of Energy Vehicle Technologies Office Advanced Engine Combustion Meeting, Southfield, Michigan, August 16, 2015.



Time-stamped images show composite injection event and illustrate fuel in sac long after pintle closes.

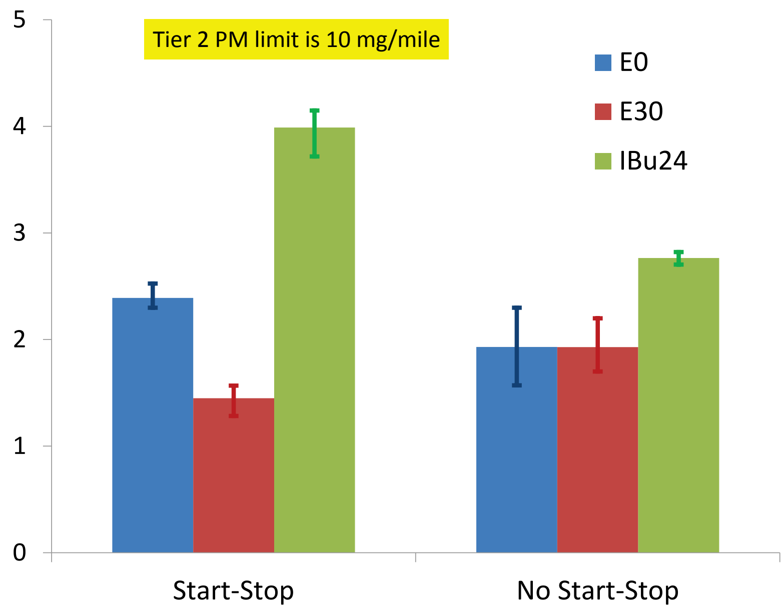
ORNL Investigates How New Fuels and Lubricants Affect Emission Systems

Contact: Todd J. Toops, toopstj@ornl.gov, 865-946-1207

ORNL researchers are investigating how new fuel blends and lubricants affect vehicle emission control systems. The aim is to determine the potential of the new chemistries, both to increase engine performance and to degrade exhaust system performance.

Experiments with engines running lean fuel mixtures (high ratios of air to fuel) showed that fuel blends containing ethanol and isobutanol (iBuOH) are readily controlled by selective catalytic reduction using a relatively inexpensive silver-based catalyst. The tests used E100, E85, and E50 ethanol-gasoline blends and pure iBuOH and iBuOH-gasoline blends. An important finding was that higher ethanol content in the fuel significantly reduced the amount of hydrocarbons that bypass the emission control system while maintaining the NOx reduction activity.

A series of measurements of particulate matter (PM) emissions focused on analyzing the performance of biofuels during start-stop conditions (a point in the cycle when PM emissions tend to be higher). Three fuels—E0 (conventional gasoline), E30, and an isobutanol blend (iBu24)—were evaluated in a 2014 Chevrolet 2.4 L gasoline direct injection engine. The results showed that E30 had the lowest level of PM emissions and was unaffected by start-stop operation. The iBu24 mixture was the only one that showed any adverse effect on PM under start-stop conditions. The tests also showed that the PM generated by the E30 blend reacts more easily with the catalyst than the PM generated by E0.



FTP composite PM emissions for E0, E30, and iBu24 under start-stop and conventional mode (no start-stop) operation.

New lubricants are being developed that reduce friction inside engines, improving efficiency and reducing wear. Ionic liquid (IL) lubricant additives, in particular, have been demonstrated to improve fuel economy. It is important to determine whether they are compatible with currently used emissions control systems. The ORNL team evaluated DEHP (diethylhexyl phthalate) phosphate, an IL that is an oil-miscible phosphorus compound, to compare its effects on a three-way catalyst (TWC) with those of the industry standard additive, ZDDP (zinc dialkyldithiophosphate). Results from a series of tests with TWCs aged under different scenarios showed that the IL additive had a somewhat less adverse impact on the catalyst than did ZDDP.

ORNL researchers, in collaboration with the engine maker Cummins, the National Renewable Energy Laboratory, and the Manufacturers of Emission Controls Association, studied the impacts of sodium impurities in biodiesel on a heavy-duty truck emission control system. A full exhaust system was operated on a test rig for more than 1,000 h using a fuel blend of 80% gasoline and 20% biodiesel doped with 14 ppm of sodium. A series of sophisticated characterization techniques showed that the primary effect of the sodium on the exhaust system was increased ash in the diesel particulate filter, but the catalysts were not directly impacted by sodium. The data from this study will be useful in determining appropriate sodium standards for biodiesel fuels.

Publications, Presentations, and Patents

1. V. Y. Prikhodko, J. A. Pihl, T. J. Toops, J. Thomas, J. E. Parks II, and B. West. 2015. "Selective Catalytic Reduction of Oxides of Nitrogen with Ethanol/Gasoline Blends over a Silver/Alumina Catalyst on Lean Gasoline Engine." SAE Technical Paper Series 2015-01-1008, SAE International, Warrendale, Pennsylvania.
2. D. W. Brookshear, J. Nam, K. Nguyen, T. J. Toops, and A. Binder. 2015. "NOx Performance of Cu-Chabazite SCR Catalysts under Severe Sulfur Poisoning from Marine Diesel Engine's Fuels." *Catalysis Today* **258**: 359–366.
3. P. Ye, C.-X. Sun, M. Lapuerta, J. Agudelo, R. Vander Wal, A. L. Boehman, T. J. Toops, and C. S. Daw. 2016. "Impact of Rail Pressure and Biodiesel Fueling on the Particulate Morphology and Soot Nanostructures from a Common-Rail Turbocharged DI Diesel Engine." *International Journal of Engine Research* **17**(2): 193–208.
4. J. M. Storey et al. 2014. "Investigation of the Potential Impact of Lubricant Contribution to the Formation of Particulate Matter with Reactivity Controlled Compression Ignition on Light-Duty Diesel Engines." *Emission Control Science and Technology* **1**(1): 64.
5. M. Lance and T. J. Toops. 2014. "Impact of Metal Impurities on Catalyst Durability." invited presentation at 2014 Biodiesel Technical Workshop, Kansas City, Missouri, October 28–29, 2014.
6. D. W. Brookshear, J. A. Pihl, B. H. West, T. J. Toops, and V. Prikhodko. 2015. "The Selective Catalytic Reduction of NOx over Ag/Al_2O_3 with Isobutanol as the Reductant." submitted to *Catalysis Today*.

Stretching Internal Combustion Engine Efficiency with New Combustion Regimes

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In continuing work on a multiyear project to increase internal combustion engine (ICE) efficiency, ORNL researchers and partners from industry, academia, and other national labs have demonstrated a fuel consumption benefit of more than 9% (approaching diesel efficiency) using an ORNL-developed operation strategy. That result fell below the researchers' expectations because the thermochemical recuperation (TCR) fuel reforming had a lower fuel conversion rate than expected; however, further efficiency improvements are anticipated as the researchers refine the operating strategy to achieve higher reforming fuel conversion.

The thermal efficiency of ICEs can be improved with exhaust gas recirculation (EGR). The problem is that combustion instabilities are induced above a certain level of EGR dilution, limiting efficiency improvements. However, the dilution limit can be extended for additional efficiency improvements with the use of high flame speed/low ignition energy components such as H_2, which stabilize dilute combustion.

In the current project, ORNL researchers are exploring two pathways to TCR to support high EGR dilution: (1) a noncatalytic in-cylinder reforming approach (Figure 1) that thermally reforms the fuel in a hot, oxygen-deficient negative valve overlap portion of an engine cycle and (2) EGR loop reforming, a strategy that relies on a catalyst (in this case rhodium on alumina) to reform the fuel in an oxygen-deficient EGR stream (Figure 2). Both approaches use waste exhaust heat to drive endothermic reforming reactions to produce a mixed reformate and EGR stream that is rich in H_2 and CO. The reformate can then be used to extend the EGR dilution limit of spark-ignited combustion for a more thermodynamically favorable engine cycle.

Parametric studies of both processes were conducted to further characterize the reforming process, H_2 generation, and engine efficiency. For the noncatalytic in-cylinder reforming process, engine efficiency improvements were observed that resulted in a decrease in fuel consumption of more than 9% relative to the baseline case. The efficiency improvements were attributable to a cylinder deactivation effect in conjunction with cooled external EGR rather than TCR. Analysis showed that the fuel conversion was lower than anticipated because of relatively cool in-cylinder temperatures, a result of high heat losses. Continuing experiments in FY 2016 will focus on decreasing heat losses to increase fuel conversion with less oxygen, which reduces the thermodynamic efficiency of the process.

For the EGR loop reforming process with the rhodium-based catalyst, it was concluded that the exhaust temperatures with EGR are insufficient to reform the fuel in the absence of oxygen (steam reforming). Thermodynamic investigations found that TCR may still be possible with some amount of oxygen present. The conditions where a high reforming efficiency is observed are not necessarily the conditions leading to the highest H_2 production. Ultimately, the thermodynamic benefits will need to be assessed in an engine, an activity that will be pursued in FY 2016.

The project, which is funded by the DOE Vehicle Technologies Office, grew out of a colloquium on engine efficiency held in 2010 [1] and focuses on high risk, high reward technologies that could have a major impact on ICEs for the foreseeable future.

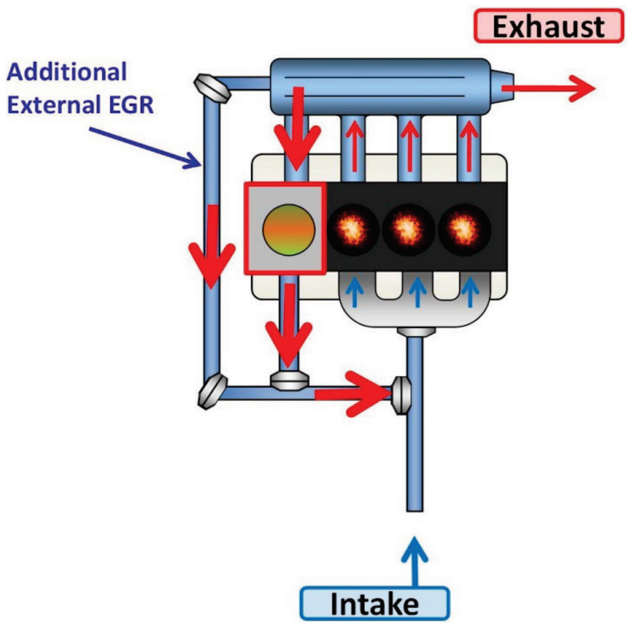

Figure 1. In-cylinder reforming process.

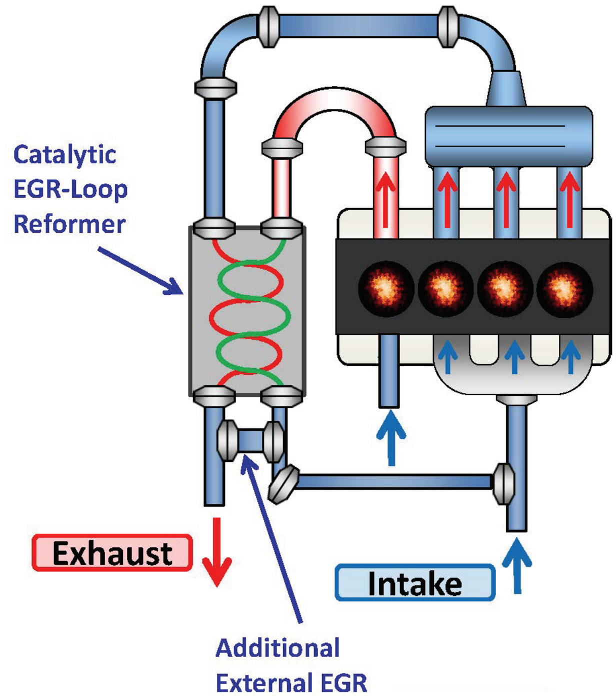

Figure 2. EGR loop reforming process.

References

1. C. S. Daw, R. L. Graves, R. M. Wagner, and J. A. Caton. 2010. *Report on the Transportation Combustion Engine Efficiency Colloquium Held at USCAR, March 3–4, 2010*, ORNL/TM-2010/265, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Publications, Presentations, and Patents

1. J. P. Szybist and D. A. Splitter. 2015. "In-Cylinder Fuel Reforming to Support High EGR Dilution in High Efficiency SI Engines." presented at the IEA Task Leaders Meeting on Combustion, St. Andrews, Scotland, August 2015.

2. I. Ekoto, B. Peterson, J. Szybist, and W. Northrop. 2015. "Analysis of Thermal and Chemical Effects on Negative Valve Overlap Period Energy Recovery for Low-Temperature Gasoline Combustion." *SAE International Journal of Engines* **8**(5): 2227–2239, doi: 10.4271/2015-24-2451.

3. J. P. Szybist. 2015. "Update of ORNL In-Cylinder Reforming Investigation." presented at the AEC Program Review Meeting, Sandia National Laboratories, February 2015.

4. C. S. Daw, J. P. Szybist, J. A. Pihl, D. A. Splitter, and G. Fisher. 2015 "Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes." presented at the 2015 DOE Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting, Washington, DC, June 18, 2015.

Using Advanced Fuels in Advanced Combustion Regimes

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Two related projects investigated the performance of several advanced fuels in different advanced combustion regimes. The advanced compression ignition (ACI) project investigated the potential for coevolution of these emerging combustion technologies and biofuels to reduce petroleum consumption in future engines. The spark ignition (SI) project analyzed methods of increasing the efficiency of gasoline-like fuels under both advanced and conventional combustion regimes.

Identifying pathways to improved engine efficiency requires understanding the thermodynamics of internal combustion engines. Many renewable and advanced fuels have unique properties that could increase fuel efficiency in both ACI and SI modes. These two projects are exploring which properties of renewable fuels can enable higher-efficiency operation.

The 2015 objectives were to

- demonstrate the potential of biofuels to obtain efficiency targets with reactivity-controlled compression ignition (RCCI),
- compare dual-fuel RCCI and single-fuel gasoline compression ignition (GCI), and
- determine the extent and causes of fuel-specific differences in exhaust gas recirculation (EGR) dilution tolerance at light-load engine conditions in an SI engine.

The ACI project met the 2015 technical target for demonstrating fuel effects of 36% brake thermal efficiency (BTE) at 2,000 rpm and 20% peak load. The ACI project compared the efficiency, load expansion, and controllability for RCCI with conventional fuels and GCI with fuels spanning a wide range of research octane numbers (RONs). The SI project showed that EGR tolerance limits can be attributed to stochastic cycle-to-cycle instabilities and fuels with faster flame speeds are more resilient to stochastic turbulence and thus able to tolerate more dilution.

ACI Research

The ACI project used a modified modern General Motors 1.9 L multicylinder diesel engine. The effects of fuel properties on both single- and dual-fuel combustion strategies on the same engine platform were considered. The 2,000 RPM, 20% peak load conditions were similar to those common in real-world driving. The 36% BTE, achieved using biodiesel and gasoline as the high- and low-reactivity fuels, respectively, is a 6% improvement over the conventional diesel combustion baseline diesel fuel (Figure 1).

In addition, GCI experiments on fuel effects were done using gasoline-range fuels supplied by Chevron Energy Technologies in partial fuel stratification (PFS) and heavy fuel stratification (HFS) modes. They investigated the effects of RONs ranging from 40 to 87 on both PFS and HFS low-temperature GCI modes. Each of seven fuels was run at 2,000 rpm, 4.0 bar brake mean effective pressure in HFS mode sweeping the amount of EGR and other key parameters.

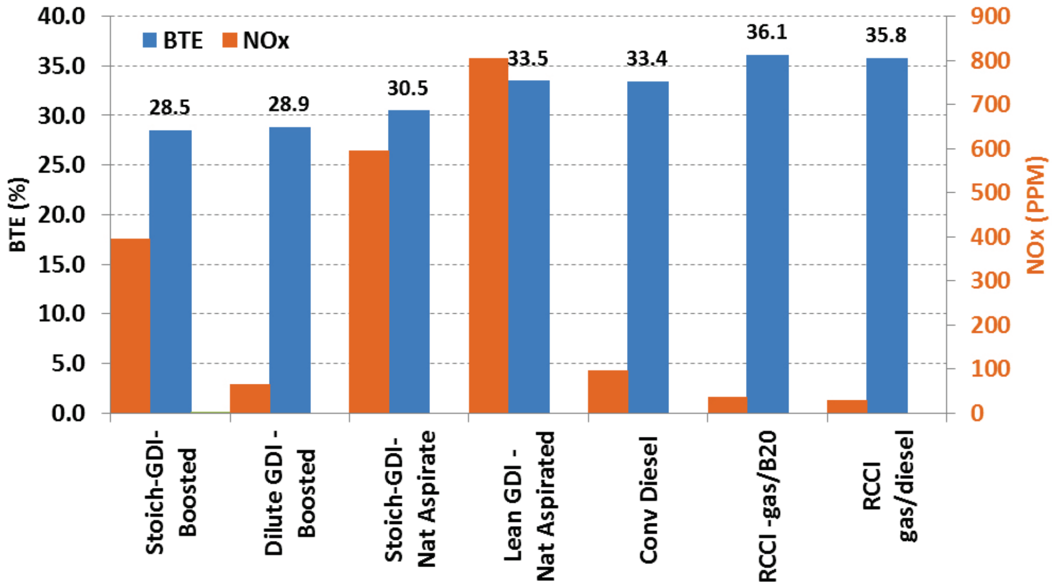

Figure 1. Comparison of FY 2015 advanced compression ignition milestone accomplishment with other combustion technologies.

SI Research

The SI project used a modern direct-injection single-cylinder research SI engine to examine six model fuel blends at a constant RON of 95 using n-heptane, iso-octane, toluene, and ethanol (Figure 2). Laminar flame speeds for the mixtures spanned a range of about 6 cm/s. The results illustrated that fuels with increased flame speeds increase EGR tolerance. Fuel blends with the highest ethanol content were the most tolerant of dilution. The fuel-specific differences in dilution tolerance allowed for a 50% relative increase in EGR (4% absolute difference) at a constant coefficient of variation of indicated mean effective pressure of 3%.

Both of these projects are being brought into the DOE Co-Optimization of Fuels & Engines initiative in FY 2016. Fuel effects on advanced combustion continue to be explored with a verity of advanced and renewable fuels. The high-efficiency SI project will continue to contribute to the understanding of fuel effects on dilution tolerance and is ready to test candidate fuels from the co-optimization initiative. Both of these projects will collaborate with other internal and external projects within the larger DOE initiative.

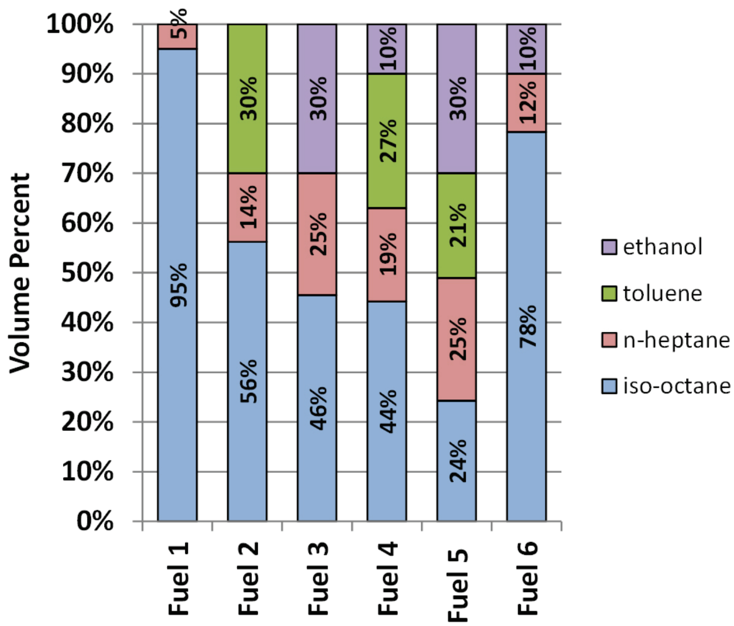

Figure 2. Compositions of the six surrogate blends used to investigate exhaust gas recirculation dilution tolerance in spark ignition engines, each with a research octane number of 95.

Publications, Presentations, and Patents

1. 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 Multicylinder Compression Ignition Engine." *J. Engineering for Gas Turbines and Power* **137**(11): 111506.

2. S. J. Curran, A. Gao, and R. M. Wagner. 2015. "Reactivity-Controlled Compression Ignition Drive Cycle Emissions and Fuel Economy Estimations using Vehicle System Simulations." *Int. J. Engine Research* **16**, 1014–1024.

3. D. A. Splitter. R. M. Wagner, A. B. Dempsey, and S. J. Curran. 2015. "The Landscape of GCI Combustion—Fuel Properties and Stratification." presented at the SAE 2015 Gasoline Compression Ignition Engine Symposium, Capri, Italy, September 17, 2015 (invited).

4. S. J. Curran, R. M. Wagner, and A. B. Dempsey. 2015. "Next-Generation Compression Ignition Engines and Future Fuel Opportunities." presented at the 2015 SAE/JSAE Powertrain Fuels and Lubricants International Meeting, Kyoto, Japan, September 1–4, 2015 (invited).

5. R. M. Wagner, A. B. Dempsey, and S. J. Curran, "Directions in High Efficiency Engine Research and Future Fuel Opportunities." presented at the 13th International Conference on Engines for Vehicles, Port Jefferson, New York, June 22, 2015 (invited).

6. D. A. Splitter and J. P. Szybist. 2015. "Fuel Effects and EGR Dilution Limits with SI Combustion." presented at the Advanced Engine Combustion Program Review, Livermore, California, February 2015.

Using High-Performance Computing to Accelerate Engine Development

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ORNL is partnering with Ford Motor Company, Convergent Science, General Motors, General Electric, and other industry stakeholders to use DOE high-performance computing (HPC) resources (Figure 1) to accelerate design and development of advanced engines to meet future emissions and fuel economy goals. Specific projects evolve in response to DOE and stakeholder priorities and as tasks and projects are completed.

Current efforts are focused on understanding and controlling cycle-to-cycle variability in highly dilute and dual-fuel combustion applications and optimizing gasoline direct injection (GDI) fuel injector design.

Figure 1. ORNL's Titan supercomputer.

Combustion instability is a potential barrier to realizing the full benefits of many advanced combustion strategies, such as dilute and dual-fuel (natural gas–diesel) combustion, which offer advantages in terms of engine efficiency, cost, and pollutant emission reductions. This past year, ORNL researchers used highly parallelized engine simulations on ORNL's Titan supercomputer to better understand the stochastic and deterministic processes driving cyclic variability in dilute combustion. Results from the simulations were used to generate metamodels to study serial combustion events and the parameters that promote combustion instability. Final analysis of the simulation results from this effort will continue in FY 2016. The approach, which uses uncertainty quantification and sparse-grids sampling, was also applied to the study of instabilities in dual-fuel locomotive applications. The extent of cyclic variability observed for dual-fuel operation was not fully captured by the initial round of simulations, which focused on variability with a limited number of inputs. An expanded study is planned for FY 2016 to examine the impact of additional stochastic inputs and deterministic feedbacks.

GDI, a type of fuel injection, is used in modern engines for improved fuel efficiency and reduced emissions. Injector design is currently a lengthy, labor-intensive process typically involving numerous hardware iterations. GDI injector design was selected for this project because of the potential to automate the design process, reducing costs and reducing the design cycle from months to weeks. The approach used involves an optimization routine to coordinate parallel fuel-spray and combustion simulations with different injector geometries to hasten convergence on an optimal design. Current efforts are focused on developing and validating a high-fidelity multiprocessor simulation tool for more accurate spray modeling to enable virtual design and optimization of injectors. Results show good qualitative agreement with experimental data over a range of operating conditions, including accurately capturing the transition to flash boiling at higher fuel temperatures and lower cylinder pressures (Figure 2). Future efforts will focus on additional refinement of the model to better predict plume mixing and the inclusion of combustion to evaluate engine performance and efficiency.

During FY 2015, the use of Oak Ridge Leadership Computing Facility HPC resources for the combustion stability studies was supported through two DOE Office of Science 2014 Advanced Scientific Computing

Research Leadership Computing Challenge awards. A Director's Discretionary Research allocation supported GDI fuel injection project efforts on Titan during FY 2015.

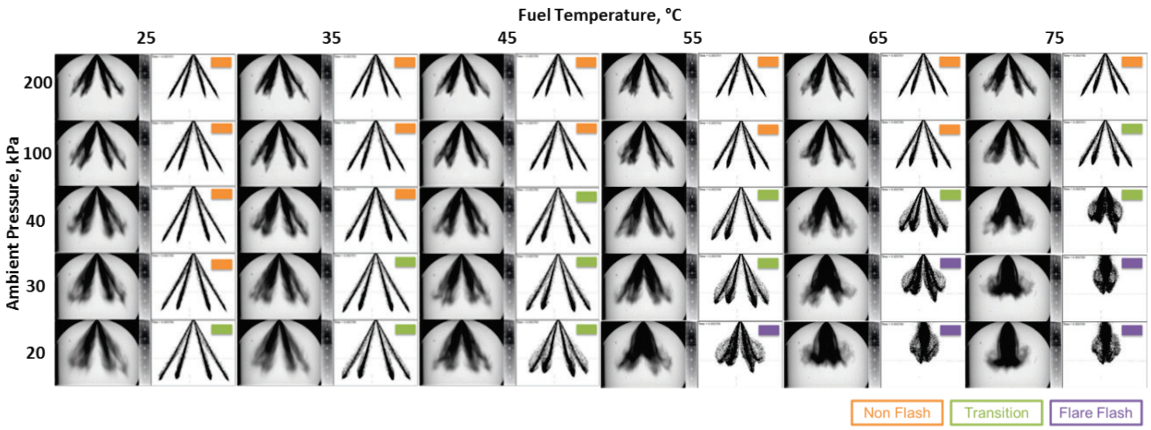

Figure 2. Improving predictive models of injector flow and cavitation. Internal nozzle flow simulations capture transition to flash boiling at high temperature and low pressure.

Publications, Presentations, and Patents

1. K. D. Edwards, C. E. A. Finney, S. Pannala, W. R. Elwasif, M. K. Stoyanov, R. M. Wagner, and C. S. Daw. 2015. "Accelerating Predictive Simulation of IC Engines with High Performance Computing" presented at the 2015 DOE Vehicle Technologies Office Annual Merit Review, Crystal City, Virginia, June 8–12, 2015.

2. R. O. Grover Jr., T. W. Kuo, W. R. Elwasif, S. Pannala, K. D. Edwards, and R. M Wagner. 2015. "Multi-Hole Injector Optimization for Spark-Ignited Direct-Injection Gasoline Engines." presented at the 2015 OLCF Users Meeting, June 23–25, 2015, Oak Ridge, Tennessee.

3. C. E. A. Finney, K. D. Edwards, M. K. Stoyanov, and R. M. Wagner. 2015. "Application of High Performance Computing for Studying Cyclic Variability in Dilute Internal Combustion Engines." accepted for presentation at the 2015 ASME Internal Combustion Engine Division Fall Technical Conference, November 8–11, 2015, Houston, Texas, as ASME ICEF2015-1172, doi: 10.1115/ICEF2015-1172.

Energy Storage

Nondestructive Evaluation Techniques for Processing High-Energy Lithium Ion Batteries

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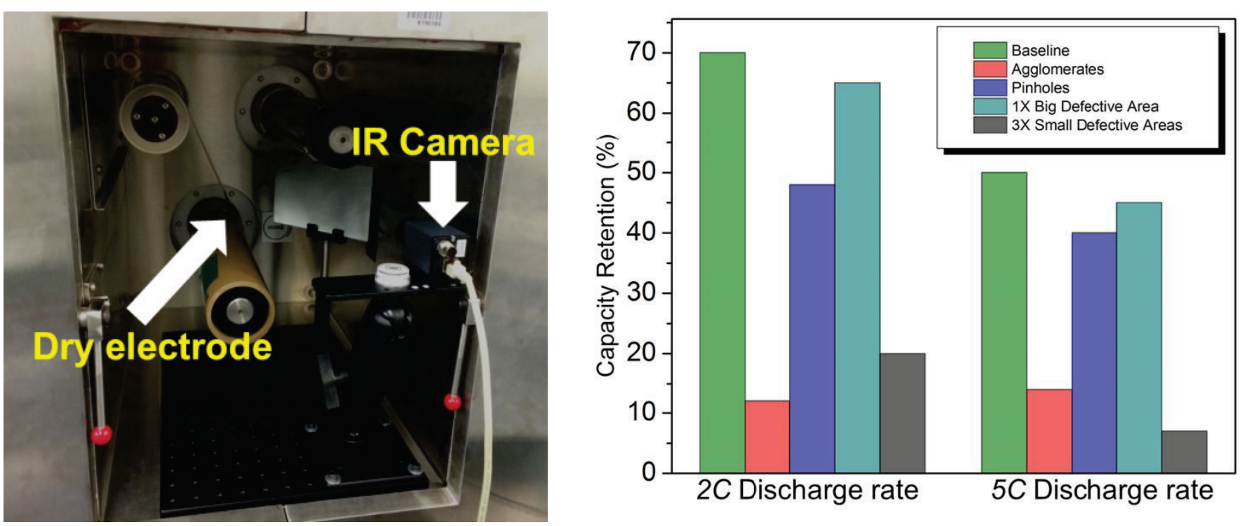
For electric vehicles to successfully compete with vehicles powered by internal combustion engines, battery efficiencies must be improved and costs must be brought down.

One way to bring production costs down and in some cases improve efficiency at the same time is through better defect control and elimination of the associated scrap and waste. Currently in-line nondestructive evaluation (NDE) techniques used in other industries have not been adapted to the roll-to-roll processing used in the lithium ion battery (LIB) industry. Continuous, in-line monitoring and NDE of the electrodes during the manufacturing process would improve overall quality and performance of LIBs and would help to avoid waste by detecting flaws and defects at or near the manufacturing step where they are created, allowing adjustments to prevent additional flaws and defects before final cell assembly.

ORNL is teaming with battery manufacturers and colleagues at the National Renewable Energy Laboratory (NREL) to develop in-line NDE techniques applicable to LIBs. In 2015 they undertook a thorough investigation of electrode coating defects, including microstructural analyses of defective electrodes, and correlated them with electrochemical performance to better understand the effects of specific defects on device performance. Such correlations are essential to establishing pass/fail criteria for NDE of electrodes.

The following defects, which diminish battery performance and shorten battery life, were investigated: agglomerates, pinholes, nonuniform coating, and metal particle contaminants. The results revealed that the type of defect determines the extent of capacity degradation at high discharge rate.



(a) Experimental setup of the infrared detection system for electrode coating defects on an ORNL slot die coater. (b) Comparison of the impacts of various types of electrode coating defects on the performance of coin cell electrodes compared with the performance of a defect-free baseline electrode after 200 full coin cell cycles.

The ability of infrared (IR) thermography to detect these defects, porosity (which plays a major role in the lithium-ion transport process and thus battery efficiency), and other battery characteristics was also investigated, with positive results. Further development of a combined defect detection and porosity measurement NDE system based on the IR thermography technology will be explored in 2016.

The findings from this research have broad applicability to advanced manufacturing processes and to other electrochemical products such as fuel cells, membrane electrolyzers, supercapacitors, flexible displays, and flexible sensors. Because of this, the technology development at NREL was funded through the DOE Fuel Cell Technologies Office to investigate quality control for fuel cell membrane electrode assembly and gas diffusion layers and at ORNL through the DOE Vehicle Technologies Office to investigate quality control for battery electrodes.

Publications, Presentations, and Patents

1. D. Mohanty, J. Li, R. Born, C. L. Maxey, R. B. Dinwiddie, C. Daniel, and D. L. Wood. 2014. "Reducing the Scrap Rate in Lithium-Ion Battery Manufacturing by Implementing In-Line Non-Destructive Electrode Evaluation Techniques." presented at the 3rd International Conference and Exhibition on Materials Science & Engineering, San Antonio, Texas, October 6–8, 2014. (Invited)

2. D. Mohanty, J. Li, S. Nagpure, D. L. Wood, III, and C. Daniel. 2015. "Correlating Electrode Defects with Electrochemical Performance of Lithium-Ion Batteries." presented at the 2015 MRS Spring Meeting and Exhibit, San Francisco, April 6–10, 2015.

3. D. Mohanty, J. Li, C. Daniel, and D. L. Wood. 2015. "Effect of Electrode Manufacturing Defects on Electrochemical Performance of Lithium-Ion Batteries; Cognizance of the Battery Failure Sources." *Journal of Power Sources* (submitted).

Patented Aqueous Processing Technology Demonstrates Performance and Durability

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

Lithium ion batteries (LIBs) are among the leading contenders to provide power for battery electric vehicles (BEVs). However, current LIBs are too expensive for BEVs to be competitive with vehicles powered by internal combustion engines. Two avenues for major cost reductions are raw materials synthesis and materials processing, which combined constitute 80% of the total cost of EV batteries.

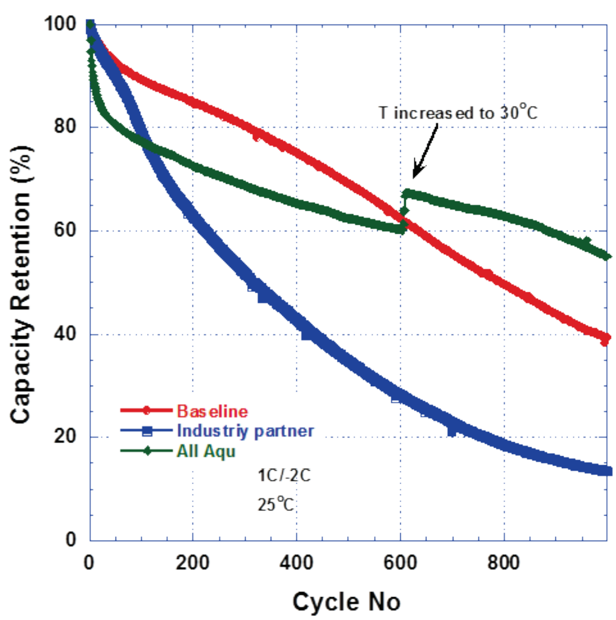
Researchers at the DOE Battery Manufacturing R&D Facility at ORNL are working with battery manufacturers, material suppliers, equipment manufacturers, and colleagues at other national labs to develop their patented TACLE (tailored aqueous colloids for lithium ion electrodes) technology to transform LIB electrode manufacturing by reducing manufacturing costs, mitigating environmental impacts, and increasing LIB energy density.

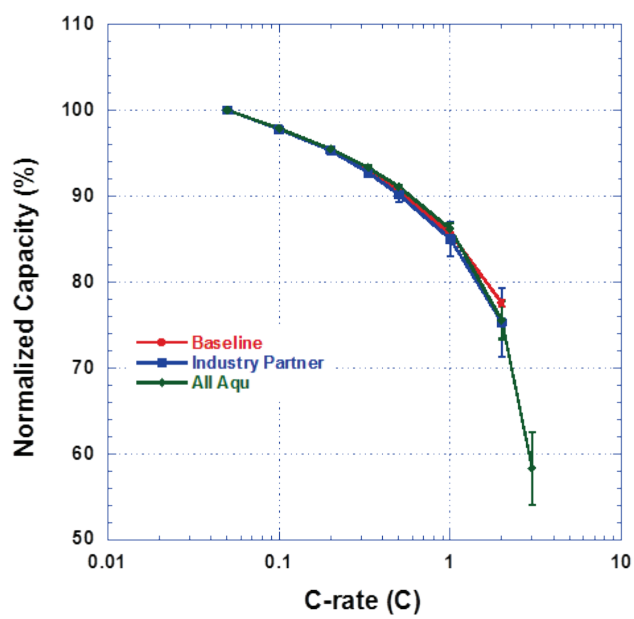
TACLE, as the definition implies, is an aqueous process for electrode manufacture. Currently most cathodes are manufactured using a costly organic solvent, N-methyl-2-pyrrolidone (NMP). NMP is both expensive (> $1.25/L) and toxic, produces flammable vapors, and requires expensive machinery and costly solvent recovery. In the ORNL TACLE process, NMP is replaced with deionized water ($0.015/L), enabling materials and processing cost savings and eliminating the costly NMP recovery process. The waterborne binders used in the process are also more environmentally friendly than conventional ones.

In 2015, project researchers concentrated on scaling up the process to larger-format pouch cells; incorporating steps and materials to increase electrode conductivity and energy density, including controlling particle-size distribution, electrode porosity, pore-size distribution, and the porosity gradient in the electrodes; investigating the effect of doubling electrode thicknesses on power density; confirming potential cost savings from the process; and comparing cell performance to cells made with conventionally manufactured electrodes.

Pouch cells with water-based electrodes exhibited similar capacity and performance to those manufactured using conventional techniques up to 600 deep-discharge cycles and were projected to outperform them in extended cycling. Also, capacity for the cells with aqueous electrodes could be boosted by increasing cell temperature from 25°C to 30°C. However, even without the temperature change, capacity retention of the all-aqueous-processed cells was much higher than the baseline cells after 1,000 cycles, confirming that the electrodes made via aqueous processing have better long-term cyclability than conventionally processed electrodes. The additional advancement of doubling electrode thicknesses not only will increase power density, but also will reduce costs through use of fewer inactive components in cells.

In addition, researchers developed step-by-step guidelines for introducing aqueous processing in existing or new LIB manufacturing plants.





Comparison of pouch cell performance with ORNL baseline electrodes, ORNL all-aqueous-processed electrodes, and aqueous-processed cathodes with conventionally processed anodes from a prominent industry partner: capacity retention under accelerated degradation (a) and rate capability (b).

Publications, Presentations, and Patents

1. J. Li, D. L. Wood, C. Daniel, and B. L. Armstrong. 2015. "Aqueous Processing of Composite Lithium Ion Electrode Material." US Patent 8,956,688 (UT-Battelle, LLC), February 17, 2015.

2. D. L. Wood, J. Li, and C. Daniel. 2015. "Prospects for Reducing the Cost of Lithium Ion Electrode Processing and Pouch Cell Formation Steps." *Journal of Power Sources* **275**, 234–242.

3. J. Li, C. Daniel, and D. L. Wood. 2015. "Effect of Interface between Current Collector and $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ Composite Cathodes on the Electrode Performance." presented at the 227th ECS Meeting, Chicago, Illinois, May 24–28, 2015.

4. J. Li, Claus Daniel, and D. L. Wood. 2015. "Coating of $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ Cathode on Various Substrates via Slot-Die Coating and Their Performance." presented at the European Coating Symposium 2015, Eindhoven, Netherlands, September 9–11, 2015.

5. D. Wood, J. Li, C. Daniel, and B. L. Armstrong. 2014. "Aqueous Colloidal Chemistry for Low-Cost Green Manufacturing of Lithium -Ion Battery Electrodes." presented at the Materials Science & Technology 2014 Symposium on Advanced Solution and Colloidal Processing for Ceramics, Pittsburgh, Pennsylvania, October 12–16, 2014 (invited).

State-of-the-Art Diagnostics Applied to High Voltage, High Capacity Lithium-Manganese-Rich Cathodes

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Affordable high voltage, high capacity batteries will be necessary for battery electric vehicles to displace other types of vehicles in transportation applications. Lithium ion batteries (LIBs) made with cathodes of lithium-manganese-rich (LMR) oxides are of particular interest because of their high initial capacity and operating voltage. However, after a minimum number of charge-discharge cycles, they undergo an irreversible structural change that severely degrades performance.

Researchers at ORNL and colleagues at Argonne National Laboratory are using state-of-the-art analytic techniques to better understand the nature of this structural change and to determine whether the change truly is irreversible.

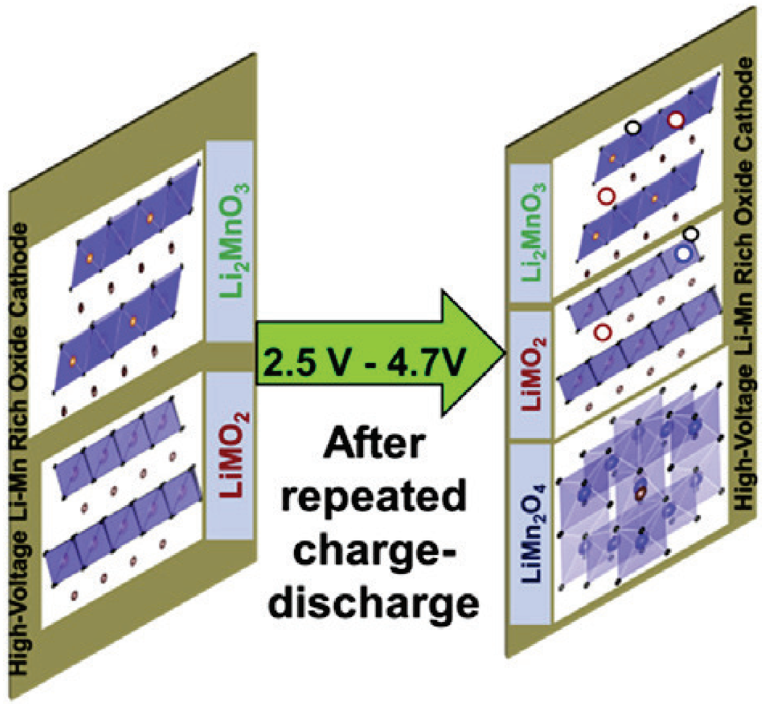
In 2015, they used the temperature-dependent magnetic susceptibility technique to study structural changes and the electronic states of the transition metal ions in the oxide lattices of cathode samples from LIB pouch cells. Magnetic susceptibility, based on whether a material is repelled by or attracted to a magnetic field, was selected because of its sensitivity in detecting structural changes and related electrical properties.

Using the technique, they were able to show direct evidence of irreversible structural changes in the LMR oxides from the pouch cells after a minimal number of charge-discharge cycles (26 in the study). The results support the hypothesis that the layered LMR material transforms from a layered to a spinel structure with $LiMn_2O_4$ as the dominant phase because of the formation of lithium vacancies and oxygen loss, which blocks the ion transport pathways in the oxide lattice, leading to capacity and voltage fading. The results also demonstrate the utility of the magnetic susceptibility technique for understanding structural changes in complex layered oxides.

Publications, Presentations, and Patents

1. D. Mohanty, J. Li, S. Nagpure, D. L. Wood III, and C. Daniel. 2015. "Understanding the Structure and Structural Degradation Mechanisms in High-Voltage Lithium-Ion Battery Cathode Oxides: A Review of Materials Diagnostics." *MRS Energy & Sustainability* **2**; doi:10.1557/mre.2015.16.

2. D. Mohanty, A. S. Sefat, E. A. Payzant, J. Li, D. L. Wood III, and C. Daniel. 2015. "Unconventional Irreversible Structural Changes in a High-Voltage Li-Mn-Rich Oxide for Lithium-Ion Battery Cathodes." *Journal of Power Sources*, **283**: 423–428.



Development of spinel structure in lithium-manganese-rich oxide cathodes with repeated cycling.

Lightweight Materials

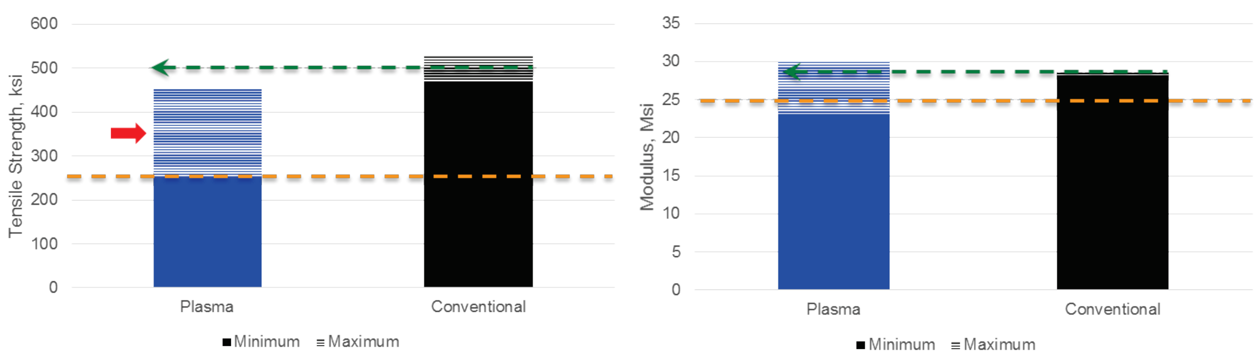
Advanced Oxidative Stabilization of Carbon Fiber Precursors

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

The total manufacturing cost of carbon fiber (CF) is one of the single largest obstacles to its incorporation in future automotive systems, and 43% of the cost is attributable to the conversion of the precursor into CF and activating the surface for resin compatibility. Conventional oxidation, part of the conversion step, 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 would appreciably lower the fiber cost.

ORNL has been working with RMX Technologies to develop a plasma-processing technique to rapidly and inexpensively oxidize polyacrylonitrile precursor fibers to produce lower-cost CF with properties suitable for use by the automotive industry. Essential to the success of this project was meeting critical technical criteria, including DOE strength goals (≥ 25 Msi tensile modulus, ≥ 250 ksi tensile strength, and ≥ 1.0% ultimate elongation in the finished fiber); repeatable and controllable processing; and significant unit cost reduction compared with conventional processing. FY 2015 was the final year of DOE funding for the project, and all project goals and technical criteria have been met.

The technology has been successfully demonstrated to a variety of companies in the CF industry, and industry interest is strong. RMX is negotiating to license ORNL's rights to the intellectual property covering plasma oxidation. (RMX already has rights to this intellectual property through co-invention.) RMX and its subsidiary, 4M Industrial Oxidation, have already begun scaling up this technology with its industry partner, C. A. Litzler Co., Inc., with the goal of demonstrating the technology to industry at a scale of 175 MT/year.



Tensile strength of plasma-oxidized, conventionally carbonized fiber vs. conventionally oxidized/carbonized fiber (a) and modulus of plasma-oxidized, conventionally carbonized fiber vs. conventionally oxidized/carbonized fiber (b). The green dashed arrows project the average conventional results to plasma results; the orange dashed lines denote the DOE program minimum. The red arrow in (a) points out the large variation in this parameter, which is due to the wide variation of carbonization conditions explored at ORNL.

Publications, Presentations, and Patents

1. F. L. Paulauskas and T. A. Bonds. 2015. "Advanced Oxidation and Stabilization of PAN-Based Carbon Precursor Fibers." presented at the 2015 US Department of Energy Hydrogen and Fuel Cells Program and Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting on June 11, 2015.

Better Predictive Engineering Tools for Improved Thermoplastic Composites

Contact: Vlastimil Kunc, kuncv@ornl.gov, 865-919-4595, and C. David Warren, warrencd@ornl.gov, 865-574-9693

The strength of fiber-reinforced composite materials is related to the length and orientation of the reinforcing fibers. Longer fibers impart greater load-bearing strength to the matrix, and such composites are typically stronger in the orientation direction of the fibers. One of the problems for automotive component design using chopped carbon fibers (CFs) is the lack of validated models.

ORNL is leading a project to validate three-dimensional models for long-fiber-reinforced, thermoplastic (LFT), injection-molded composites containing CF. Advanced characterization techniques are being used to generate a database of experimental results for the CF orientation and CF length distribution within a component. Computational models that have been validated using a part with features representative of an automotive component and the database of results will be made available to the general public via the World Wide Web. Additionally, this predictive technology led to the creation of a demonstration part that led to production implementation of a CF-LFT oil pan by Ford Motor Company.

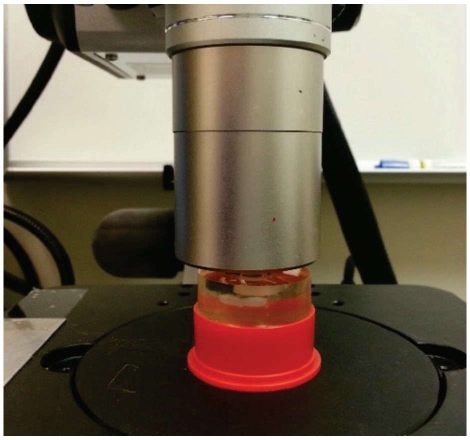
In FY 2015 the project team molded plaques and complex parts with four material compositions using qualified equipment and a combination of fast and slow fill speeds and high and low back pressures. Fiber orientations and fiber lengths were measured using previously reported techniques. Most of the experimental work has been completed, and predictions for complex parts can now be finalized before the experimental results for the complex part are released for comparison. During FY 2016, the team anticipates completing flow simulation for the complex part and reporting on the comparison of flow simulations and experimental measurements for the part.

The fiber orientation and fiber length prediction models validated in this project will be commercially available through Moldex 3D Northern America Inc. Experimental data used for validation will be available in a publically accessible format. Additionally, other industry participants on the project have indicated production intent.

Ultimately, the results of this project will enable the optimal design of lightweight automotive structural components using injection-molded LFTs.

Publications, Presentations, and Patents

None to report this period.



Fiber orientation distribution (FOD) sample being imaged (a) and example FOD image (b).

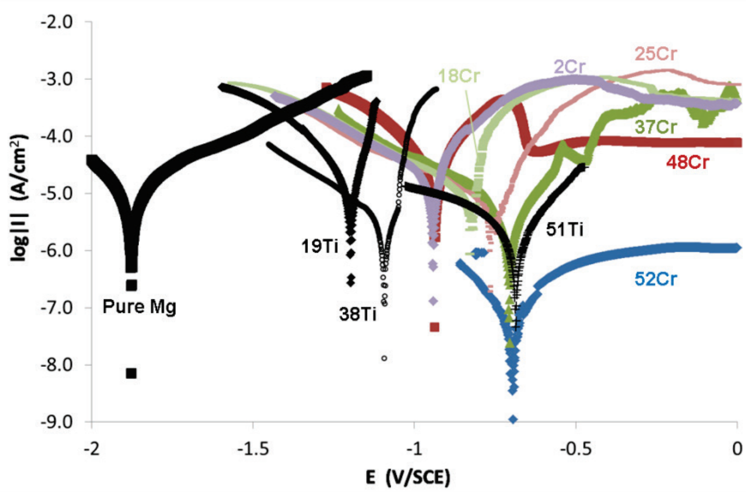
Corrosivity and Passivity of Metastable Magnesium Alloys

Contact: M. P. Brady, bradymp@ornl.gov, 865-574-5153

One way to improve fuel economy is to make vehicles lighter, sometimes referred to as "lightweighting." The high strength-to-weight ratio and castability of magnesium, the lightest of the structural metals, make it a good candidate for automotive lightweighting; however, traditionally its use has been low. One reason is its low corrosion resistance. Coupled with this is the fact that it is prone to galvanic corrosion when in contact with other metals—as is the case in many vehicle applications.

ORNL researchers have made significant efforts to understand the corrosion behavior and to improve the corrosion performance of magnesium alloys. Surface alloying offers the potential to dramatically enhance corrosion resistance without significantly altering a material's bulk properties and density. It may be possible to obtain a corrosion-resistant magnesium alloy through alloying with passivating elements such as Cr, Ti, Al, and Ni. The matrix phase, which is weakly corrosion resistant and thus preferentially attacked by corrosion, is a critical factor in magnesium alloy corrosion. Passivating the matrix phase through alloying with a strong passivating element would be a significant step toward improvement in overall corrosion resistance of magnesium alloys.

In this project the possibility of forming a passive film on magnesium alloys through adding strong passivating elements in metastable magnesium solid solution was investigated. The project manufactured and compared the behavior of ingot and magnetron-sputtered pure magnesium relative to magnetron-sputtered magnesium-titanium (Mg-Ti) and magnesium-chromium (Mg-Cr) alloys. A transition to passive-like behavior was observed for both Mg-Ti and Mg-Cr; however, the transition only occurred if the level of Ti or Cr exceeded that of the Mg (in atomic percent)—effectively shifting the alloy to Ti or Cr base. While this is of limited utility for conventional magnesium alloy design, insights from this research might prove beneficial to new classes of complex, multiple-element, high-entropy alloys. The findings may also provide guidance for coating approaches that enrich the local surface of an Mg alloy in Cr or Ti as both elements are commonly used in conversion coating strategies.



Polarization curves for pure magnesium and select magnetron-sputtered Mg-Cr and Mg-Ti alloys in saturated $Mg(OH)_2$ + 0.1 wt % NaCl solution. Alloy polarization curves shifted to the right and downward on the plot compared to the pure magnesium control curve, indicating an improved degree of corrosion resistance.

Publications, Presentations, and Patents

1. G. L. Song and K. A. Unocic. 2015. "The Anodic Surface Film and Hydrogen Evolution on Mg." *Corros. Sci.* **98**: 758–765.

2. G. L. Song, K. A. Unocic, H. M. Meyer III, E. Cakmak, M. P. Brady, P. E. Gannon, P. Himmer, and Q. Andrews. 2016. "The Corrosivity and Passivity of Sputtered Mg-Ti Alloys." *Corros. Sci.* **104**: 36–46.

3. G. L. Song and P. E. Gannon. 2016. "The Surface Films and Their Possible Roles for Mg Corrosion." presented at the 2016 TMS Annual Meeting and Exhibition, February 14–18, 2016, Nashville, Tennessee, and published in *Magnesium Technology 2016* (A. Singh, K. Solanki, M. V. Manuel, and N. R. Neelameggham, eds.), 285–290, John Wiley & Sons, Inc., Hoboken, New Jersey; doi: 10.1002/9781119274803.ch56.

DOE Carbon Fiber Technology Facility Continues to Chart Low-Cost Fiber Course

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

ORNL is home to the DOE Carbon Fiber Technology Facility (CFTF), a 42,000 ft^2 innovative technology facility offering a unique, highly flexible, highly instrumented carbon fiber line for demonstrating advanced technology scale-up and for producing market-development volumes of prototypical carbon fibers. CFTF serves as a national test bed for government and commercial partners to scale up emerging carbon fiber technology.

CFTF has been focused on addressing technical challenges that impact the cost per unit volume of carbon fiber. Significant advancements have been made in this area and in increasing the performance of textile-based polyacrylonitrile (PAN) carbon fiber precursors. During 2015, the following significant advances were made with textile-based PAN precursors and the carbon fibers made from them.

Modulus of the textile-based carbon fiber was increased to 41 Msi, with tensile strength of 423 ksi and greater than 1% strain. This meets the strength requirements of the automotive industry for carbon fiber composite structural applications. In addition, CFTF doubled the throughput volume of these same textile-based carbon fibers, which will have a significant impact on reducing operational cost per unit volume of carbon fiber.

CFTF conducted a 2-week nonstop baseline run with standard 24 K industrial-grade commercial PAN precursor to demonstrate process consistency and equipment reliability in a long continuous run. During this trial, 1,293 lb of carbon fiber was produced with an average tensile strength of 517 ksi (standard deviation 37.9) and tensile modulus of 34.1 Msi (standard deviation 0.4). The carbon fiber scrap rate was 2.1% of total carbon fiber produced. The start-up and shutdown precursor waste rate was 11% of total precursor consumed.

Four bands of large tow fibers entering the oxidation ovens.

A precursor prestretch simulation was performed to demonstrate the value to the conversion process of prestretching textile PAN and other alternative precursors. The initial simulation showed that the mechanical properties were unaffected by the prestretching vs. oxidative stretching, but the line speed could be increased by 20%. Additional trials are needed to engineer the equipment specifications of the prestretch station.

In addition, 650 visitors representing 110 companies toured CFTF, and CFTF produced 15,165.2 kg of carbon fiber, 12,407.2 kg of which was transferred to outside companies and research organizations for further research.

Future directions include developing multiple alternative precursor materials and economically attractive processing conditions to support them.

Publications, Presentations, and Patents

1. R. Ott. 2014. "Carbon Fiber Technology Facility Update." presented to the Oak Ridge Carbon Fiber and Composites Consortium, Knoxville, Tennessee, October 28, 2014.

2. C. Jackson. 2014. "Manufacturing of Low-Cost Carbon Fiber from Unmodified Textile PAN Fiber." presented at the Composites World 2014 Conference, La Jolla, California, December 10, 2014.

3. R. Ott. "ORNL Manufacturing Demonstration Facility and Carbon Fiber Technology Facility." presented at the American Carbon Society Workshop, Oak Ridge, Tennessee, April 16, 2015.

4. R. Chambers, J. Crabtree, and C. Jackson. *Method of Measuring Density of Oxidized and Carbonized Fibers In-Situ*. Invention disclosure 201503593, September 2015.

5. C. Jackson. *Method of Producing Carbon Fibers from Multipurpose Commercial Fibers*. Invention disclosure 201503583, September 2015.

6. C. Jackson. *Modular Line Configuration for Carbon Fiber Conversion*. Invention disclosure 201403438, December 2014.

Laser-Assisted Joining Process for Aluminum and Carbon Fiber Components Enables Use in Primary Automotive Structures

Contact: Adrian Sabau, sabaua@ornl.gov, (865) 241-5145

ORNL has demonstrated a breakthrough laser-structuring technology for joining carbon fiber polymer composites (CFPCs) and aluminum components. The innovations included texturing the aluminum and CFPC surfaces using a laser-interference technique, engineering rough surfaces before an adhesive bonding operation. 3M Company provided the adhesives; Plasan Carbon Composites, Inc., provided the composite; and Cosma, Inc., provided the aluminum.

Joining carbon fiber composites and aluminum for lightweight cars and other multimaterial high-end products could become less expensive, and the joints could be more robust because of this new method, which harnesses a laser's power and precision. Using an interference-based laser technique to either structure the surfaces or remove layers of material from surfaces before bonding improves the performance of the joints and provides an efficient, repeatable production process that can be automated for high-volume use.

ORNL's research effort focused on demonstrating the effect of the laser-interference structured surfaces of the aluminum and CFPC materials on joint performance. The following quality indicators were used for assessing joint performance: shear-lap strength, maximum load, displacement at which the maximum load was recorded, energy stored in the joint during tensile testing, and mode of failure (failure in the adhesive or failure in one component).

A significant increase in the mechanical properties of the shear-lap joints, which were made with laser-structured surfaces, compared to the baseline data demonstrated the proof of concept for the use of laser-structuring and/or laser-ablation technology for surface preparation of both CFPC and aluminum coupons before adhesive joining.

For a bondline thickness of 0.85 mm, the mechanical testing results showed that shear lap strength, maximum load, and displacement at maximum load were increased by 40%, 28%, and 100%, respectively, over those measured for the baseline joints. Also, joints made with laser-structured surfaces were found to absorb about 200% more energy than the conventionally prepared baseline joints. The maximum possible mechanical strength for the double-lap aluminum-CFPC joints was attained with 50% of the failure points occurring in the aluminum coupon, away from the joint.

Ultimately, two project participants, Cosma and Plasan, have the ability to commercialize this technology, which is attractive because the use of lighter weight, adhesively joined materials in automotive applications would reduce gas consumption and production of greenhouse gasses.

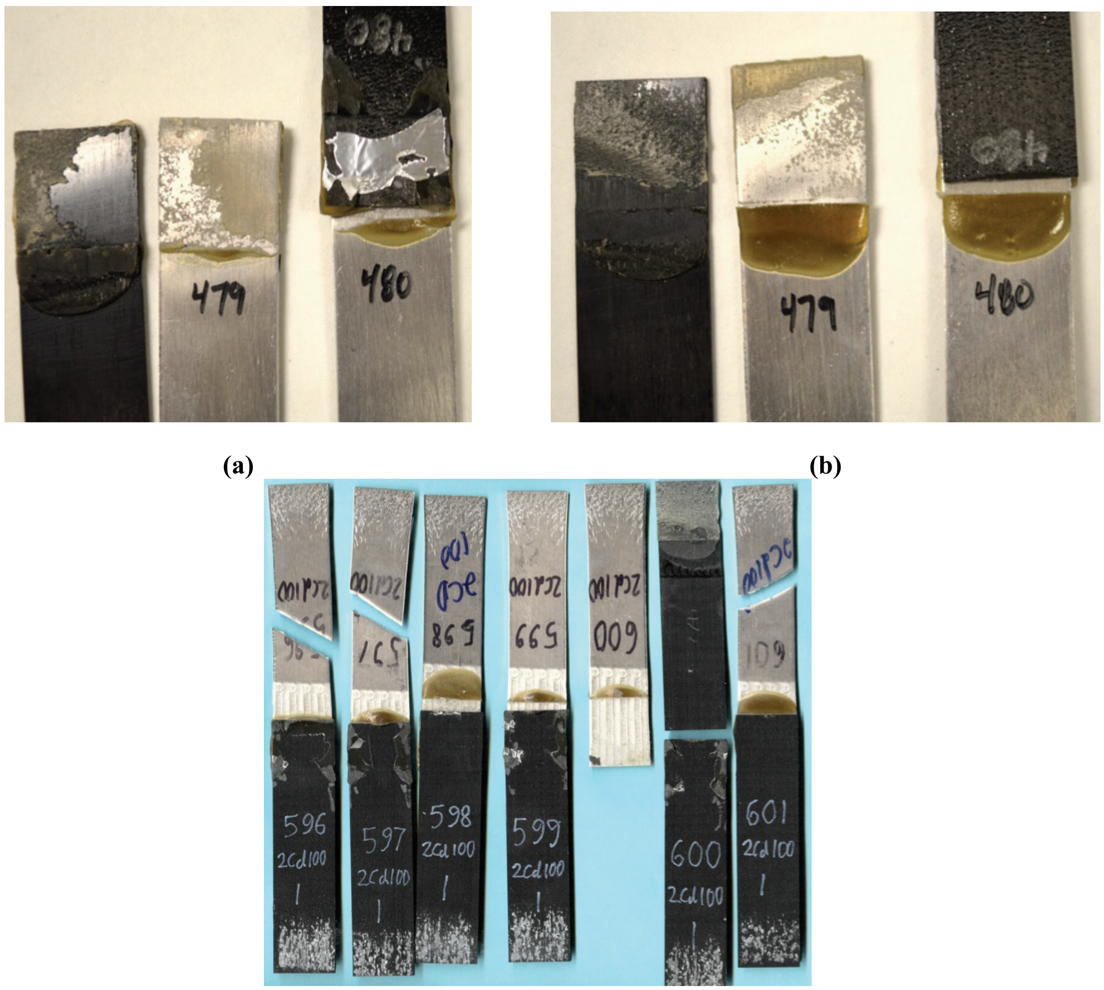
Publications, Presentations, and Patents

1. S. Sabau, C. M. Greer, J. Chen, C. D. Warren, and C. Daniel. 2016. "Surface Characterization of Carbon Fiber Polymer Composites and Aluminum Alloys after Laser Interference Structuring." *JOM* **68**: 1882–1889.

2. S. Sabau, J. Chen, C. D. Warren, D. L. Erdman III, C. Daniel, T. Skszek, and M. Caruso Dailey. 2016. "Laser Interference-Based Surface Treatment of Al and Carbon Fiber Polymer Composites for Enhanced Bonding." paper LB15-0070, SAMPE Conference and Exhibition, Long Beach, California, May 23–26, 2016.

3. J. Chen, A.S. Sabau, J. F. Jones, A. Hackett, G. D. Jellison, C. Daniel, and D. Warren. 2015. "Aluminum Surface Texturing by Means of Laser Interference Metallurgy." in 2015 TMS Annual Meeting & Exhibition, Proceedings: Light Metals 2015: Aluminium Processing, Orlando, Florida.

4. A. S. Sabau, J. Chen, J. F. Jones, A. Hackett, G. D. Jellison, C. Daniel, D. Warren, and J. D. Rehkopf. 2015. "Surface Modification of Carbon Fiber Polymer Composites after Laser Structuring." in *Advanced Composites for Aerospace, Marine, and Land Applications II*. T. Sano and T. S. Srivatsan, eds., John Wiley & Sons, Inc., Hoboken, New Jersey; doi: 10.1002/9781119093213.ch23.



(a) **(b)**

(c)

Pictures taken after mechanical testing of double-lap joints bonded with adhesive DP810 showing fracture surfaces and/or failure modes: (a, b) baseline joints (c) joints with laser-structured surfaces using a laser beam size of 6 mm.

Enabling Multimaterial Next-Generation Vehicles

Contact: C. David Warren, warrencd@ornl.gov, 865-574-6098; Michael P. Brady, bradymp@ornl.gov, 865-574-5153; and Zhili Feng, fengz@ornl.gov, 865-576-3797

DOE has estimated that using lightweight components and high-efficiency engines in just a quarter of vehicles on the road could save more than 5 billion gallons of fuel annually by 2030. While lightweight materials are making inroads in vehicles, most vehicles are still nearly 50% conventional steel. The multimaterial enabling project at ORNL is aimed at removing barriers to greater use of lightweight materials in vehicles, including lowering costs and developing enhanced processing techniques to handle these materials. Currently the project consists of three separate tasks: (1) developing a deeper understanding of protective film formation in magnesium alloys, (2) developing and commercializing a rapid, in-line, nondestructive evaluation (NDE) method for inspecting spot welds in an automotive production environment, and (3) developing a novel method for mitigating weld fatigue in advanced high-strength steels (AHSSs).

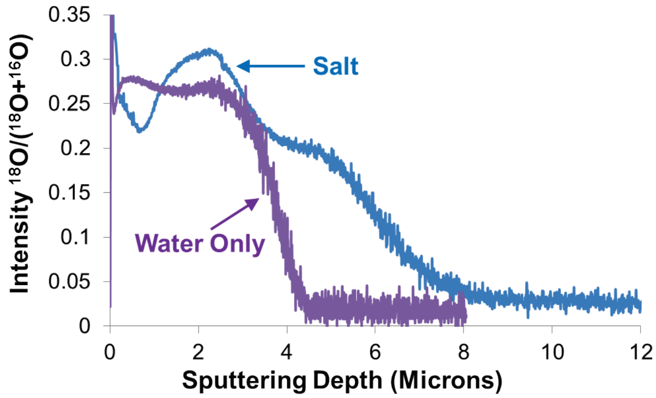
Protective film formation in magnesium alloys

Magnesium alloys are of interest to automotive manufacturers because of their high strength-to-weight ratio (highest of all structural metals), castability, and recycling potential. However, they are susceptible to corrosion, particularly in harsh automotive environments. The inability of magnesium alloys to establish a continuous and fully protective surface film under many exposure conditions is a key factor underlying their 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.

The goal of this task is to develop an improved understanding of how alloy composition, microstructure, and exposure conditions affect the establishment, continuity, nature, and growth of protective films on magnesium alloys. To accomplish this goal, researchers have used advanced characterization techniques not previously widely applied to magnesium surface film formation, and a major ancillary goal of the project is to assess which advanced characterization techniques are most amenable to providing new insights into film formation on magnesium alloys. These results will then serve as baseline information for evaluation of more corrosive environments (e.g., salt species), modified alloy compositions, and conversion coatings.

Work in FY 2015 focused on three main magnesium corrosion activities: (1) secondary ion mass spectrometry (SIMS) isotopic tracer aqueous film growth studies in the presence of salt; (2) studies of hydrogen uptake in aqueous exposures as a function of Al, Nd, and Zr alloying additions to Mg; and (3) studies on the effect of substrate composition on conversion coating formation in the as-conversion-coated condition and after subsequent e-coating.

Cross-section transition electron microscopy with sample preparation by focused ion beam techniques has proven particularly useful in understanding film/coating structure and chemistry. Application of the SIMS isotopic tracer study approach to magnesium corrosion is a key outcome of this project, with feasibility established for aqueous conditions with and without salt species and for elevated-temperature, humid-air oxidation. Given the formation of oxide-hydroxide films by magnesium, tracers incorporating both ^{18}O and deuterium can provide unique insights not achievable by other techniques. An unexpected finding was enhanced hydrogen uptake as a result of aqueous exposure in magnesium alloys containing zirconium and neodymium. This is potentially relevant to magnesium alloy design from a hydrogen embrittlement and stress corrosion cracking perspective and to functional use of magnesium alloys (e.g., in batteries or hydrogen storage). Although further work is needed, this research suggests a number of paths forward to more corrosion-resistant magnesium alloys, including advanced characterization of substrate–alloy-coating interfaces to optimize the synergy between alloy composition and subsequent conversion coating chemistry and structure and possible modification of coating parameters to avoid degradation of the initially formed conversion coating surface.



Fraction $^{18}O/(^{18}O+^{16}O)$ secondary ion mass spectrometry data (counts per second vs. sputtering depth) for commercial alloy Elektron 717 (a rare earth–zirconium magnesium alloy). Water-only exposure was 4 h D_2O + 20 h ^{18}O water. Salt exposure was 4 h D_2O + 20 h ^{18}O water with 0.01 wt % NaCl. Zero sputtering time corresponds to the film surface. The dip in the salt exposure data indicates a shift to mixed outward/inward film growth compared to inward-dominated film growth in pure water.

Online Weld NDE with Infrared Thermography

The development of resistance spot welding (RSW) for AHSSs is critical for enabling the broader implementation of AHSSs in vehicle structures for lightweighting and crashworthiness. Variations in welding conditions, part "fit-up," and other production conditions can result in out-of-tolerance joints that impair the quality and performance of vehicles. The increasing use of AHSSs and other lightweight metals is expected to pose even more stringent requirements on joint quality in the future. Thus, reliable quality inspection techniques are crucial for determining the quality of joints on the assembly line.

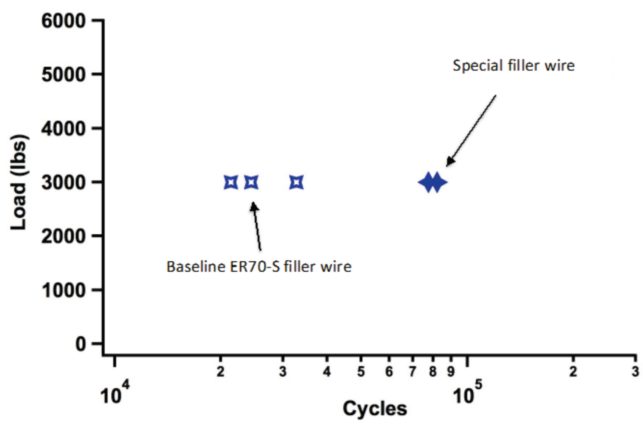
In FY 2011–2014, a prototype infrared-based system was developed for both real-time (online) and post-weld (online/offline) inspection applications. The inspection cycle is 1–2 seconds, fast enough to measure each weld made during the welding operation and to provide industry with a low-cost, nondestructive method for monitoring welds in real time. The system was extensively tested in the laboratory, where tests showed that it was able to positively identify welding defects, including lack of fusion and excessive indentation. In FY 2015, this technology was licensed by APLAIR Manufacturing Systems, a Tennessee-based company. ORNL is assisting APLAIR in scaling up the technology and prototype system to a commercial product. APLAIR plans to have a commercial product within 2 years.

The net result is that automakers now have an efficient method for sending immediate feedback to the production lines to correct weld quality issues, potentially saving the US automotive industry hundreds of millions of dollars per year. This new ORNL technology is a key enabler for automaker adoption of advanced high-strength, lightweight auto-body materials, which are more difficult to weld and inspect but will improve the fuel efficiency and safety of the vehicle fleet. As RSW is the primary auto-body assembly process for automotive companies worldwide, this new NDE technology has the potential to revolutionize the welding and assembly of automotive body structures.

Improving Fatigue Performance of AHSS Welds

Durability is one of the primary metrics in designing and engineering automotive body structures. Fatigue performance of welded joints is critical to the durability of body structures because the likeliest locations for fatigue failure are often at welds. Today's weld fatigue improvement techniques are mostly post-weld based. The added steps are cost prohibitive in the high-volume mass-production automotive environment, and large variability exists in the fatigue life achieved by the postweld–based techniques. In this project, ORNL and industry partner ArcelorMittal worked together to develop effective in-process ways to control and mitigate the key factors governing the fatigue life of AHSS welds, including weld residual stress, weld profile, and weld microstructure/chemistry. The joint research used state-of-the-art integrated computational welding engineering; neutron, synchrotron, and other advanced residual stress measurement techniques; and fatigue testing and microstructure analysis capabilities at ORNL to perform project R&D.

The project was successfully completed during FY 2015. Weld fatigue life improvements of 3 to 5 times and 5 to 10 times were demonstrated using two novel approaches developed during the project to control and mitigate the weld residual stresses. The improvements in weld residual stresses could also drastically change the welding-induced distortion in thin sheet steels used for auto-body structural components. The potential of ORNL–US Army–developed low transformation temperature weld wires to mitigate hydrogen-induced cracking in welding of high-strength steels was also demonstrated during the project. While the project focused on AHSSs, the techniques developed may also be applicable to welding of other lightweighting materials such as aluminum and magnesium alloys.



Comparison of weld fatigue lives of baseline ER70-S filler wire vs. the new filler wire developed during this project.

Publications, Presentations, and Patents

1. M. P. Brady, M. Fayek, H. M. Meyer, D. N. Leonard, H. H. Elsentriecy, K. A. Unocic, L. M. Anovitz, E. Cakmak, J. R. Keiser, G.-L. Song, and B. Davis. 2015. "Tracer Study of Oxygen and Hydrogen Uptake by Mg Alloys in Air with Water Vapor." *Scripta Materialia* **106**: 38–41.

2. M. P. Brady, G. Rother, L. M. Anovitz, K. C. Littrell, K. A. Unocic, H. H. Elsentriecy, G. L. Song, J. K. Thomson, N. C. Gallego, and B. Davis. 2015. "Film Breakdown and Nano-Porous Mg(OH)2 Formation from Corrosion of Magnesium Alloys in Salt Solutions." *Journal of the Electrochemical Society* **162**(4): C140–C149.

3. J. Chen, Z. Feng, and W. Zhang. W. Software, *IR Spot Weld Inspector*. Copyright 50000074, April 2014.

4. Z. Feng, Z. Yu, S. David, and D. Tzelepis. *High-Strength Weld Wire for Hydrogen Embrittlement Control*. US Patent Application 14/614,439, Filed February 5, 2015.

5. G.-L. Song, et al. 2014. "Film Evolution on Mg Alloys." presented at Materials Science & Technology 2014, Pittsburgh, October 12–16, 2014.

6. Z. Wang, Z. Yu, and Z. Feng. 2015. "Effect of Low Transformation Temperature Welding Consumables on the Weld Microstructure and Mechanical Properties." presented at the 2015 AWS Annual Convention, Chicago, 2015.

7. Z. Wang, Z. Yu, Z. Feng, and S. Liu. 2014. "Effect of Low Transformation Temperature Welding Consumables on Mechanical Properties of Lap Joints." presented at the 2014 AWS Annual Convention, Atlanta, 2014.

Power Electronics and Electric Motors

ORNL Demonstrates 10 kW Bidirectional Wireless Power Transfer System

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

ORNL developed and demonstrated the world's first level 2 (10 kW) bidirectional wireless power transfer system. The system achieved efficiencies greater than 90% and charging speeds equivalent to plug-in charging.

The bidirectional wireless charging system offers flexibility with several architectures available along with dc and ac interfaces for energy storage and grid applications. As part of the development process, researchers conducted simulations and experimental evaluation of the use case scenarios. The bidirectional wireless charger can transfer power between the stationary (home) energy storage system and the vehicle battery. The vehicle can be powered from the grid, and the vehicle can power the building loads, or power can be transferred to the grid.

With this capability, the vehicle can be used as an emergency backup power source, and several benefits can be realized on the customer side of the meter (e.g., peak shaving; improvements in power factor, load factor, and power quality; reactive power compensation; time-of-use energy management; demand charge management; and renewables integration). The system can also provide a target amount of power to the grid, which enables the grid ancillary services such as regulation, spinning/nonspinning reserves, and voltage control.

ORNL demonstrated the bidirectional wireless charging technology through the Additive Manufacturing Integration Energy (AMIE) project. AMIE leveraged expertise across the ORNL programs funded by the DOE Office of Energy Efficiency and Renewable Energy, bringing together researchers and resources focused on vehicles, manufacturing, and buildings. The team created a novel printed utility vehicle (PUV) and a building that exchange energy via smart controls and bidirectional wireless power transfer.

The AMIE PUV generates energy using a hybrid electric powertrain with a small (5.5 kW) engine/generator fueled by two compressed natural gas storage tanks. Energy flows from the generator to the PUV battery to the charging coil attached to the underside of the car. When the PUV is parked, the vehicle charging coil sends energy across an air gap to a wireless charging pad on the ground. Inductive charging transfers the energy from coil to coil. The charging pad sends electricity to the building, where it can power appliances or recharge the home's battery.

The AMIE project offers a platform for evaluating new technologies and integrated energy systems that increase efficiency for transportation, buildings, and the grid.

Publications, Presentations, and Patents

1. M. Chinthavali, O. C. Onar, S. L. Campbell, Z. Wang, C. P. White, and L. Seiber. 2016. "A 10-kW Level-II Bidirectional Wireless Power Transfer System for Grid Services and Export Power." submitted to the IEEE Applied Power Electronics Conference and Exposition, March 2017.

2. J. M. Miller, P. T. Jones, J.–M. Li, and O. C. Onar. 2015. "ORNL Experience and Challenges Facing Dynamic Wireless Power Charging of EVs." *IEEE Circuits and Systems Magazine* **15**(2) 40–53. May 2015.

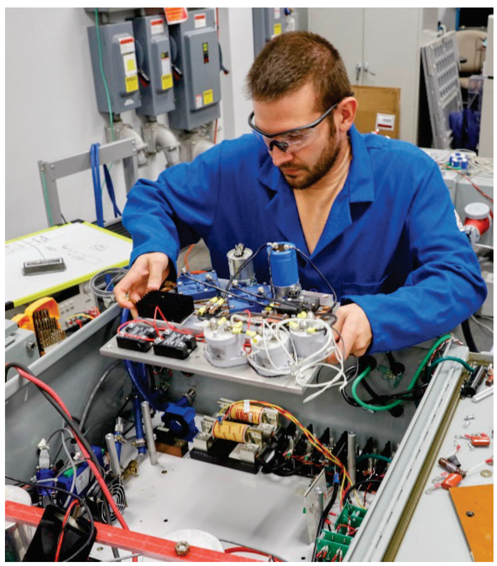
3. J. M. Miller, O. C. Onar, and M. Chinthavali. 2014. “Primary Side Power Flow Control of Wireless Power Transfer for Electric Vehicle Charging.” *IEEE Journal of Emerging and Selected Topics in Power Electronics—Special Issue on Wireless Power Transfer* **3**(1), 147–162. December 2014.

4. O. C. Onar. 2015. “Recent Advances in Wireless Power Transfer Systems.” IEEE Applied Power Electronics Conference and Exposition, Industry Special Session on Recent Development in Wireless Power Transfer, March 2015, Charlotte, NC.

5. J. M. Miller (Moderator), T. Bohn, O. C. Onar, J. Taiber, and M. de Rooji. 2015. “Wireless Power Transfer: Facts and Fictions.” RAP Session at the IEEE Applied Power Electronics Conference and Exposition, March 2015, Charlotte, NC.

6. O. C. Onar. 2014. “Electric Vehicles without Plugging-In.” Presentation at the University of Tennessee Science Forum, November 2014, Knoxville, Tennessee.

7. O. C. Onar.2014. “Electric Vehicles without Plugging-In” Presentation to the Technical Society of Knoxville, November 2014, Knoxville, Tennessee.



Steven Campbell works with the electronics that enable wireless controls and communications between the grid and the wireless charging coils in the ORNL bidirectional wireless power transfer system.

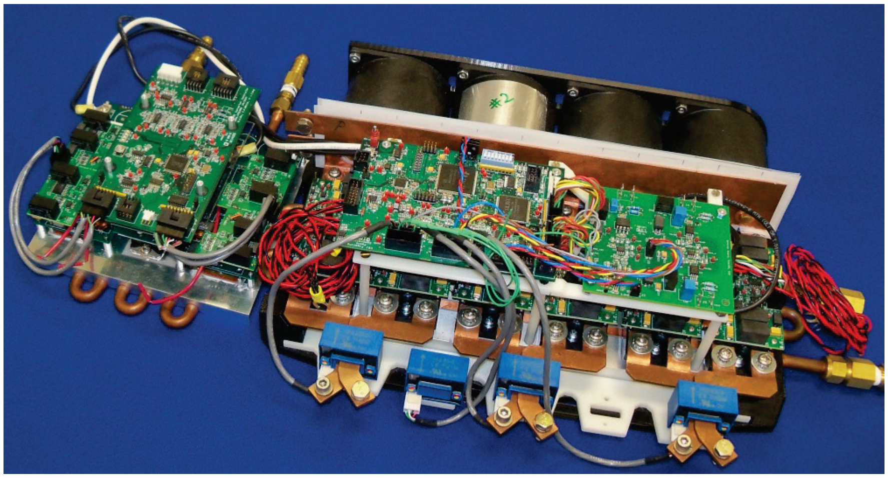
Bidirectional wireless charging technology enabled energy to flow between this novel printed vehicle and building as part of the Additive Manufacturing Integrated Energy demonstration project.

ORNL's Innovative Onboard Battery Charger Technology: Double the Power Density at Half the Cost

Contact: Gui-Jia Su, sugj@ornl.gov, 865-946-1330

The stand-alone onboard battery chargers (OBCs) and 14 V dc-dc converters that are currently prevalent in 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. In addition, they are unidirectional; that is, they can charge the battery but are not capable of vehicle-to-grid support, a highly desirable function for future smart grids. ORNL plans to leapfrog these limitations in a multiyear project to replace current silicon-based charger technology with wide bandgap (WBG) silicon carbide (SiC) devices, advanced magnetic materials, and a novel integrated charger architecture and control strategy.

A major task for FY 2015 was designing, building, and testing an all-SiC 6.8 kW bidirectional OBC prototype that integrates a 6.8 kW isolation converter into a 100 kW segmented traction inverter. The architecture reduces the number of components significantly (a 47% reduction in power circuit components alone, not counting savings in the gate driver and control logic circuits), translating to a 50% reduction in cost and volume compared with existing stand-alone OBCs. In addition, SiC-based devices are used in the converter and inverter to further reduce the cost, weight, and volume of the passive components and improve system efficiency. The isolation converter has a built-in 2 kW, 14 V buck (voltage-reducing) converter to meet vehicle accessory electrical loads and an ORNL-developed control strategy to reduce the battery ripple current that is inherent in single-phase ac-dc converters. Test results show that 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. Test results also showed a high charging efficiency with a peak value of 96.5% and an improvement of more than 2% over a silicon-based counterpart. Work planned for FY 2016 will focus on further reducing the weight and volume of the isolation converter by using gallium nitride devices and advanced packaging technology.



ORNL's all-SiC 6.8 kW bidirectional OBC prototype with integrated 6.8 kW isolation converter and 100 kW segmented traction inverter.

Publications, Presentations, and Patents

1. G. J. Su. 2014. "Innovative Technologies for Converters and Chargers." presented at the DOE Vehicle Technologies Office Electric Drive Technologies Advanced Power Electronics and Electric Motors R&D FY 2015 Kickoff Meeting, Oak Ridge, Tennessee, November 18–20, 2014.

2. G. J. Su. 2015. "Innovative Technologies for Converters and Chargers." presented at the 2015 DOE Hydrogen and Fuel Cells Program and Vehicle Technologies Office Annual Merit Review and Peer Evaluation Meeting, Arlington, Virginia, June 8–12, 2015.

3. G. J. Su and L. Tang. 2015. "An Integrated Onboard Charger and Accessory Power Converter using WBG Devices." in Proceedings of the 7th IEEE Energy Conversion Congress and Exposition (ECCE 2015), 6306–6313, Montreal, Canada, September 20–24, 2015.

Sintered-Silver Interconnect Technology for High-Performance Wide-Bandgap Devices

Contact: Andrew Wereszczak, wereszczakaa@ornl.gov, 865-946-1543, or Zhenxian Liang, liangz@ornl.gov, 865-946-1467

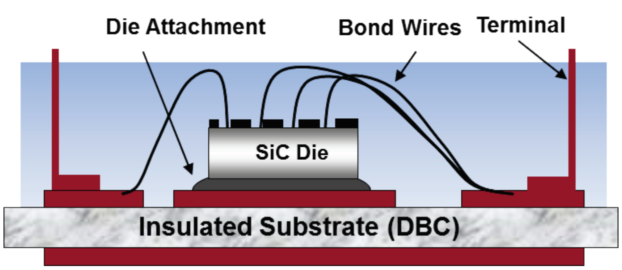
Wide-bandgap (WBG) semiconductors such as those made from silicon carbide (SiC) permit devices to operate at much higher temperatures, currents/voltages, and frequencies—making power electronic modules using these materials significantly more powerful and energy efficient than those made from conventional silicon semiconductors. They also offer greater efficiency in converting electrical power and in operating the electric traction drive during vehicle use.

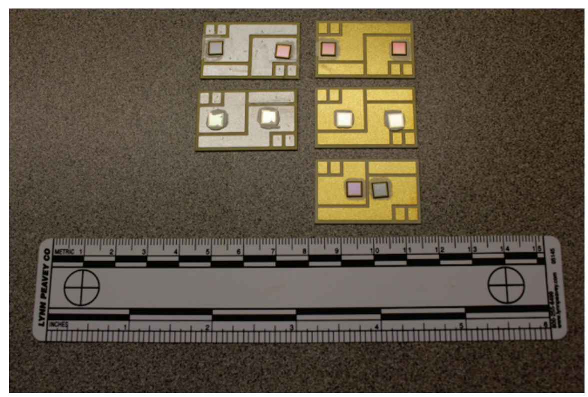
Sintered-silver die bonding or interconnection is part of a comprehensive ORNL program, sponsored by the DOE Vehicle Technologies Office, to bring all-SiC power modules to market through advanced packaging technologies that exploit SiC's superior performance in such devices.

Current state-of-the-art interconnects (die bonds) are soldered, but the sintered-silver interconnect is quite different. The silver bond forms from a paste (composed of micron and submicron silver particles and other additives) during the sintering process and is known to be a superior die attachment material compared with a solder layer. It offers much better electrical, thermal, and especially thermomechanical properties for power module packaging. These properties are especially critical to SiC power devices, allowing them to operate at temperatures higher than those of silicon devices. Silver sintering currently also includes an additional process of mechanically pressing the stack of dies and substrates during heating that ORNL is attempting to eliminate via other process modifications. The quality of the bond formed between die and substrate can be affected by many factors, such as finishing metals on the die and substrate, geometry of the die, patterns on the substrate, and process parameters—pressure, heating temperature, and heating time. The ORNL-led research is aimed at a deeper understanding and process refinement of sintered-silver interconnection. The ultimate goal is to determine the elements necessary to consistently produce reliable sintered-silver joints as economically as possible.

During 2015, custom-designed sintered-silver test coupons were fabricated to enable measurement of shear strength, perform failure analyses, and examine the effect of coefficient-of-thermal-expansion–induced residual stress on sintered-Ag joints and the onset of delamination of the interconnect.

The shear strengths of sintered-silver interconnect systems were on the order of 40 to 50 MPa—about twice the strength of soldered joints. Preliminary failure analysis showed the concurrency of different failure mechanisms that limit those strengths. It also indicated that power electronic devices having sintered-silver interconnects should be designed so that the maximum service stress is some fraction (safety factor) of the measured shear stress. Additional efforts are planned for FY 2016 that will further increase the versatility of and confidence in the processing and that will promote greater receptiveness to this technology.





Sintered-silver technology: (a) cross-sectional schematic of an SiC die bonded onto a direct-bonded copper (DBC) substrate, showing where the silver-sintering process is used for die attachment, and (b) examples of preliminary sintered-silver bonding of SiC to either silver- or gold-plated DBC substrates.

Publications, Presentations, and Patents

1. A. 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**: 158–165.

2. A. A. Wereszczak, Z. Liang, and T. A. Burress. 2015. “Enabling Materials for High-Temperature Power Electronics.” presented at the 2015 VTO AMR, Arlington, Virginia, June 10, 2015.

3. A. A. Wereszczak, S. B. Waters, and W. Carty. *Transfer Method for Printed Sinterable Paste Having Nonaqueous Solvent*. Invention Disclosure Number 201503508, DOE S-138,140, April 4, 2015.

4. A. A. Wereszczak and W. Carty. *Drying Method for Sinterable Paste Used for Bonded Joints*. Invention Disclosure Number 201503507, DOE S-138,139, April 3, 2015.

USDrive–DOE, Delphi Partner on New Chevrolet Volt Inverter

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

The 2016 Chevrolet Volt uses a second-generation "Voltec" extended-range electric powertrain with a traction power inverter module (TPIM) designed to increase efficiency, performance, and durability. Technology innovations developed as part of a USDrive-DOE cofunded project contributed to the design of Delphi's novel dual-side cooled package, which is used as the power device in the Volt TPIM.

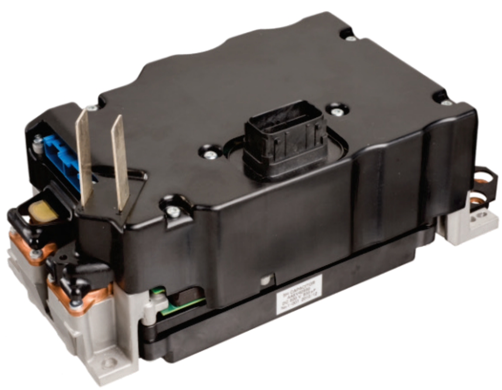
Key to the project's success was Delphi's development of a silicon dual-side cooled power device package. The Delphi device delivers more uniform current density than traditional single-sided power modules and is composed of a material stack in which the coefficients of thermal expansion (CTEs) of the layers are matched. (Failure in a power module typically is caused by thermal cycling. Mismatching CTEs can lead to adhesion issues and cracks and can make layers detach.) Both sides of the device are attached to ceramic substrates that are CTE-matched to the silicon.

ORNL developed a test plan for evaluating the final power module prototype built by Delphi, and the testing was completed in collaboration with Delphi. ORNL evaluated the 600 V package over a wide range of temperatures (25°C to 150°C), currents (10 A to 300 A), and voltages (250 V to 325 V). The device level test data were used to develop behavioral loss models that were incorporated into the system-level model.

The National Renewable Energy Laboratory also contributed to the project, providing thermal modeling of various polymeric thermal interface materials for use in the Delphi thermal stack.

Publications, Presentations, and Patents

None to report this period.



Power-dense, robust traction power inverter for the second-generation Chevrolet Volt extended-range electric vehicle.

Propulsion Materials

Stronger, Lower Cost Alloys for Higher Temperature Exhaust Valves Improve Vehicle Efficiency

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

Exhaust valve temperatures are anticipated to increase in future high-efficiency engines. Temperatures could increase from 870°C today to 950°C in 2025 and to 1,000°C by 2050 in light-duty vehicles and from 700°C today to 900°C by 2050 in heavy-duty vehicles.

Alloys that can withstand these temperature ranges are needed so that car manufacturers can produce vehicles with higher-efficiency engines employing modified internal combustion regimes. Use of such engines would improve the fuel economy of passenger vehicles by 25% and would improve the efficiency of commercial vehicle engines by at least 20%. Barriers to introducing new, high-performance material in these high-efficiency engines include the cost of existing high-performance alloys that can withstand the extreme conditions of downsized, turbocharged engines and the long lead times required for commercialization of new alloys.

ORNL has developed lower-cost, higher-strength nickel-based alloys that are capable of withstanding more extreme temperatures than the alloys currently used in exhaust valves (e.g., alloy 751). Use of the new alloys will enable higher efficiencies without incurring a significant cost penalty. The new alloys have been designed to contain up to 40% less Ni and to achieve high strength without the addition of other expensive alloying elements. They possess high strength and good oxidation resistance at temperatures up to 950°C.

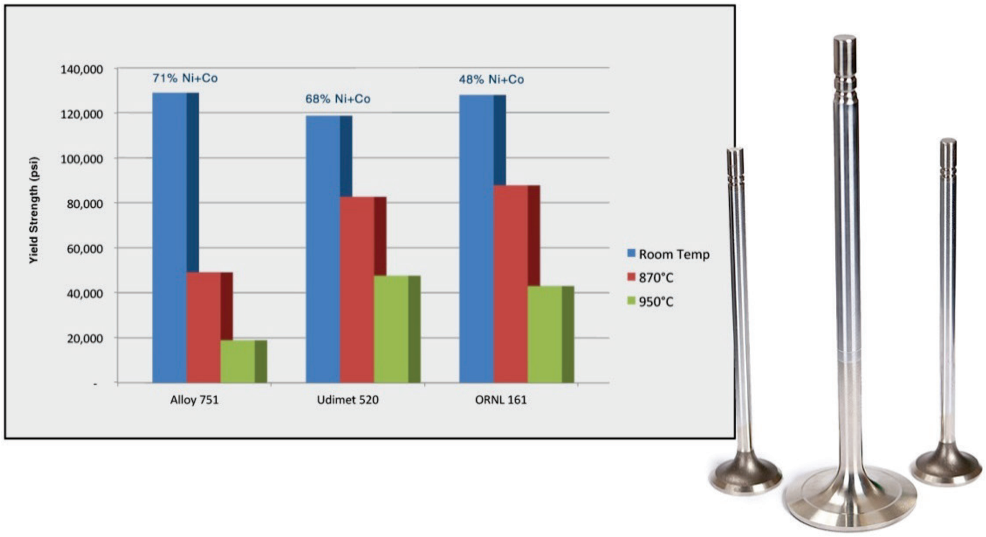
A computationally guided approach was used to develop this new class of lower-Ni alloys with higher strength at temperatures up to 950°C. A similar approach was used earlier to develop other cost-effective alloys for use at temperatures up to 870°C. Several experimental strategies to improve oxidation resistance in the 950°C alloys were also proposed and evaluated.

Oxidation was shown to lessen with the additions of trace amounts of reactive elements. Transmission electron microscopy and X-ray scattering is being used to understand the effect of precipitation on strengthening and will ultimately help in minimizing the levels of strengthening additions that can adversely affect oxidation resistance. Testing showed that changes in processing temperature favorably affected the ductility of alloys during industrial processing.

Experiments are on-going to understand the optimum process temperatures for industrial processing of the new ORNL alloys.

Publications, Presentations, and Patents

1. G. Muralidharan. “Computation-Aided Development of High Temperature Structural Alloys.” First International Symposium on Structural Materials for Innovation, February 26, 2015, Tokyo, Japan.



ORNL's nickel-based alloys can be used in exhaust valves and show high strength and good oxidation resistance at temperatures 950°C and above.

Novel In Situ Electron Microscopy Developed for Characterizing Catalyst Behavior Under "Real" Reaction Conditions

Contact: Lawrence F. Allard, allardLFjr@ornl.gov, 865-607-1144

ORNL collaborated with Protochips Inc., based in Raleigh, North Carolina, and led the development of a novel in situ reactor holder for electron microscopes. The reactor, called the Atmosphere 200, is a complete environmental gas cell that frees researchers from the confines of the transmission electron microscope vacuum.

Based on unique semiconductor technology, the Atmosphere 200 operates at up to 1 atm of pressure within a "closed-cell" specimen holder, while maintaining atomic resolution. It features ultralow-drift heating and automated closed-loop temperature control that can quickly reach and maintain temperatures of 1,000°C.

Through its novel design, evaluated through several generations of development at ORNL, the Atmosphere 200 is compatible with the most advanced spectroscopic systems and turns any electron microscope into a high-performance gas-reaction system, allowing scientists to explore the composition of materials at very small scales (nano to atomic) at elevated temperatures and at high pressures in gas environments. The device enables new research avenues, including in situ study of single-atom catalysts.

Publications, Presentations, and Patents

1. L. F. Allard et. al. "Novel MEMS-Based Gas-Cell Heating Specimen Holder Provides Advanced Imaging Capabilities for *In Situ* Reaction Studies." *Micros Micoranal* **18**(04), 2012, 656–666.

Researcher Larry Allard works with the Atmosphere 200 on ORNL's JEOL 2200FS aberration-corrected electron microscope.

ORNL Develops Advanced Alloys for Turbochargers and Manifolds

Contact: Phillip J. Maziasz, maziaszpj@ornl.gov, (865) 574-5082

Automotive exhaust components, which experience temperatures as high as 950°C, require materials with better heat-resistance than current commercial SiMo or D5S cast irons.

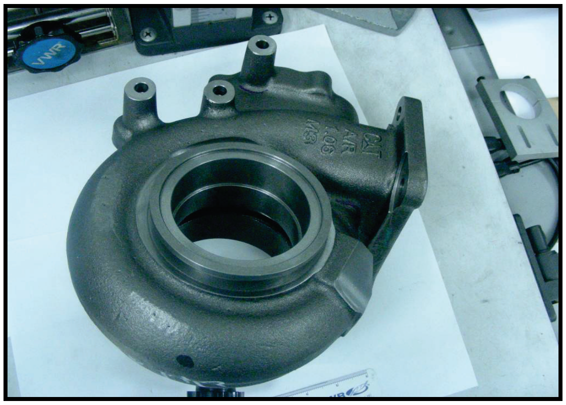
ORNL's CF8C-Plus cast stainless steels with ~20Cr and 12Ni were developed for advanced diesel exhaust components and exhibited very good mechanical properties up to at least 850°C. CN12-Plus cast austenitic stainless steel had 25Cr, slightly increased Ni, and more C+N (0.8), resulting in better tensile and creep strength than most commercial austenitic alloys for applications up to 950°C.

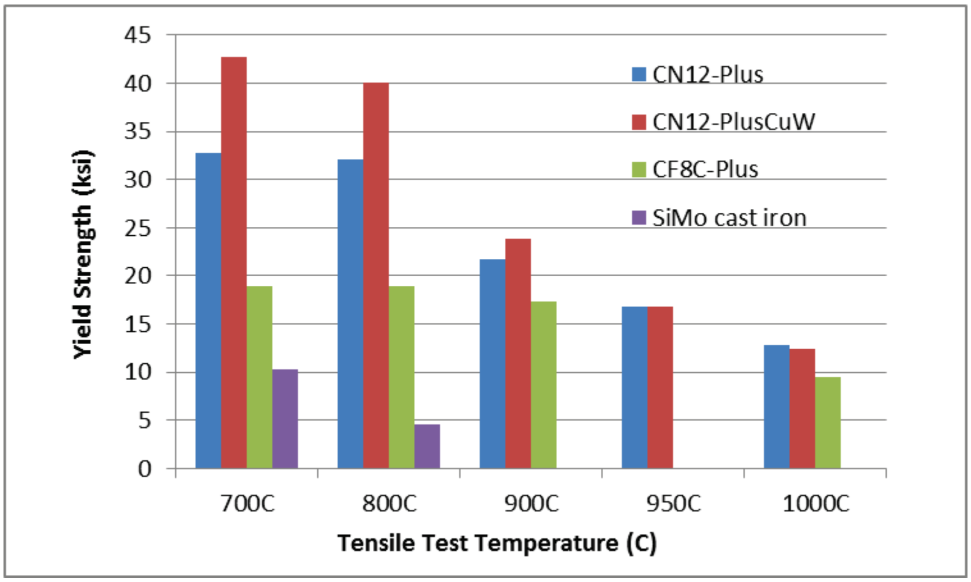
CN12-Plus was scaled up to commercial heats in 2015. Tensile testing occurred up to 1000°C, and creep-rupture evaluation occurred at 850°C to 950°C. Oxidation testing occurred in air+H_2O at 850°C to 950°C.

CN12-Plus improved yield strength vs. CF8C-Plus and exhibited a better combination of yield strength and ductility than CN12-PlusCuW. CN12-Plus also provided a better base alloy matrix for modifying with aluminum additions to further improve oxidation resistance at 950°C.

Publications, Presentations, and Patents

1. None to report this period.





Cast iron and austenitic stainless steel tensile properties at elevated temperatures.

ORNL, Industry Partners Use High-Performance Computing to Drive Alloy Design

Contact: Amit Shyam, shyama@ornl.gov, (865) 241-4841

A team of researchers from ORNL, FCA US LLC, and Nemak of Mexico used integrated computational materials engineering (ICME) to speed the development of affordable new high-temperature aluminum alloys for automotive cylinder heads. ICME enabled researchers to tailor new alloys at the atomic level to achieve desired properties such as strength and ease of manufacture.

The project is focused on engineering a material that is 25% stronger than current alloys and durable at temperatures 50°C higher than existing baseline alloys, a necessity for next-generation engines. The real challenge is to accomplish this while keeping costs low for automotive manufacturers and consumers.

ORNL broke new ground by scaling ICME to run on DOE’s Titan supercomputer, the second-fastest computer in the world. Using Titan’s speed and parallel-processing power, ORNL researchers predictively modeled new alloys and selected only the best candidates for further experimentation. This predictive capability dramatically reduced the time, energy, and resources devoted to casting trial alloys.

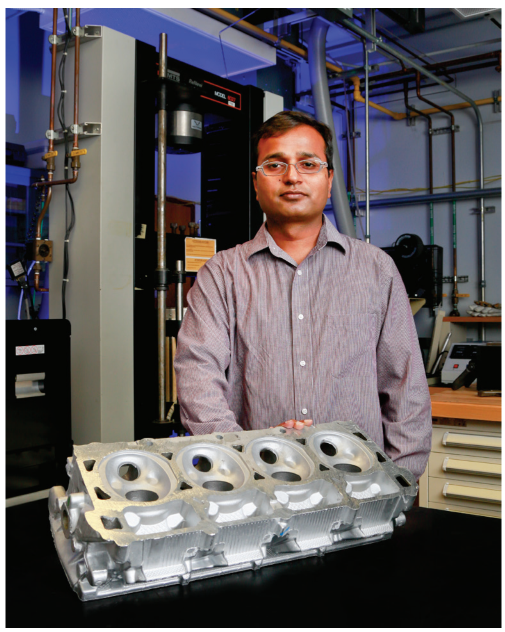
Before the shift to Titan, a Linux cluster was used with approximately 300 cores creating atomistic simulations of single elements diffusing to intermetallic precipitates within the alloy. Researchers achieved larger-scale simulations on Titan that are much closer to real-world scenarios.

The team verified the computational models through atomic-scale imaging and analytical chemistry measurements. ORNL's scanning transmission electron microscopy and atom probe tomography allowed researchers to identify and examine the location and chemistry of each atom in the alloy matrix, the precipitates, and the interfaces between them.

ORNL and collaborators also created a database capturing their aluminum alloy materials discoveries. This "materials genome" approach helped guide efforts to improve ICME capabilities and accelerated the development of new high-performance materials.

Publications, Presentations, and Patents

1. A. Sabau, W. Porter, R. Shibayan, and A. Shyam. "Process Simulation Role in the Development of New Alloys Based on an Integrated Computational Materials Engineering Approach." AMSE 2014 International Mechanical Engineering Congress & Exposition, November 14–0, 2014, Montreal, Quebec, Canada



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

Vehicle Systems

Advanced Combustion and Emission Control Technology Analysis and Evaluation

Contact: Zhiming Gao, gaoz@ornl.gov, 865-946-1339

To meet 2025 Corporate Average Fuel Economy standards, EPA Tier III emissions regulations, and Renewable Fuel Standard requirements will require integration of numerous advanced technologies such as high-efficiency clean combustion engines, leading-edge catalysts, and renewable fuels. That integration will require a deep understanding of the complex processes involved, fostered not only by experimentation, but also by analysis, modeling, and simulation.

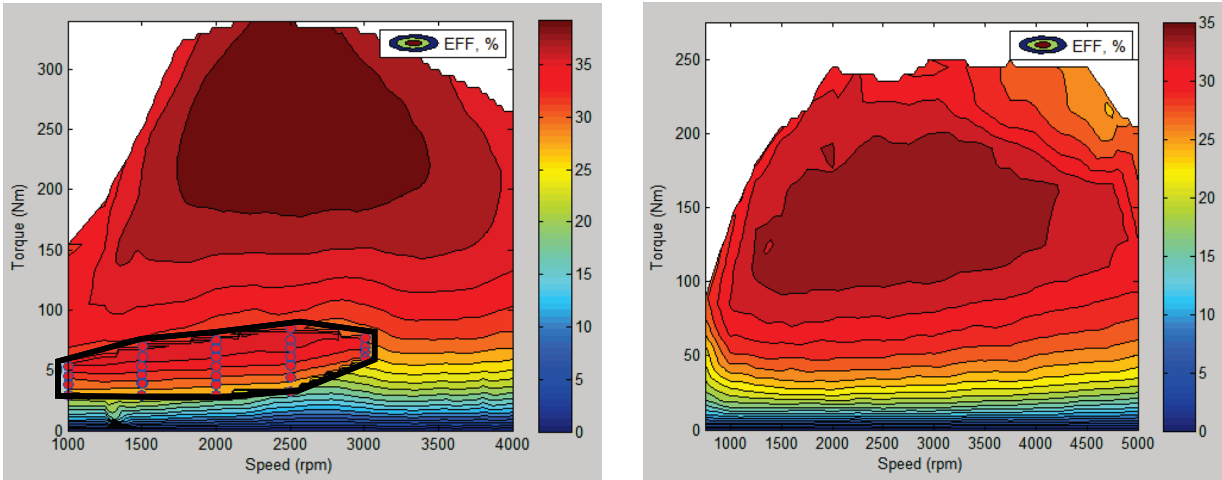
The goal of this project is to assist with this process by providing comprehensive vehicle system simulations that support DOE R&D efforts in evaluating and identifying innovative technologies and to leverage activities that will assist US automakers in meeting future fuel economy standards and emissions regulations. The models and simulations developed as part of this program rely on measurements from multiple facilities at ORNL and can be implemented directly in simulation platforms such as Autonomie. These models also provide guidance to experimental teams in targeting future measurements. This close interaction between simulation and experimentation provides DOE with the best possible basis for identifying promising vehicle technologies that maximize energy efficiency and minimize any negative environmental impacts from transportation.

In FY 2015 the project team continued to collaborate with partners at ORNL; in the DOE Advanced Combustion Engine, Fuel and Lubricant Technologies, and Vehicle Systems Simulation and Testing Programs; and in various other research programs to evaluate and identify the impacts of multiple reactivity-controlled compression ignition (RCCI) regimes on fuel economy and emissions from conventional and hybrid vehicles.

Two sets of new engine maps were constructed for 1.9 L GM engines enabled with mixed-mode operation between conventional diesel combustion (CDC) and RCCI and for a Ford EcoBoost 1.6 L turbocharged gasoline direct injection engine. Simulation results indicate that this RCCI implementation can boost fuel economy by nearly 30% compared to port fuel injection (PFI), which is consistent with the DOE FY 2015 Joule milestone.

Comparison of various RCCI fueling strategies was also carried out in conventional and hybrid vehicles. Results indicate renewable fuels such as E30 and B20 are capable of extending the RCCI operating regime and enhancing engine efficiency over city and highway driving cycles. The results also indicate that actual fuel economies of RCCIs are substantially higher than PFI gasoline, but differ little from CDC fuel economy levels.

A one-dimensional diesel oxidation catalyst (DOC) model that uses a new global kinetic reaction mechanism was developed, refined, and validated. The model accounts for CO, hydrocarbon, and nitrous oxide oxidation for CDC and RCCI exhausts during cold-start and the transition to mixed-mode operation and has been used in exploring sophisticated RCCI utilization strategies. The simulated results show that RCCI utilization strategies that manage CDC–RCCI switches via regulating exhaust temperature could significantly improve the performance of conventional DOCs during transient drive cycles involved in RCCI utilization.



(b)

Example of steady-state engine maps for (a) the 1.9 L GM engine with the RCCI-enabled zone highlighted and (b) the 1.6 L Ford turbocharged gasoline direct injection (GDI) stoichiometric engine. The pink circles in (a) indicate measured reactivity-controlled compression ignition operating conditions.

Publications, Presentations, and Patents

1. Z. Gao, S. Curran, J. E. Parks, D. E. Smith, et al. 2015. "Drive Cycle Simulation of High Efficiency Combustions on Fuel Economy and Exhaust Properties in Light-Duty Vehicles." *Applied Energy* **157**: 762–776 (invited).

2. Z. Gao, D. E. Smith, C. S. Daw, K. D. Edwards, et al. 2015. "The Evaluation of Developing Vehicle Technologies on the Fuel Economy of Long-Haul Trucks." *Energy Conversion and Management* **106**: 766–781.

3. S. Curran, Z. Gao, and R. M. Wagner. 2015. "Reactivity-Controlled Compression Ignition Drive Cycle Emissions and Fuel Economy Estimations Using Vehicle System Simulations." *International Journal of Engine Research* **16**: 1013–1024.

4. Z. Gao, S. Curran, C. S. Daw, D. E. Smith, and J. E. Parks. 2015. "Comparison of the Simulated Light-Duty Drive-Cycle Fuel Economy and Engine Exhaust Properties for Three Different RCCI Fuel Combinations." presented at the 9th US Combustion Meeting, May 2015.

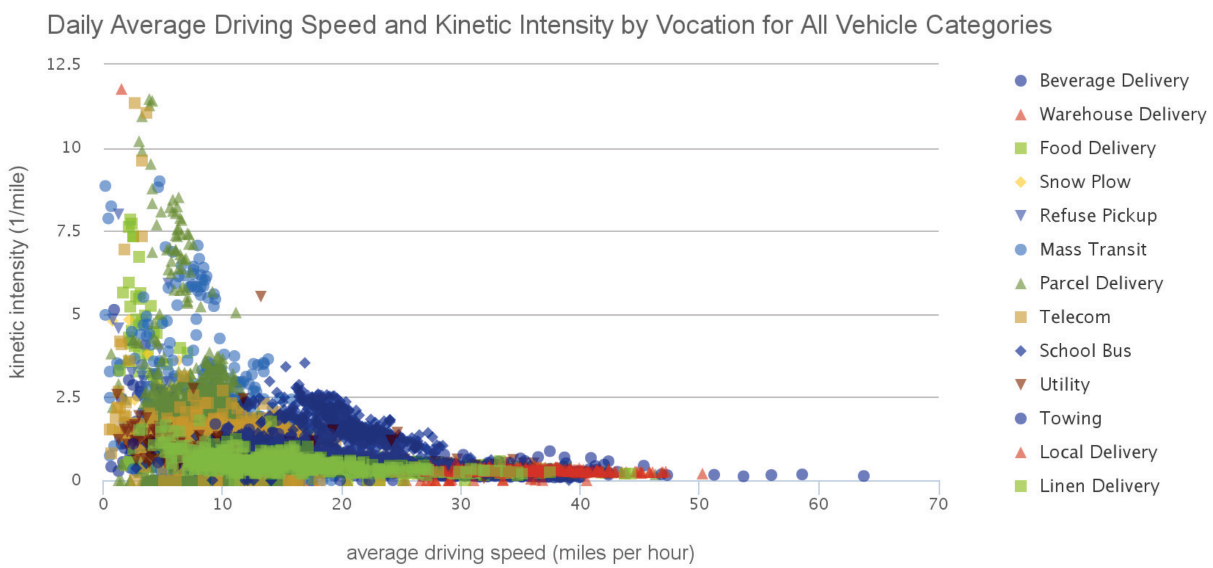
5. S. Curran, Z. Gao, D. E. Smith, and C. S. Daw. 2015. "Impacts of Advanced Combustion Engines." presented at the 2015 DOE Hydrogen Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting, June 9, 2015.

Fleet DNA Database Development and Support

Contact: Oscar Franzese, franzeseo@ornl.gov, 865-946-1304

A lot of information on medium and heavy truck real-world duty cycles (MTDCs and HTDCs) has been generated by ORNL as part of DOE-sponsored projects. Other DOE laboratories, various state and federal agencies, and private industry [original equipment manufacturers (OEMs) and fleets] have also generated duty cycle information, although not as extensively as the DOE MTDC and HTDC projects. The problem is that the data are in multiple locations, in multiple formats, with no common means of access. With this in mind, in 2012 the Vehicle Systems Simulation and Testing (VSST) project within the DOE Vehicle Technologies Office funded the Fleet DNA project to provide a common location for storage and basic analysis of this type of information. ORNL and the National Renewable Energy Laboratory (NREL), VSST's primary medium- and heavy-duty truck data collection laboratories, were authorized to assemble previously collected data in a common database (Fleet DNA); develop data analysis and access techniques to make the data available to OEMs, fleets, and others; and develop methods for collection and processing of future data from various organizations.

During the first phase of this project, ORNL worked with NREL to merge the existing ORNL MTDC and HTDC databases into the Fleet DNA data repository at NREL in accordance with project guidelines. The data were parsed, and selected channels were extracted and filtered using different techniques and methods developed exclusively for this project. This work generated the base Fleet DNA database, which covers specific vocations, long-haul operations, regional delivery, public transit (buses), electrical utility vehicles, and tow and recovery vehicles.



Sample Fleet DNA database information. This graph shows the relationship between daily average driving speed and kinetic intensity, which is a measure of how a vehicle drives, starts, and stops. High kinetic intensity means the vehicle starts and stops often during its route. Low kinetic intensity means the vehicle does not start and stop as often. A vehicle with high kinetic intensity and low-speed is a good candidate for hybridization because the regenerative brakes charge the battery effectively. [Fleet DNA project data courtesy of the Fleet DNA database, http://www.nrel.gov/fleetdna.]

In the second phase of the project, completed in 2015, ORNL developed methods and algorithms to build searching tools that would allow extraction of information from the ORNL Fleet DNA database duty cycles based on user-defined criteria.

This and future efforts will provide OEMs and fleets, other DOE programs, and other federal agencies with valuable drive cycle information to make decisions about and deploy and design advanced technology vehicles.

Publications, Presentations, and Patents

None to report this period.

MD and HD Accessory Hybridization for Fuel Savings and Emissions Control

Contact: Dean D. Deter, deterdd@ornl.gov, 865-576-8620

Medium-duty (MD) and heavy-duty (HD) trucks, used for home delivery of goods and HD freight hauling, are the main means by which material and goods are transported in the United States and might justifiably be called the workhorses of our society. Modern trucks have become much more advanced in terms of engine, aftertreatment, and transmission technologies, which have greatly reduced both fuel consumption and emissions. However, HD line haul trucks, which account for about 20% of total US truck fuel use, often idle for long periods in traffic and overnight for "hotel loads," which include cab cooling and power for things such as televisions, refrigerators, and phone chargers. This causes unnecessary amounts of fuel to be burned and releases additional emissions into the atmosphere.

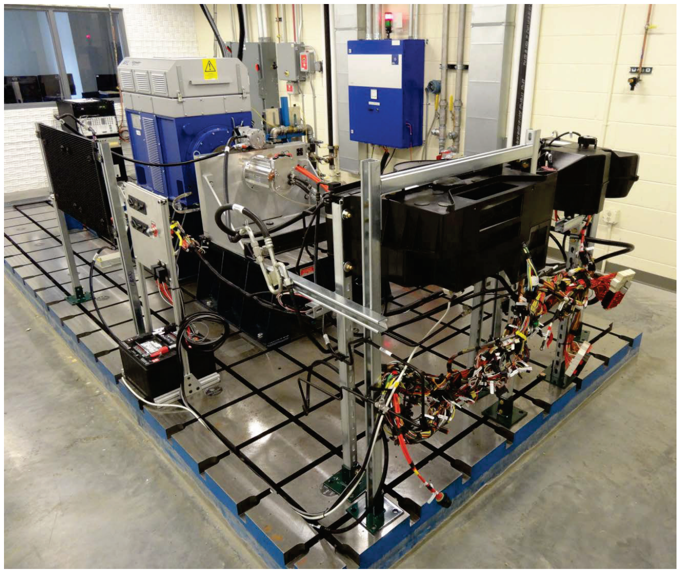
A unique cooperative research and development agreement between ORNL and Cummins, a global leader in the design, manufacture, and distribution of diesel and natural gas engines and related components, seeks to address this problem and in so doing reduce fuel consumption and emissions. An ancillary goal for ORNL was determining which technologies would be most readily accepted by fleet owners and industry. Using ORNL's Vehicle Systems Integration (VSI) Laboratory, the team was able to test prototypes at both component and systems levels for initial development and validation, which was quicker, safer, and more cost effective than using a test vehicle.

Line haul drivers are required to spend 10 hours' down time between each haul (typically overnight). During down time, the truck will idle during the night's hotel stay (8 to 10 hours) and will use 4 to 7 gal of diesel fuel if the driver needs air conditioning or power for phone chargers, TV, radio, etc. That does not account for time spent idling when trucks are preparing to load or unload cargo or sitting in traffic.

Currently, idle mitigation is handled with auxiliary power units (APUs), but they are generally aftermarket units that are added rather than built into the original truck systems, so they are not maximally efficient and in some cases contribute to maintenance issues. In addition, the units are only advantageous when trucks are not running.

The ORNL-Cummins proposed solution will be an integrated system that will allow elimination of overnight idling, connectivity with shore power, engine start/stop capability, optimized cooling capacity via electric fans, and regenerative braking. The prototype APU system is currently undergoing testing in a Cummins test vehicle.

When the project was initiated, physics-based MD and HD accessories models—for such things as air conditioning, power steering, fans, and pumps— were not available, so among the first things researchers had to do were to collect data on all accessories and to develop physics-based mechanical and electrical accessory models, which were then integrated into vehicle models. After air conditioning became a focal point of the study, the National Renewable Energy Laboratory's CoolSim modeling tool was adopted to provide a high-fidelity physics-based air conditioning model for validation of the conventional and prototype systems. The model will be validated and updated using data from this project for use in future projects.



ORNL VSI Component Test Cell. Using ORNL's Vehicle Systems Integration Laboratory, testing prototypes at both a component and powertrain level instead of using a test vehicle, allows for quicker, safer, and more cost-effective development and validation.

Publications, Presentations, and Patents

1. M. M. Kumar, G. L. Parker, S. Varigonda, J. E. Paquette, B. D. Padgett, W. B. Fields, P. C. Mualidhar, V. A. Sujan, D. D. Deter, and D. E. Smith. *Apparatus and System for Controlling Power to an Air Conditioning Compressor for a Vehicle*. US Patent Application 62/354,364, filed June 24, 2016.

ORNL Collecting Important Data on Electric Vehicle Charging

Contact: Melissa Lapsa, lapsamv@ornl.gov, 865-576-8620

Widespread electric vehicle (EV) use is such a recent phenomenon that statistics on factors of interest such as recharging patterns, peak times of recharging station use, and optimal placement of charging stations are needed. Such factors are important to developing the charging infrastructure necessary to help power a sustainable transportation future.

Thanks to the 2009 DOE American Recovery and Reinvestment Act, related ECOtality grants, and regional cost-share investments, ORNL has been able to explore these factors in greater detail. The original project, which at the time was the largest deployment of EVs and charging infrastructure in history, allowed for the deployment of more than 15,000 charging systems (solar- and non-solar-powered) to support EVs in strategic markets in six states (Arizona, California, Oregon, Tennessee, Texas, and Washington) and Washington, DC. One of the goals of the original project was to collect and analyze data to characterize EV use under diverse topographic and climatic conditions.

The original project ended in FY 2014, but in 2015 ORNL received additional DOE funding to continue collecting, analyzing, and reporting EV charging data for Tennessee, specifically the 44 charging stations (solar and nonsolar) at ORNL and, to the degree possible, solar-assisted installations across the state. (Note: Since completion of the original project, data on some of the charging stations across the state are no longer available.)

Major areas for tracking and analysis have been energy consumption, times of connect and disconnect, duration of charging, and overall use of the stations. Energy consumption and duration of charging provide insights on the state of charge of car batteries at the start of charging and the associated recharging patterns. Connect and disconnect times provide information on peak times of station use and, again, recharging patterns at ORNL and in public settings. The insights gained will be useful in determining the need for and locations of additional stations at ORNL and elsewhere in the state.

Electric cars plugged in at the ORNL solar-charging facility.

Findings

The following are among the findings so far.

1. At ORNL, the distributed charging stations (i.e., those located near major office areas) have higher use rates than the centrally located stations.
2. Based on monthly power consumption for EVs charging at ORNL, it is estimated that fuel savings exceed 700 gal of gasoline each month.
3. Use at most of the ORNL-installed EV charging station sites has increased rather steadily since they were first installed—something that would be expected with greater familiarity with the sites over time and the growing number of EVs on the site.
4. Longer use data are needed to draw additional conclusions about statewide use trends, and this work is continuing in 2016.

Publications, Presentations, and Patents

None to report this period.

Powertrain Controls Optimization for Heavy-Duty Hybrid Line Haul Trucks

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

Hybrid medium- and heavy-duty powertrains have great potential for reductions in fuel consumption, criteria pollutants, and greenhouse gases through integrated diesel hybridization, analytical modeling, regenerative braking, hybrid energy storage, and supervisory controls development. This project seeks to leverage advances in these multiple research areas on a single vehicle platform. In addition, advanced combustion technologies such as reactivity-controlled compression ignition will be implemented into an advanced hybrid powertrain for a Class 8 line haul application.

There are four focus areas for the project, ranging from advanced combustion regimes and engine control strategies to emissions control technologies, pulsed energy storage systems (dual energy storage systems), and advanced energy management and supervisory controls.

In 2015, progress was made in the following areas.

- **Engines and emissions data.** Engine fuel consumption and emissions data were enhanced by leveraging other ongoing projects in the ORNL Vehicle Systems Integration (VSI) Laboratory. A complete test matrix was executed (and repeated for accuracy) for developing more reliable engine and emissions data. Fuel consumption data were verified through comparison of actual fuel measurement, J1939 engine network data, and emission/air fuel calculations.

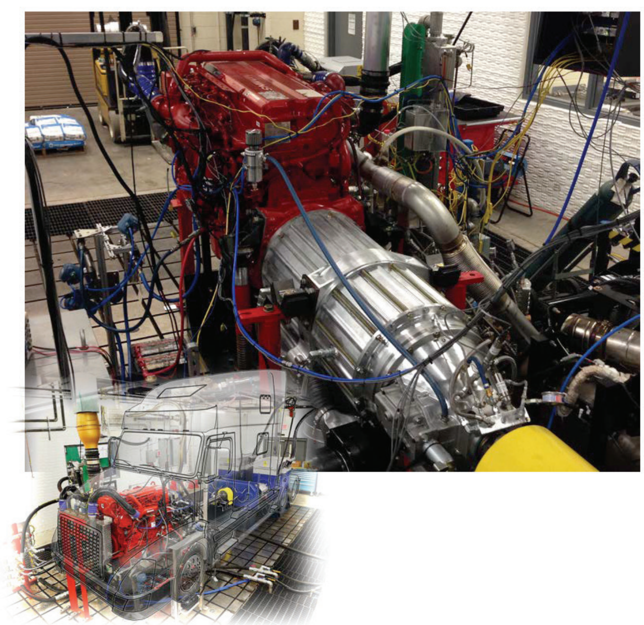
- **Engine system models.** ORNL has implemented past transient engine modeling experience to develop a transient model for use in Autonomie of a Cummins ISX-450 15 L engine and an associated emissions aftertreatment system. Emphasis was placed on completing development and validation of the aftertreatment models for this powertrain in FY 2015. Data were logged from the actual components in the ORNL VSI Laboratory and were used to validate the resulting empirical models over a host of drive cycles.

- **Hybrid energy storage system.** The simulation model for the dual energy storage system has been completed, including voltage mode control of boosting and buck modes and the addition of an ultracapacitor parameter extraction tool that, given an appropriate single-pulse-discharge data set, facilitates voltage-dependent modeling of any manufacturer's ultracapacitor.

The project is being refocused in FY 2016 to align research more closely with 21st Century Truck Partnership needs, which will include powertrain optimization of conventional line haul vehicles through controls integration and optimization of both the engine and the transmission.

Publications, Presentations, and Patents

None to report this period.



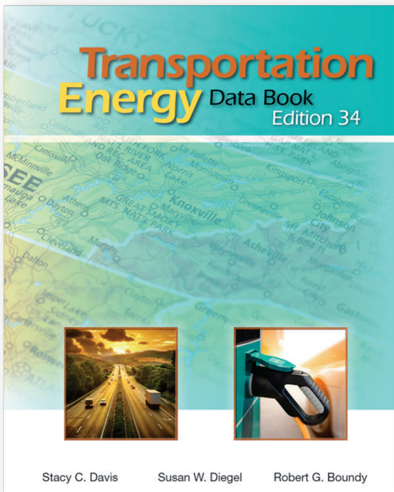
Researchers leveraged experimental powertrain results from the ORNL Vehicle Systems Integration Laboratory to complete enhanced engine and aftertreatment models for this project.

Vehicle Technologies Office Communications

ORNL Publications Support Outreach Efforts and Meet Data Needs of the DOE Vehicle Technologies Office

Contact: Stacy Davis, davissc@ornl.gov, 865-946-1256

ORNL continued to support the DOE Vehicle Technologies Office (VTO) public communication efforts in 2015 with publication of the *Transportation Energy Data Book*, the *Vehicle Technologies Market Report*, and the "Fact of the Week" for the VTO home page.



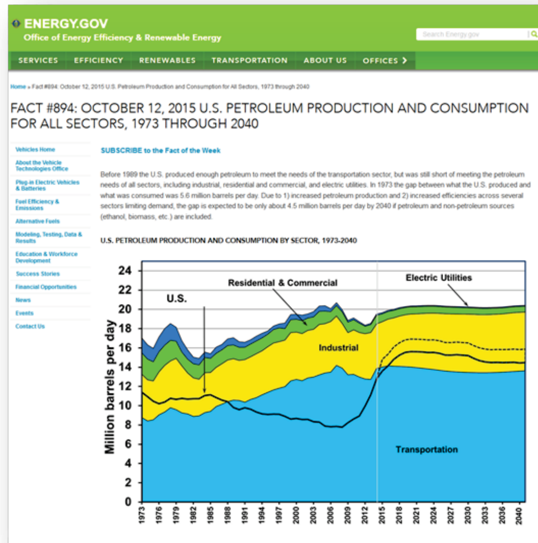
The ***Transportation Energy Data Book*** (TEDB), published in September, is the 34th edition of the data collection that ORNL publishes for VTO. This long-running project has been active at ORNL since 1975; the first edition was published in 1976. The TEDB website (http://cta.ornl.gov/data/index.shtml) allows visitors to download TEDB in pdf format, download any of the Excel spreadsheets in the book individually, or request a hard copy of the report free of charge. Between 6,000 and 8,000 visits to the website are logged each month. In addition, TEDB was printed and distributed to a nationwide mailing list.

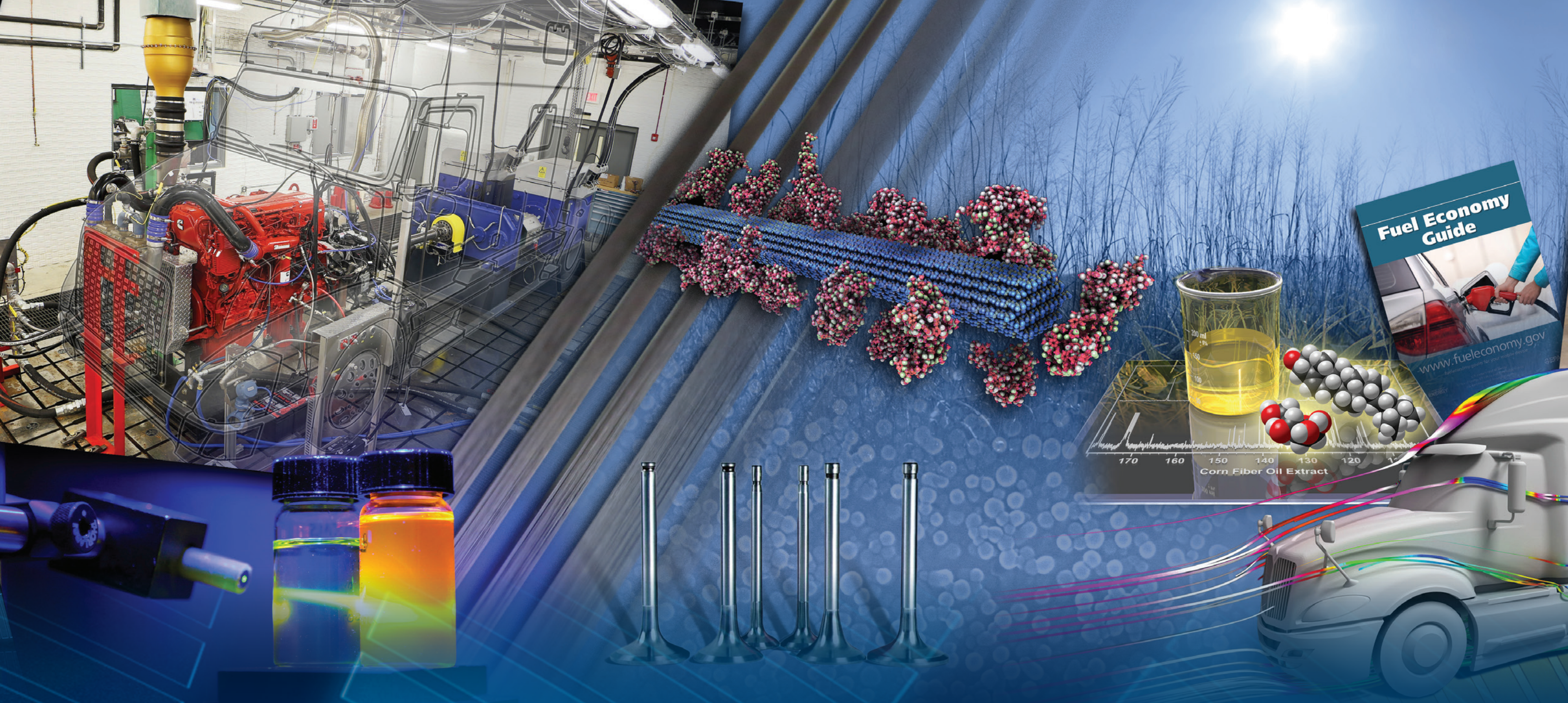
The document supports VTO public outreach, allowing VTO staff to provide quick responses to queries on transportation energy use. The goal is to produce a comprehensive document with transportation data from diverse sources for use in answering transportation energy questions and resolving data conflicts and inconsistencies.

TEDB's historical data tables provide a foundation for the analyses 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 2015 ***Vehicle Technologies Market Report*** was the sixth 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 3,700 visitor 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. In 2015, the site allowed users to subscribe to receive an email every Monday with the weekly fact. In the first 6 months, more than 1,300 people subscribed.





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