Sustainable Transportation Program

2013 Annual Report

Oak Ridge National Laboratory

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Sustainable Transportation Program 2013 Annual Report

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Introduction

Oak Ridge National Laboratory's (ORNL's) Sustainable Transportation Program (STP) performs research and development (R&D) leading to new vehicle and transportation system technologies. The program's R&D portfolio includes advanced combustion engines, advanced materials, alternative fuels, efficient vehicle components, intelligent transportation systems and operations, transportation electrification, and vehicle systems integration. ORNL also provides data and analysis to guide policies and decisions of the Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) and the Department of Transportation (DOT).

The focus of Sustainable Transportation is clean, efficient, intelligent paths to reducing petroleum consumption and vehicle emissions, and to replacing imported petroleum with affordable, diverse domestic fuels to revitalize the US economy and improve US energy security. Millions of vehicles on US roadways are more durable and more efficient because of materials technologies developed at ORNL, and government agencies and consumers make transportation decisions every day using data collected and analyzed by ORNL.

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

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

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

These efforts are directed toward attaining

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

Transportation is a key factor in the energy and environmental future of the United States. Highway transportation (light-, medium-, and heavy-duty vehicles) accounted for more than 25% of US greenhouse gas emissions [1] and about 60% of US petroleum consumption in 2011.[2] 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 econo-

[1] S. C. Davis, S. W. Diegel, and R. G. Boundy, *Transportation Energy Data Book: Edition 32*, ORNL-6989, Table 11.4, 2013.
[2] Ibid, Table 1.17.

my regulations—light commercial trucks and heavy trucks are projected to use almost 45% more energy in 2040 than in 2011.[3] 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.

In support of the Vehicle Technologies Office (VTO) in FY 2013, ORNL researchers implemented a user-friendly online calculator that supplies personalized estimates of energy costs and gas station visits for a specific plug-in hybrid electric vehicle (EV); manufactured a lithium-ion battery using a process that replaces a toxic, expensive, chemical with deionized water; determined that blending as much as 30% ethanol with regular gasoline may improve fuel efficiency in conventional gasoline vehicles; developed cost-effective nickel-based alloys for valves in high-temperature automotive applications, using a materials-by-design approach incorporating computation and experiment; developed a robust, highly efficient 10 kW wide-bandgap inverter for use in EVs; and completed the installation of several major pieces of test equipment in the Vehicle Systems Integration Laboratory, which can test conventional and hybrid powertrains for architectures ranging from light-duty vehicles to fully loaded Class 8 trucks.

An ORNL effort sponsored by the Bioenergy Technologies Office (BETO) is studying the impacts of short-rotation tree farming for bioenergy, examining the effects of intensive silviculture practices on watersheds. It is a collaboration with the US Forest Service and several universities. In concert with industrial and academic partners, ORNL produced a low-cost, highly efficient "clean cookstove" with a metal combustor that is more durable against corrosion than earlier versions of the stove. The efficient, affordable stove dramatically reduces harmful combustion gases and fuel use compared with the traditional biomass-fueled fires and stoves that are widely used in the developing world. The Regional Feedstock Partnership assessed biomass crop yields across the country to gather regional crop productivity data for models and databases supporting biomass feedstock supply and logistics systems.

In research supporting the Fuel Cell Technologies Office (FCTO), ORNL researchers produced melt-spun carbon fibers that met a major go/no-go performance milestone. Carbon fiber composites are a prime candidate material for hydrogen storage tanks if they can satisfy cost and performance targets. The melt-spinning approach promises to be much less costly than the process currently used, and the ORNL fibers demonstrated the required tensile strength and modulus of elasticity. In another project, materials scientists established analytical methods for using advanced electron microscopy and spectroscopy to characterize fuel cell membrane electrode assemblies so that materials can be selected or modified to improve membrane performance. The techniques were used to reveal the mechanisms of carbon corrosion. A study of market prospects for fuel cell plug-in hybrid EVs conducted using ORNL's MA3T model found that the vehicles have the potential to succeed in the marketplace in both the near and the long term.

Research sponsored by DOT included the launch of the Intelligent Transportation Systems (ITS) Asset Viewer, an online application that uses visual mapping technology to identify the locations of ITS transportation tools such as message boards, traffic sensors, and road

[3] US Energy Information Administration, *Annual Energy Outlook 2013 with Projections to 2040*, US Department of Energy, Washington, D.C., Table A7, 2013.

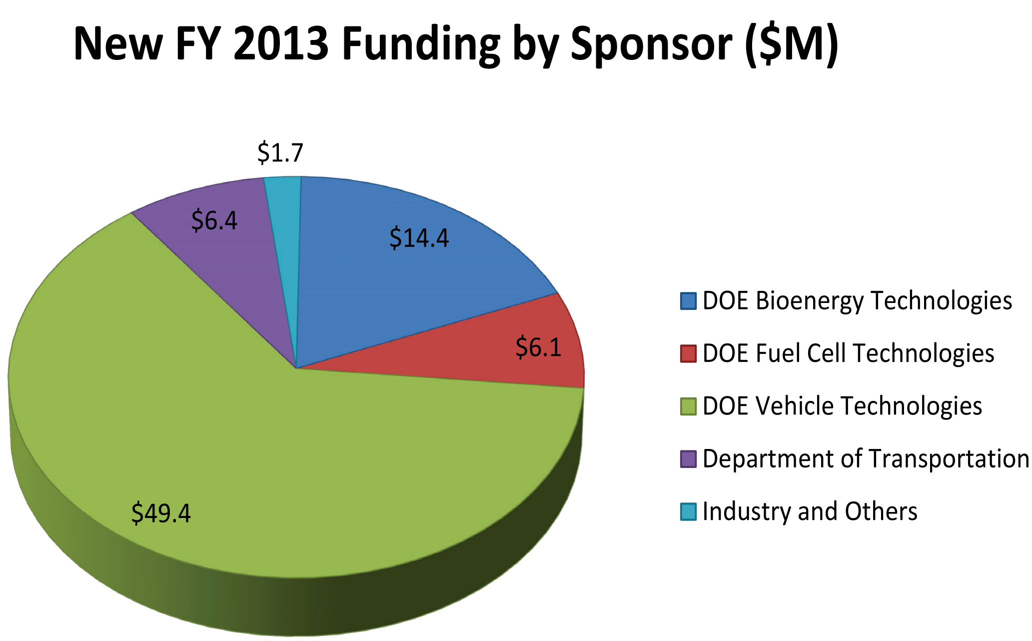
weather information systems. Data from the system will enable DOT to analyze the impacts of ITS technologies. ORNL analysts worked with the Federal Motor Carrier Safety Administration to help identify policy and process weaknesses related to motorcoach safety and suggest needed changes. And ORNL assisted the Federal Motor Carrier Safety Administration in evaluating its formulae for granting financial assistance to the states.

Highlights of these and other STP R&D efforts begin on page 13.

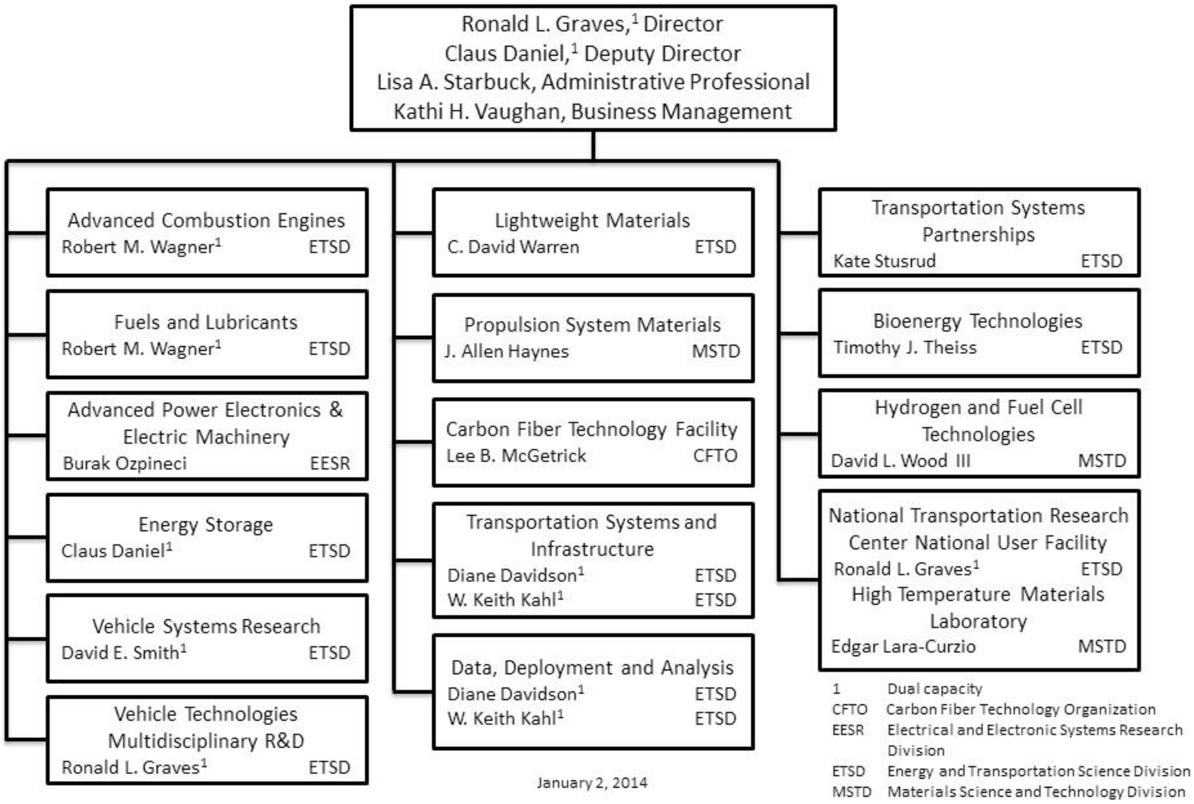
Program Metrics

Funding

The STP received $78M in new budget funding in FY 2013. Approximately $23M, or 30%, is funding for projects that were competitively awarded by DOE EERE via Funding Opportunity Announcements. DOE VTO remains the largest sponsor of the ORNL program. DOT and DOE FCTO budgets remained stable in FY 2013, while funding from the DOE BETO grew compared with FY 2012.



Program funding provided significant support for more than 165 scientific and technical staff in 10 technical divisions, reflecting the broad, multidisciplinary character of the ORNL program. The STP team leaders are shown in the following organization chart.



Industry Impact

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

CRADAs

STP researchers supported 17 CRADAs in FY 2013 with 13 different companies, developing an array of technologies including new materials for high-efficiency engines, advanced combustion regimes, alternative fuels, and hybrid and EV components and systems. In FY 2013, our industry partners contributed about $7M in materials and services toward these efforts, nearly half of the total funding for the projects.

WFO Agreements

ORNL worked with 16 industrial companies, 14 federal and state government entities, and 4 universities under 52 separate WFO agreements in FY 2013. In total, these agreements were valued at about $8M.

Technology Licensing

US-based all-electric vehicle manufacturing startup Arcimoto has exclusively licensed a combination of three ORNL technologies—an innovative ac-dc inverter, a battery system charger, and a dc-dc inverter—to enable Arcimoto to build a drivetrain that eliminates the need for a stand-alone external charger. The technologies also let the system operate at higher temperatures by significantly reducing undesirable motor torque ripple. The Arcimoto–ORNL partnership was the focus of an article titled "A Promising New Electric Car Is on the Horizon" that appeared in *Innovation Magazine Online*.

User Facility Agreements

Four nonproprietary user projects were approved for the National Transportation Research Center (NTRC).

Los Alamos National Laboratory—Robust Nitrogen Oxide/Ammonia Sensors for Vehicle On-Board Emissions Control

The goal of this project is to develop robust electrochemical sensors capable of reliably detecting 1–500 ppm nitrogen oxides and 1–50 ppm ammonia in a vehicle exhaust stream. The Los Alamos National Laboratory (LANL) team completed two sets of experiments with their sensor on the NTRC's unique engine research platform. Results were very promising, with LANL's sensor demonstrating the ability to distinguish different pollutant gases in real exhaust. Results were presented during a Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Focus Group teleconference, and further presentations and publications are planned.

Texas A&M University—Characterization of Surface Area and Kinetic Oxidation of Particulate Matter from Advanced Gasoline Direct Injection Engine Technologies

Texas A&M University seeks to characterize the surface area and oxidation kinetics of particulate matter (PM) or "soot" generated from an advanced gasoline direct injection (GDI) engine to better understand how PM can be controlled in aftertreatment devices. Texas A&M collected PM from the NTRC GDI engine platform during the combustion of alternative fuels and is analyzing the nature of the PM as it relates to oxidation processes that enable control of the PM in emission control systems.

Pacific Northwest National Laboratory—Detailed Characterization of PM from Advanced Combustion Engines

Researchers from Pacific Northwest National Laboratory (PNNL) brought the Single Particle Laser Ablation Time-of-Flight Mass Spectrometer (SPLAT) to the NTRC for a two-week sampling campaign. SPLAT is able to physically and chemically characterize individual particles, thus giving a complete picture of the particle emissions from an engine. The combination of SPLAT and the advanced, unique engine platforms at the NTRC produced an unprecedented examination of exhaust emissions from lean GDI, partially premixed charge gasoline compression ignition, and reactivity-controlled compression ignition under a variety of light-duty operating conditions. The studies will provide a better understanding of how to control the unique PM from these fuel-efficient engine concepts. Preliminary results were presented to the U.S. DRIVE[4] Advanced Combustion and Emissions Control Tech Team, and ongoing data analysis will yield more results for inclusion in presentations and publications.

[4] U.S. DRIVE is a cooperative partnership between DOE and industry to accelerate the development of clean, advanced, energy-efficient technologies for cars and light trucks and the infrastructure needed to support their widespread use.

3M Company—Thermal Insulation in Automotive Exhaust Systems for Advanced Combustion Engines

3M Company has a specific interest in the use of insulating materials for thermal management to control emissions. The user project was approved in FY 2013 and scheduled for January 2014, but an engine water coolant line failure occurred during uncommon freezing temperatures. The campaign was delayed to a more suitable time for the engine platform of interest and is now planned for the summer of 2014.

Patents and Invention Disclosures

ORNL research sponsored by DOE's VTO, FCTO, and BETO resulted in 40 invention disclosures and 11 patent applications. Twelve patents were issued based on earlier filings, as shown in Table 1. Patent applications filed in FY 2013 are shown in Table 2.

Table 1. Patents awarded during FY 2013

Inventor(s)	Title	Number	Sponsoring EERE Office
David Joseph Singh	Alkaline earth filled nickel skutterudite antimonide thermoelectrics	8,487,178 B2	VTO
Jy-An Wang, Zhili Feng, Lawrence M. Anovitz, and Kenneth C. Liu	Apparatus and method for fatigue testing of a material specimen in a high-pressure fluid environment	8,453,515 B2	FCTO
Chaitanya K. Narula and Claus Daniel	Solid lithium ion conducting electrolytes and methods of preparation	8,449,790 B2	VTO
Govindarajan Muralidharan, Yukinori Yamamoto, and Michael P. Brady	Cast alumina forming austenitic stainless steel	8,431,072 B2	VTO
Gui Jia Su	Electrical motor/generator drive apparatus and method	8,373,372 B2	VTO
John S. Hsu	Substantially parallel flux uncluttered rotor machines	8,330,319 B2	VTO
John S. Hsu	Flux control and one-hundred and eighty degree core systems	8,319,464 B2	VTO
James E. Parks and William P. Partridge	Optical backscatter probe for sensing particulate in a combustion gas stream	8,451,444	VTO

Table 1. Patents awarded during FY 2013 (continued)

Inventor(s)	Title	Number	Sponsoring EERE Office
Roman I. Pankiw, Govindarajan Muralidharan, Vinod Kumar Sikka, and Philip J. Maziasz	Cast heat-resistant austenitic steel with improved temperature creep properties and balanced alloying element additions and methodology for development of the same	8,318,844	VTO
Matthew B. Scudiere	Off-resonance frequency operation for power transfer in a loosely coupled air core transformer	8,310,202	VTO
John S. Hsu	Brushless machine having ferromagnetic side plates and side magnets	8,294,321	VTO
James P. Szybist and James C. Conklin	Highly efficient 6-stroke engine cycle with water injection	8,291,872	VTO

Table 2. Patent applications filed during FY 2013

Inventor(s)	Title	Number	Sponsoring EERE Office
Jy-An Wang, Zhili Feng, and Wei Zhang	Hydrogen storage container	13/940,567	FCTO
Amit K. Naskar, Felix L. Paulauskas, Claude C. Eberle, Christopher J. Janke, and Charles D. Warren	Sulfonated polyolefin-based flame retardant material	61/762,489	VTO
William P. Partridge and James E. Parks II	EGR distribution and fluctuation probe based on CO_2 measurements	13/912,462	VTO
Amit K. Naskar	Controlled chemical stabilization of polyvinyl precursor fiber, and high strength carbon fiber produced therefrom	13/860,188	VTO
Felix L. Paulauskas	Atmospheric pressure plasma processing of polymeric materials using close proximity indirect exposure	13/680,406	VTO
Michael D. Kass, Shean P. Huff, Samuel A. Lewis Sr., Timothy J. Theiss, Steven J. Pawel, and Christopher J. Janke	System for determining biofuel concentration	13/939,479	VTO

Table 2. Patent applications filed during FY 2013 (continued)

Inventor(s)	Title	Number	Sponsoring EERE Office
Chaitanya K. Narula and Claus Daniel	Solid lithium ion conducting electrolytes and methods of preparation	13/886,542	VTO
Madhu S. Chinthavali	Gas cooled traction drive inverter	14/016,327	VTO
Sreekanth Pannala, Chaitanya K. Narula, Raymond R. Unocic, Nancy J. Dudney, and Jagjit Nanda	High energy density secondary lithium batteries	13/651,322	VTO
Nancy J. Dudney	Lithium-conducting sulfur compound cathode for lithium-sulfur batteries	13/974,854	VTO
Timothy A. Burress and Curtis W. Ayers	Reluctance motor	13/944,731	VTO

Staff Awards and Honors

Program research staff members were honored with an array of awards and professional recognitions, reflecting meaningful contributions to research, technology development, and service to professional societies. A selection of the most significant is shown in Table 3.

Table 3. Significant awards and professional honors received by STP researchers

ORNL Awardee Name(s)	Name/Type of Award
Scott Curran	R&D Technology Award from the DOE Vehicle Technologies Office
	Best Presentation at the 2012 Fall Technical Conference from the American Society of Mechanical Engineers Internal Combustion Engine Division
Virginia H. Dale	Distinguished Landscape Ecologist Award from the U.S. Regional Association of the International Association for Landscape Ecology
Claus Daniel	"40 Under 40" award from the Greater Knoxville Business Journal
Claus Daniel, Curt Maxey, David Wood, Beth Armstrong, Jianlin Li, Amit Shyam, Harry Meyer, Ralph Dinwiddie, Wally Porter, Cristian Contescu, Edgar Lara-Curzio, Hsin Wang, Rosa Trejo, Jane Howe	R&D100 Award for Symmetrix HPX-F
C. Stuart Daw	Fellow, American Institute of Chemical Engineers
Nancy J. Dudney	Fellow, Electrochemical Society

Table 3. Significant awards and professional honors received by STP researchers (continued)

ORNL Awardee Name(s)	Name/Type of Award
Zhili Feng	Fellow, American Welding Society
Ronald L. Graves	R&D Technology Award from the DOE Vehicle Technologies Office
David L. Greene	Distinguished Career Service Award from the DOE Fuel Cell Technologies Office
David L. Greene	Roy W. Crum Distinguished Service Award from the Transportation Research Board of the National Academies
Janet Hopson	R&D Technology Award from the DOE Vehicle Technologies Office
Hua-Tay Lin	Honor Medal of Aurel Stodola, Slovak Academy of Sciences
Hua-Tay Lin	Distinguished Engineering Achievement Award from The Engineers' Council
Hua-Tay Lin	Appointment to the Advisory Board of the World Academy of Ceramics
Philip J. Maziasz	William Hunt Eisenman Award from ASM International for "outstanding success in the development of new heat-resistant stainless steel and alloys with significant commercial impact in advanced transportation, coal-fired generation, and nuclear power generation"
Karren L. More	R&D Technology Award from the DOE Fuel Cell Technologies Office
Mitchell Olszewski	North Atlantic Treaty Organization Applied Vehicle Technology Fall 2012 Panel Excellence Award
William P. Partridge, James E. Parks II, David Sims	R&D100 Award for Da Vinci Fuel-in-Oil (DAFIO™) Measurement System
Shahabaddine Sokhansanj	Standards Developer Award from the American Society of Agricultural and Biological Engineers
	Fellow, Engineers Canada
John M. Storey	Fellow, SAE International
Leon Tolbert	Fellow, IEEE
Todd J. Toops, Michael J. Lance	Researchers of the Year from 2012 Biodiesel Technical Workshop
Robert M. Wagner	Fellow, SAE International
Brian H. West	Fellow, SAE International

Infrastructure and Facility Investments

Battery Manufacturing Facility (BMF). The BMF demonstrated double-sided electrode manufacturing of $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ cathodes. This success significantly enhanced the BMF's capability in electrode manufacturing and completed an industry-ready pilot scale in spring 2013. The BMF also demonstrated DOE's first fully water-processed lithium-ion battery, reducing pack cost by 15–20%, and it won an R&D100 Award for a new separator technology developed through an industrial collaboration with Porous Power Technologies.

Carbon Fiber Technology Facility. All key performance parameters committed to DOE in the Project Execution Plan were proved. Several successful conversion runs prior to commissioning produced carbon fibers in 12K, 24K, and 48K tow format. A ribbon cutting ceremony was held in March 2013. The facility includes a nearly 400 foot long line for producing carbon fiber in pre-commercial quantities, and it will explore more efficient and less costly carbon fiber production methods in an effort to bring down the cost of carbon fiber for vehicle applications.

Commercial Motor Vehicle Roadside Technology Consortium (CMVRTC). ORNL proposed and DOT approved expansion of the Consortium (formerly "Corridor"; the name was changed October 1, 2013) to include 30 sites in 5 states and more than 2,400 miles of interstate highway. Sites in Alabama, Georgia, Kentucky, and North Carolina are now a part of this real-world test bed for commercial vehicle operation. The first project to take advantage of the expanded facility is the Wireless Roadside Inspection Field Operational Test.

Energy Storage. ORNL built a pinch simulation testing system used at the Naval Surface Warfare Center in Carderock, Maryland, to conduct internal short-circuit testing of 18 and 25 ampere-hour lithium-ion cells. The tests were successful in distinguishing the safety factor of lithium-ion cells with different chemistries and capacities.

Fuels, Engines, and Emissions Research Center (FEERC). FEERC is partnering with Ford Motor Company to investigate the potential for the use of high-octane fuels to enable greater fuel economy. Ford provided FEERC with a state-of-the-art 1.6 liter Ecoboost® 4-cylinder engine to support the work. ORNL's work will focus on increasing the compression ratio of the engine to improve low-load fuel economy, while using the increased anti-knock properties of high-octane fuels to reduce fuel consumption due to knock avoidance at high-load conditions.

Lightweight Materials Research. ORNL researchers designed an alternate fixture for holding magnesium sheet during dome testing. The new design, which uses a ring-in-groove mechanism, is more effective at clamping and holding samples to prevent draw-in of the sheet during dome testing. The dome test simulates the common failure strain states in sheet metal forming processes.

Performance-based Brake Tester (PBBT). A newly refurbished PBBT was received for use in the CMVRTC. The refurbishment includes a new generator set and new trailer for mobility. Tennessee Highway Patrol officers were trained in use of the equipment by the equipment vendor and ORNL. The new PBBT supports a number of ORNL-led research efforts within the CMVRTC, including the Brake Causation and Abatement Study, the Infrared-based Selection System, and Vehicle Out-of-Service Data Collection. There are now five fixed and portable PBBTs in use by the Tennessee Highway Patrol.

Vehicle Systems Integration (VSI) Laboratory. The AVL powertrain dynamometer test system demonstrated full functionality using a conventional Class 8 heavy-duty powertrain making up a Cummins 15L ISX engine. The hardware-in-the-loop system was commissioned for both engine- and powertrain-in-the-loop configurations. Both conventional and hybrid powertrain architectures were successfully demonstrated. Two sets of emission analyzers were commissioned to measure raw, engine-out emissions and post-aftertreatment (tailpipe) emissions. The AVL eStorage system (battery emulator) has been installed, and an AVL high-speed dynamometer and a modular bed plate have been ordered for the VSI component test cell. The bed plate and dynamometer provide features to support two separate, simultaneous experimental setups. Commissioning of the component test cell and the battery emulator is planned for FY 2014.

Clean Cookstove Reduces Toxic Emissions from Biomass

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

Half of the world's population cook their food by burning biomass fuel over open fires or rudimentary, inefficient stoves. The toxic emissions produced cause more than 4 million premature deaths a year and account for 20% of the world's black carbon, contributing significantly to regional and global climate change. ORNL is part of a partnership that has developed and continues to improve on a low-cost, highly efficient cookstove to help solve this complex problem.

ORNL has worked with Envirofit International (EI) and Colorado State University (CSU) since 2008 to develop metallic materials for use as combustor components in clean cookstoves for the developing world. ORNL researchers identified suitable commercially available, low-cost metal combustor alloys that are durable in the harsh operating environment of the combustor, at sufficiently low cost to permit widespread adoption. The combustor component in the EI design must resist temperatures up to 800–900°C (1,470–1,650°F) in the presence of aggressive corrosive compounds from varied biomass fuels. ORNL also pursued ways of optimizing the specification of combustor alloy composition, impurity level, and heat treatment for durability at the lowest possible alloy cost.

The key technological aspect of this cookstove is a combustor chamber (patent pending by EI, CSU, and ORNL) with design features, geometry, and materials to enable cleaner, more efficient combustion. Compared with the ceramic combustor used in the previous generation of EI cookstoves, the metal combustor is more mechanically robust and better able to withstand transportation and delivery to remote locations without component breakage. The use of a metal for the combustor also permits the use of a thin orifice plate, which further reduces emissions.

Envirofit G-3300 clean cookstove using low-cost iron-base alloy combustor (photo courtesy of Envirofit).

The resulting EI G-3300 clean cookstove is a low-cost, low-emission alternative to cooking methods now prevalent in developing countries. It reduces smoke and harmful gases by 80%, fuel use by 60%, and cooking time by 50% compared with traditional cooking fires and stoves. EI has integrated the core metal combustor technology developed for the G-3300 across six models of wood and charcoal stoves. To date EI has sold more than 700,000 cookstove units in the developing world, most of which use the metal combustor component.

The continuing ORNL-EI-CSU collaboration is devoted to improving understanding of combustion and heat transfer in cookstove metallic combustors to guide cookstove design and improve materials durability for a wide range of biomass feedstocks. Key activities will include public dissemination of corrosion and durability findings as a function of alloy type and biomass feedstock and evaluation of optimized alloys and/or coatings for a targeted 40% durability improvement over existing materials.

ORNL Examines the Sustainability of Silvicultural Practices for Bioenergy

Contact: Natalie Griffiths, griffithsna@ornl.gov, 865-576-3457

An important goal of bioenergy is environmentally sustainable feedstock production with minimal impact on soil and water resources. ORNL is leading an effort to evaluate the sustainability of high-intensity, short-rotation forestry for bioenergy that involves mechanical planting and annual or biannual fertilization and herbicide application.

The study is using both a watershed-scale experiment (at three watersheds in South Carolina) and a watershed modeling approach. Baseline water and soil data were collected from all three watersheds for two years (2010–2012). Starting in spring 2012, more than 40% of two watersheds was harvested, prepared for planting, and then planted with loblolly pine seedlings (winter 2013). Intensive silviculture activities (weed control and fertilization) necessary to achieve high yields are occurring in the two treatment watersheds (2013–2018). The third watershed is not manipulated and serves as a reference to account for variations in hydrology, water quality, and soil quality over time. Indicators of environmental sustainability are measured across the watersheds to assess whether short-rotation pine practices affect water and soil resources and whether current forestry best management practices are adequate for more intensive silviculture.

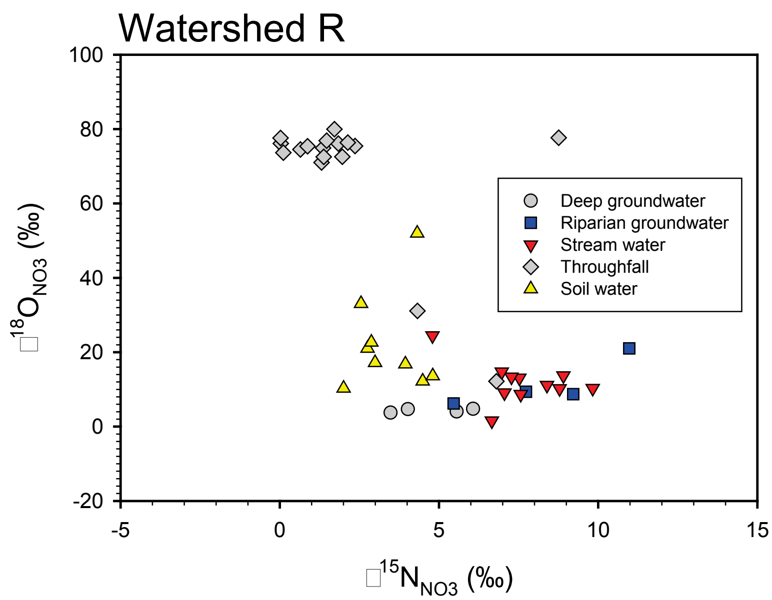
Hydrology and water quality data are also used to parameterize watershed-scale hydrological models. The goal of the modeling effort is to scale up the watershed observations to determine how woody feedstocks for bioenergy will affect hydrology and water quality at larger temporal and spatial scales.

To date, the project has been successful in characterizing baseline water quality and quantity in the three watersheds and has begun to examine short-term effects of the silviculture practices. Baseline water quality and hydrology data have been critical in determining the dominant flow paths in the watersheds, helping infer the fate of fertilizers and herbicides applied. Baseline measurements, experiments, and modeling together show that overland and lateral flows through soils are rare, suggesting that upland areas and streams are rarely connected hydrologically. Groundwater and stream flow observations,

Loblolly pine seedlings after planting in 2013.

coupled with isotopic and water chemistry data, show that riparian groundwater is a dominant source of stream flow. These results suggest that fertilizers and herbicides applied on the pine plantations in the upland areas are more likely to enter the groundwater than to be directly transported via lateral flow or overland flow to streams. These inferences from the baseline measurements and modeling efforts will be tested as the experiment proceeds.

This project is a collaboration between ORNL, the US Forest Service, the University of Georgia, Oregon State University, and the University of Saskatchewan.



Dual isotope biplot of δ18O and δ15N of nitrate in various water pools measured in reference (unmanipulated) watershed in the pre-treatment period. Overlap in the stable isotope signatures of nitrate in stream water (red triangles) and groundwater from the surrounding riparian zone (blue squares) suggests groundwater is the source of stream water nitrate. In contrast, nitrates in soil water (yellow triangles) and stream water have different stable isotope signatures, suggesting disconnect between upland areas and stream.

Presentations

1. N. A. Griffiths, P. J. Mulholland, C. R. Jackson, J. J. McDonnell, J. I. Blake, E. Du, J. Klaus, and M. H. Langholtz, "Biogeochemistry of forested watersheds in the Southeastern U.S. prior to conversion to short-rotation pine for bioenergy," presented at American Geophysical Union Conference, San Francisco, December 3–7, 2012.

2. K. B. Vache, C. R. Jackson, M. Bitew, J. Blake, J. J. McDonnell, and N. A. Griffiths, "Potential impacts of intensive cellulosic biofuel production on water quality and quantity in the Upper Coast Plain," presented at American Geophysical Union Conference, San Francisco, December 9–13, 2013.

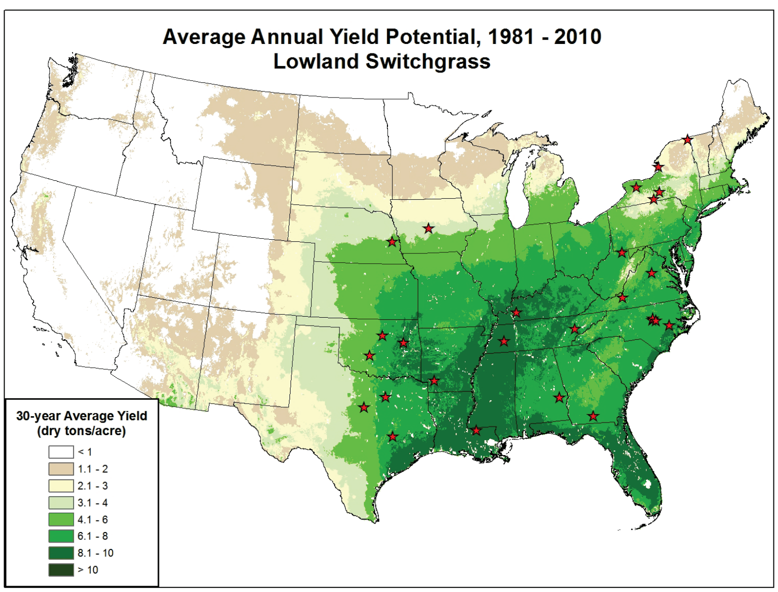
Sun Grant Regional Feedstock Partnership

Contact: Laurence Eaton, Oak Ridge National Laboratory, eatonlm@ornl.gov

The Sun Grant Initiative's Regional Feedstock Partnership commenced in 2007 with the goal of supporting the commercialization of biomass and biotechnology to meet a billion-ton annual supply as envisioned in DOE's 2005 Billion-ton Report. The partnership includes more than 100 feedstock field trials and regional resource assessments focused on agricultural residues (e.g., corn stover) and a suite of likely dedicated energy crops, including switchgrass.

In 2013–2014, a series of meetings was held across the United States with each of six crop teams and the resource assessment team to review yield trials in order to map crop productivity nationally across all soils and climatic regions. The analysis contributes to data models within ORNL's Bioenergy Knowledge Discovery Framework and the biomass chemical and physical characterization within the Idaho National Laboratory's Biomass R&D Resource Library. Together, these data collections provide empirical support of feedstock supply and logistics systems. The temporal and spatial data for biomass yield and compositional traits support the advancement of efficient, cost-effective system designs for conversion of biomass to renewable fuels, biopower, and industrial bioproducts.

Switchgrass harvested at the Cornell trial of the Regional Feedstock Partnership (Source: North Central Sun Grant Center, http://ncsungrant.sdstate.org/)



Potential annual yield of lowland switchgrass varieties at maturity estimated at 4 km resolution across all land types and use classifications. Red stars represent Regional Feedstock Partnership locations and historical field trials used to transform model predictions to absolute yield estimates. The map grid was generated using Oregon State University's PRISM-EM. (Source: Oregon State University, PRISM Climate Group)

Evaluation of Heavy and Overweight Commercial Vehicles

Contact: Adam Siekmann, siekmanna@ornl.gov, 865-946-1528

Research conducted by ORNL for federal highway safety agencies provides evidence of the danger presented by overweight commercial vehicles on the highways. It also found about a third of heavy vehicles inspected to have dangerous defects.

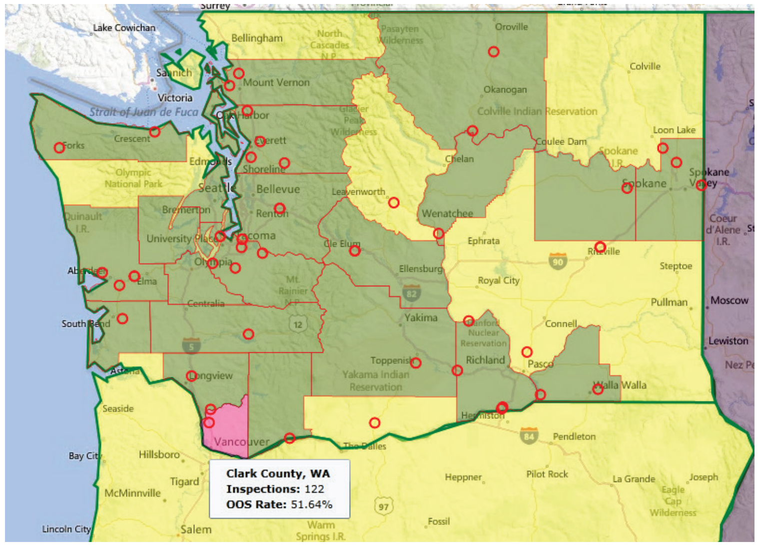
Trucks account for approximately 64% of the total freight weight moved in the United States each year. Currently, most combination commercial vehicles (tractor-trailer trucks) are allowed a maximum of 80,000 lb gross weight when traveling on the interstate. Exceeding the allowable gross weight not only damages infrastructure but also is potentially dangerous when heavy vehicles make emergency stops with faulty equipment.

ORNL is in the final year of a 3 year study funded by the Federal Highway Administration and Federal Motor Carrier Safety Administration (FMCSA) to evaluate the safety of heavy and overweight interstate commercial motor vehicles. Data were retrieved from roadside vehicle inspections performed on a voluntary basis by individual states specifically for this study. Currently, 30 of the 50 states have participated in the data collection with a total of 7,842 vehicle inspections. The ORNL researchers developed software to analyze the raw data using mapping capabilities and custom filters to better understand trends in the results.

Many heavy vehicles are weighed using static and in-motion scales installed along the interstates. However, many of these vehicles are not physically inspected because the resources are not available to inspect every one.

The study provides evidence that commercial vehicles operating on the highway system are potentially more dangerous when they exceed recommended weight limits. Analysis also showed that 35% of the heavy vehicles inspected as part of this study were found to have vehicle defects that FMCSA considers sufficient to deem the vehicles unsafe to operate, or take them out-of-service. This is higher than the national out-of-service rate for all commercial vehicles (25%).

The brake system of the vehicle was determined to be the main problem in nearly 60% of the heavy vehicles placed out of service. Tires are the second highest at 10%. The results of the analysis suggest a need for more resources directed toward the inspection of heavy vehicles and stricter maintenance procedures to detect problems on potentially dangerous vehicles before they are operated. Also, there is a need to develop new tire and brake materials that support heavier loads to allow more freight to safely be moved along US highways.



View of summary results from Washington state using the software developed. Washington had 317 inspections with a 52.4% out-of-service rate.

Publication

1. A. Siekmann and G. J. Capps, *Heavy and Overweight Vehicle Defects Interim Report,* ORNL/TM-2012/575, Oak Ridge National Laboratory, 2012.

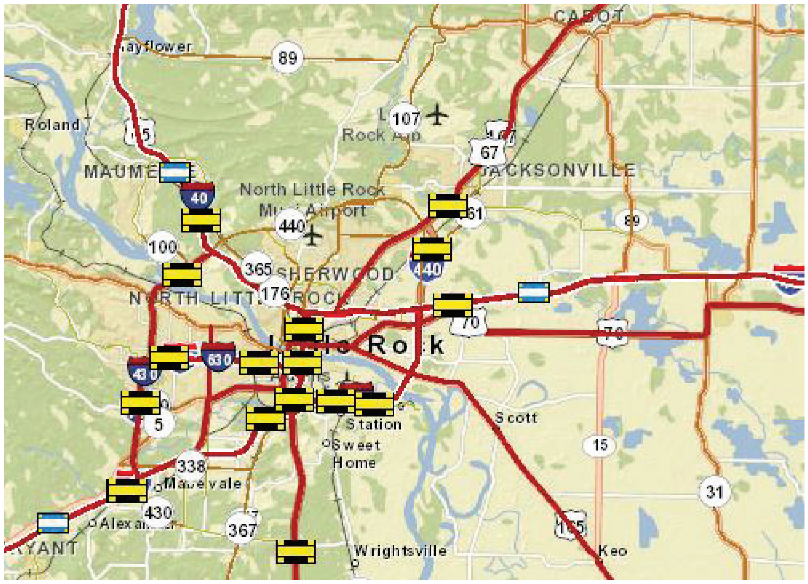
Intelligent Transportation Systems Asset Viewer

Contact: Steve Gordon, gordonsr@ornl.gov, 865-946-1313

At the annual Intelligent Transportation Society of America meeting held in April 2013, the US Department of Transportation (DOT) unveiled the Intelligent Transportation Systems (ITS) Asset Viewer, an online application that uses visual mapping technology to identify the locations of specific ITS technologies. These technologies include assets like message boards, cameras, traffic sensors, and road weather information systems. This system was developed by ORNL staff as part of the ITS Deployment Tracking Project in which ORNL tracks and analyzes progress in deployment of ITS technology for DOT.

Mike Schultze and Steve Gordon of ORNL developed the viewer, and they helped provide demonstrations during the meeting.

This is an important new resource for DOT to use in analyzing the impact of investments in technology within cities as well as rural areas nationally. Where previously only the number of assets within major cities was available, now the spatial array of deployment can be seen on the road network, showing which road segments are covered by technology as well as the existence of gaps in coverage. Asset Viewer data will be integrated with other spatial data to permit analysis of the use of technology along road segments such as evacuation routes, high-traffic areas, areas with a high incidence of crashes, designated snow routes, and corridors supporting commercial trucking. The web site is already equipped with a number of utilities to support analysis, and future development will expand these features with a focus on making the site a key DOT analysis tool.



ITS assets in Little Rock.

The launch of ITS Asset Viewer was noted in the *Research and Innovative Technology* newsletter and in the Secretary of Transportation blog:

> One new tool that transportation fans might find interesting is RITA's [Research and Innovative Technology Administration] ITS Asset Viewer, launched just this week for the ITS-A meeting. This online, web-only app shows the wide range of intelligent transportation resources already in use from coast to coast—tens of thousands of highway messaging signs, traffic control devices, and more. And all of these items—overlaid in the app atop a map of the nation—are working to keep Americans and our economy moving as fast and as safely as we can. It is an impressive collection of items that demonstrates just how thoroughly ITS innovation is embedded into our national transportation system.

DOT is funding a significant effort to further develop the site for 2014.

ORNL Helps Federal Motor Carrier Safety Administration Assess Funding

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

ORNL is providing technical assistance to the Federal Motor Carrier Safety Administration to evaluate its Motor Carrier Safety Assistance Program (MCSAP) basic and incentive funding formulae, which determine the amount of funding each state receives under the program. The goal is to determine whether these formulae are still effective at providing financial assistance to states in a manner that maximizes commercial motor vehicle safety. ORNL will provide recommendations on changes that will allow MCSAP to better support the financial needs of states and to assess what impact revised formulae would have on states.

MCSAP, a federal grant program, provides financial assistance to states to reduce the number and severity of crashes involving commercial motor vehicles. Investing grant monies in appropriate safety programs will increase the likelihood that safety defects, driver deficiencies, and unsafe motor carrier practices will be detected and corrected before they become contributing factors to accidents.

MSCAP also contributes to more uniform enforcement programs among states. It sets forth conditions for grant participation by state and local jurisdictions and requires that they adopt rules and standards compatible with the federal Motor Carrier Safety Regulations and Federal Hazardous Material Regulations for both interstate and intrastate motor carriers and drivers. The core national program elements are (1) driver/vehicle inspections, (2) traffic enforcement, (3) compliance reviews, (4) public education and awareness, and (5) data collection.

ORNL uses an evidential reasoning approach in its evaluation. There is no single piece of information that enables reviewers to determine whether the MCSAP grant formula still allocates an appropriate amount of funds to states. However, much like in a court of law, numerous pieces of evidence can be assembled to support a determination. One piece of evidence is the correlation between crashes experienced by each state in FY 2011 and the number of road miles in that state. Another is the correlation between crashes in each state and the other three formula variables: estimated population, total vehicle miles traveled, and consumption of special fuels. Other statistics also are useful, such as percentage changes in the number of crashes over time and number of fatalities over time.

The study will conclude in the spring of 2014.

ORNL is helping MCSAP analyze the effectiveness of the funding it provides to states to reduce commercial motor vehicle crashes.

ORNL Analysts Work to Strengthen Motorcoach Safety

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

From 2004 to 2012 more than 31,000 bus crashes occurred in the United States. As a result, the Federal Motor Carrier Safety Administration (FMCSA) has increased its oversight and enforcement activities related to motorcoach transportation. It has turned to ORNL for help in reviewing its statutory authority, regulations, policies, processes, and tools for motorcoach safety.

ORNL's evaluation effort includes four interrelated tasks:

1. Conduct a quantitative data analysis of the motorcoach industry to provide quantitative views of its state
2. Conduct a legislative and regulatory review of motorcoach authorities and regulations to determine if new authorities and regulations are needed and if some existing ones are unused or underused
3. Review FMCSA motorcoach safety policies and processes to provide information on key safety issues and identify changes that could enhance motorcoach safety
4. Conduct a gap analysis of the results of these reviews to identify legislative, regulatory, policy, and process weaknesses (i.e., gaps) and make recommendations for resolving them

ORNL provided FMCSA with recommendations for improving the safety of travel on motorcoaches like this one.

The effort's primary product is a list of 61 gaps and suggested recommendations for their resolution. Several observations and conclusions were made in the course of developing the list.

- FMCSA's statutory authorities regarding motorcoach safety are sufficiently broad and flexible that they can be interpreted in ways that can meet almost any safety issues FMCSA needs to address.
- New authorities are needed in certain motorcoach safety areas.
- Most identified gaps involved issues relating to FMCSA motorcoach safety policies and processes rather than statutory authority and regulation. Increased effort should be directed toward five gap areas cited most often in the policy and process review: information technology tool interoperability, hours of service and driver fatigue, en-route inspections, ticket brokers and leasing agents, and public outreach on motorcoach safety awareness.
- Other important issues identified include
  - uniformity of enforcement
  - retention of the most effective aspects of the Quick Strike program (mentors, working in teams, vehicle inspections, and the conduct of more thorough investigations)
  - evolution of FMSCA to a more science-based approach and risk-based inspection program to push the safety bar higher

Advanced Microscopy Reveals Details of Proton Exchange Membranes

Contact: Karren More, morekl1@ornl.gov, 865-574-7788

Cost and durability are the major technical challenges facing proton exchange membrane fuel cells (PEMFCs) for automotive applications. ORNL is developing novel methods to examine the material components within PEMFC membrane-electrode assemblies (MEAs) to uncover the underlying causes of their performance losses and thereby improve durability through careful materials modification and/or selection.

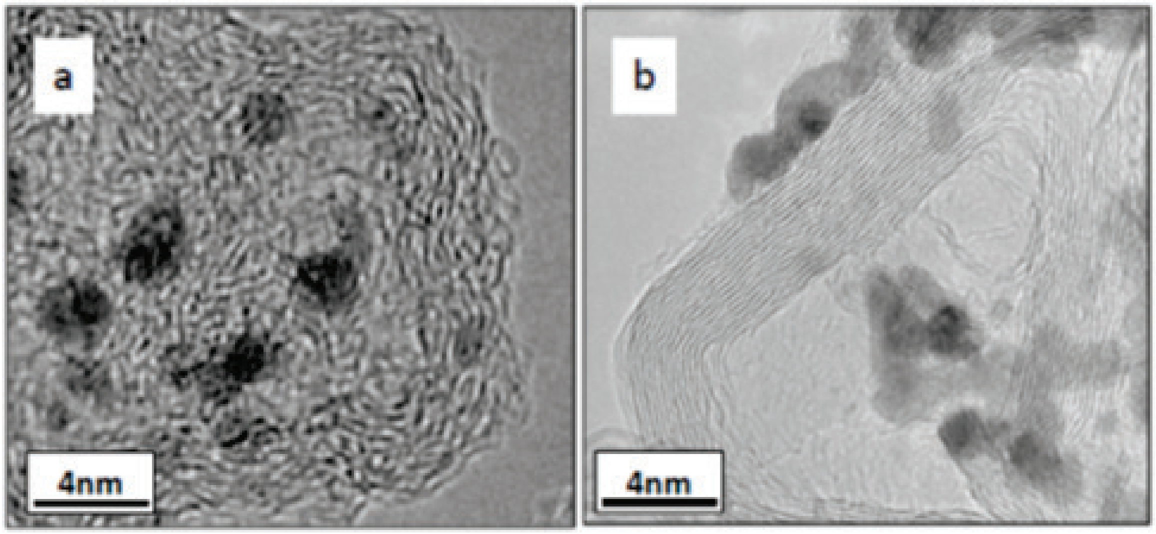
The platinum (Pt) cathode catalyst, in particular, significantly affects cost, since it is responsible for the highest fraction of the fuel cell material cost. State-of-the-art cathode catalysts consist of Pt or Pt-alloy nanoparticles dispersed on a carbon support material. A higher-performance catalyst could reduce the total amount of Pt required for the electrodes; however, catalysts that demonstrate high performance at beginning of life are many times less durable during use. It is imperative to develop a fundamental understanding of individual MEA materials degradation mechanisms to enhance performance and durability through materials optimization. ORNL has established analytical methodologies for characterizing PEMFC MEAs using state-of-the-art high-resolution transmission electron microscopy (TEM), scanning transmission electron microscopy (STEM), and spectroscopy.

Recently, ORNL contributed to understanding the mechanism(s) of carbon corrosion, a significant contributor to performance loss of the cathode. ORNL demonstrated how carbon support microstructures are correlated with initial catalyst dispersions—mechanisms by which carbon oxidizes and corrodes—and how carbon corrosion affects catalyst performance and stability. Cathode degradation at high potential holds is due to carbon corrosion and the concomitant loss of Pt as a result of Pt encapsulation in the densified/oxidized cathode layer, as well as Pt dissolution and subsequent migration into the membrane.

The degree of carbon corrosion relies specifically on the graphitization level of the carbon support. High-surface-area carbon (HSAC) is highly disordered with a defective meso-graphitic outer shell and an amorphous core that make it highly susceptible to oxidation. On the other hand, low-surface-area carbon (LSAC) comprises a highly ordered/faceted graphitic shell with a hollow core. LSAC exhibits significantly greater stability at high potentials and resists carbon corrosion as a result of the higher graphitization of the surface.

Electrochemical surface area loss of Pt is controlled by Pt coalescence, which depends on the initial Pt particle dispersion and is a direct result of the carbon support material used. A higher Pt dispersion is achieved on HSAC than on LSAC, where the catalyst particle dispersion is essentially controlled by the surface defect density of the carbon support. Thus the most critical structural factor affecting cathode durability is ultimately the defect density present on the carbon surface, which is controlled by the extent of graphitization of the support and dictates the nanoparticle dispersion. The graphitization and defect structure of the carbon support show better correlation with corrosion rate than the Brunauer–Emmett–Teller surface area of the carbon.

In addition to this work, through multiple collaborations with industry and academia, ORNL has continued to serve the analytical needs of fuel cell researchers by developing novel microscopy techniques and analytical methodologies.



TEM images of cathode catalyst materials, Pt particles dispersed on HSAC (a) and LSAC (b).

Melt-spun PAN Fibers for Gas Storage Tanks Meet Program Milestone

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

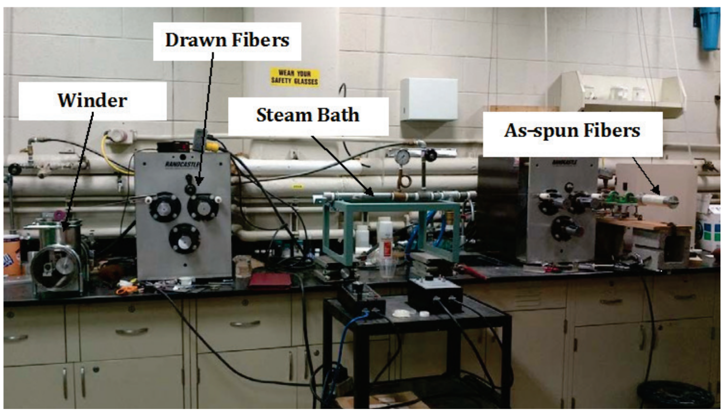
ORNL achieved a major milestone during FY 2013 by producing carbon fiber from melt-spun polyacryolnitrile (PAN) with properties that meet go/no-go decision points for the hydrogen program. The achievement demonstrates the initial feasibility of this approach.

The exceptional strength-to-weight ratio of carbon fiber composites makes them prime candidates for both mobile and stationary storage tanks for use with materials-based, cryogenic, or high-pressure gas. Cost is the primary issue for composite tanks, and carbon fiber cost and manufacturing cost are the key challenges. Current projections of the manufactured cost per unit for production volumes are about a factor of nine above storage system targets. The base cost of the carbon fiber accounts for an estimated 40–70% of the unit cost; the precursor accounts for ~40% of that and thermal processing of the precursor the rest. Melt spinning of precursor fiber could be much less expensive than the solution spinning process exclusively used today.

This project consists of tasks focused on precursor development led by Virginia Tech and conversion process improvements led by ORNL. Melt-spinnable PAN is the primary precursor option. If successful, melt spinning is expected to be significantly less costly than wet spinning and to produce high-quality, relatively defect-free precursor. Reaching that goal requires concurrent activities to develop melt-stable PAN copolymers and blends and the processes necessary to successfully spin them into filamentary tows.

For this demonstration, some baseline high-molecular-weight PAN-based formulations are being used that, while representative of processing requirements ultimately required to meet program goals, probably cannot themselves be converted into carbon fiber meeting those goals. Development of an adequate precursor formulation is a major goal for the next phase. Significant engineering obstacles have been overcome using the simple experimental equipment available in the project to demonstrate this approach is feasible, including improved spinneret design and construction, improved filtration, means of maximizing the use of small samples by integrating purging materials to maintain open holes as the sample is expended, enhanced extrusion barrel heating, a larger spinning pressure chamber, and indexed take-up winding patterns. Most recently, a capability for precursor fiber drawing in a separate process between spinning and conversion has been incorporated.

The drawn PAN/vinylacetate fibers were successfully converted to carbon fibers. The carbonized fibers have a tensile strength of over 150 ksi and a modulus higher than 15 msi, meeting the goal of the critical go/no-go milestone for feasibility demonstration. Other samples significantly exceeded this critical milestone target, including one with over 250 ksi and 25 msi. The next phase will demonstrate larger quantities of carbon fiber with improved properties through continued development of precursor formulations, spinning techniques, and carbon fiber conversion recipes.



New continuous fiber drawing system with steam bath.

Publications and Presentations

1. F. L. Paulauskas and R. E. Norris, "Melt processable PAN precursor for high strength, low-cost carbon fibers," *Fuel Cell Technologies FY 2013 Annual Progress Report*, US Department of Energy, 2013.

2. F. L. Paulauskas, "High strength carbon fibers and status report," presented at Hydrogen Storage Tech Team Meeting, April 18, 2013.

3. F. L. Paulauskas, "High strength carbon fibers," presented at 2013 DOE Hydrogen Program and Vehicle Technologies Annual Merit Review and Peer Evaluation Meeting, May 13–17, 2013.

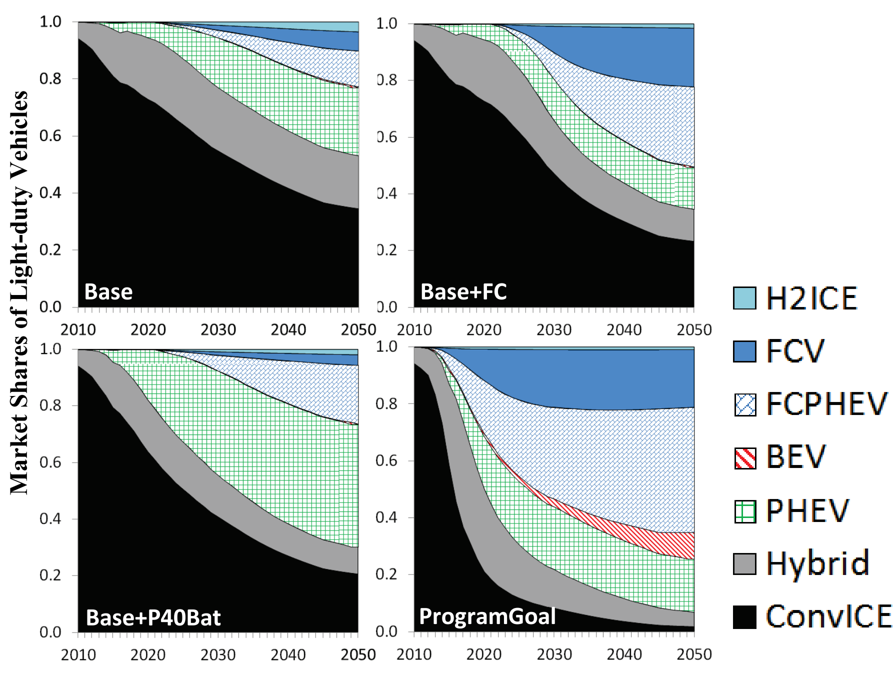
Market Prospects of Fuel Cell Plug-in Hybrid Electric Vehicles

Contact: Zhenhong Lin, linz@ornl.gov

A study conducted at ORNL found that fuel cell plug-in hybrid electric vehicles (FC PHEVs) could be competitive both in the near term and in the long run for several reasons. In the near term, when few hydrogen refueling stations are available, the plug-in battery will reduce refueling inconvenience for FC PHEV users. In the long run, both FCs and plug-in batteries will become cheaper and the FC PHEV could become a competitive powertrain.

The study, published in the *International Journal of Hydrogen Energy*, used the ORNL MA3T model to predict future sales of 40 vehicle powertrain choices among 1,458 consumer segments. Vehicle data are based on output from Argonne National Laboratory's Autonomie model.

The chart shows market shares predicted through 2050 for conventional gasoline and diesel vehicles (ConvICE), hybrid electric vehicles (HEV), gasoline plug-in hybrid electric vehicles (PHEV), battery electric vehicles (BEV), hydrogen engine vehicles (H2 ICE), fuel cell vehicles (FCV), and FC PHEVs. The four scenarios include Base, the baseline scenario; ProgramGoal, in which all DOE technical targets are met on time; Base+FC, only FC and hydrogen-related targets met on time; and Base+P40Bat, only battery and motor targets met on time.



Market shares of four scenarios by technology category.

Both FCs and plug-in batteries could dominate the light-duty vehicle market. That is, either could capture more than a 50% market share (as a result of the FC PHEV, which includes both components). If all DOE technical targets are met on time (ProgramGoal case), FCs could capture about 64% of the market and plug-in batteries about 72%.

The remarkable synergy between the FC and the plug-in battery is mainly due to their shared powertrain option—the FC PHEV—which appears to be competitive across all scenarios in both the short and long term, for some reasons common across both periods and some that differ. Low energy cost is a common reason. The FC PHEV has lower energy costs than a spark ignition (SI) PHEV (a PHEV with a gasoline engine) because it uses hydrogen fuel, which is cheaper (partly because of subsidies) and more efficient than gasoline. The FC PHEV also achieves lower energy costs than an FCV by fueling some miles with slightly cheaper electricity from the utility grid. Compared with BEVs, FC PHEVs have a longer driving range. Compared with FCVs, FC PHEVs consume less hydrogen fuel and thus require less frequent refueling, an important advantage in the early market with low hydrogen availability.

Over time, this range advantage of FC PHEVs will diminish as the hydrogen infrastructure expands, but then a long-term advantage emerges—a competitive price for the FC PHEV due to technological progress in both FCs and plug-in batteries. By 2045, an FC PHEV with a 10 mile all-electric range is predicted to be slightly less expensive than an SI PHEV with a 10 mile all-electric range if all technical targets are met on time. The competition among SI PHEVs, FCVs, and FC PHEVs reflects tradeoffs among vehicle price, energy cost, and refueling inconvenience.

Publication

1. Z. Lin, J. Dong, and D. L. Greene, “Hydrogen vehicles: Impacts of DOE technical targets on market acceptance and societal benefits,” *International Journal of Hydrogen Energy*, **38**(19), 7973–7985 (2013).

2. D. L. Greene, Z. Lin, and J. Dong, “Analyzing the sensitivity of hydrogen vehicle sales to consumers’ preferences,” *International Journal of Hydrogen Energy*, **38**(36), 15857–15867 (2013).

Analysis

My Plug-in Hybrid Calculator @www.fueleconomy.gov

Contact: Zhenhong Lin, linz@ornl.gov

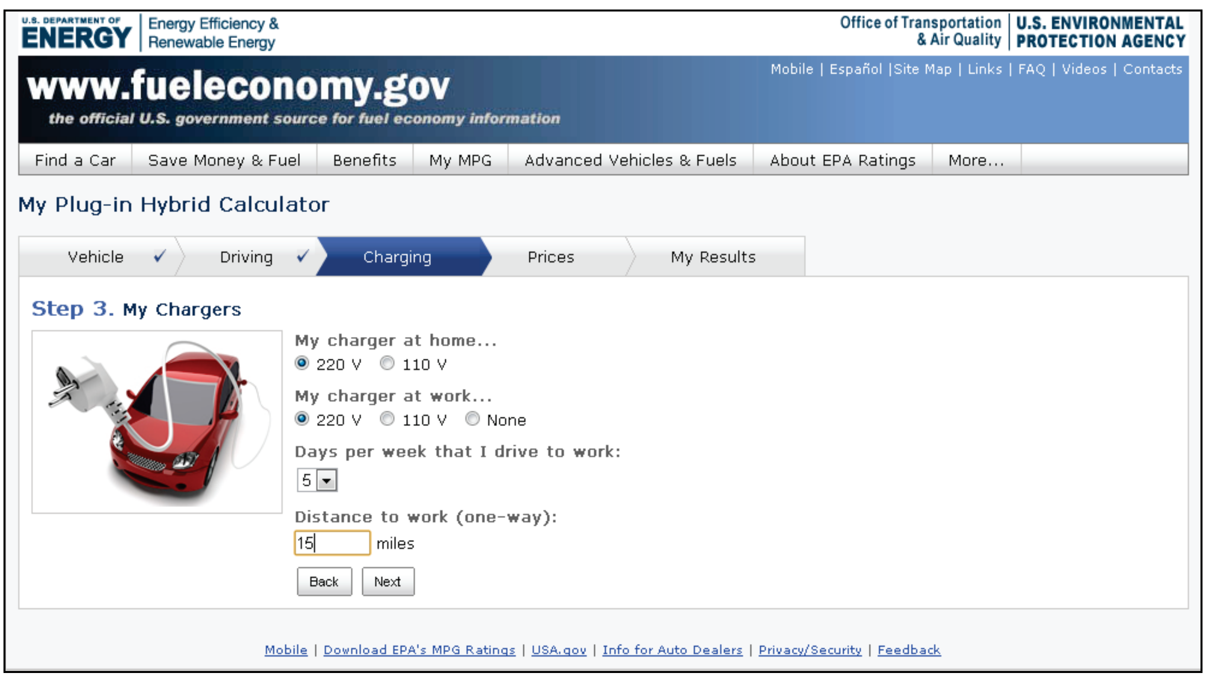
ORNL has implemented an online calculator, *My Plug-in Hybrid Calculator*, on the website www.fueleconomy.gov. The website, operated by ORNL for DOE, provides official Environmental Protection Agency fuel economy data for more than 1000 vehicle models.

Using this flexible and user-friendly tool, consumers need only answer a few questions to obtain personalized estimates of energy costs and gas station visits for operating a specific plug-in hybrid electric vehicle (PHEV).

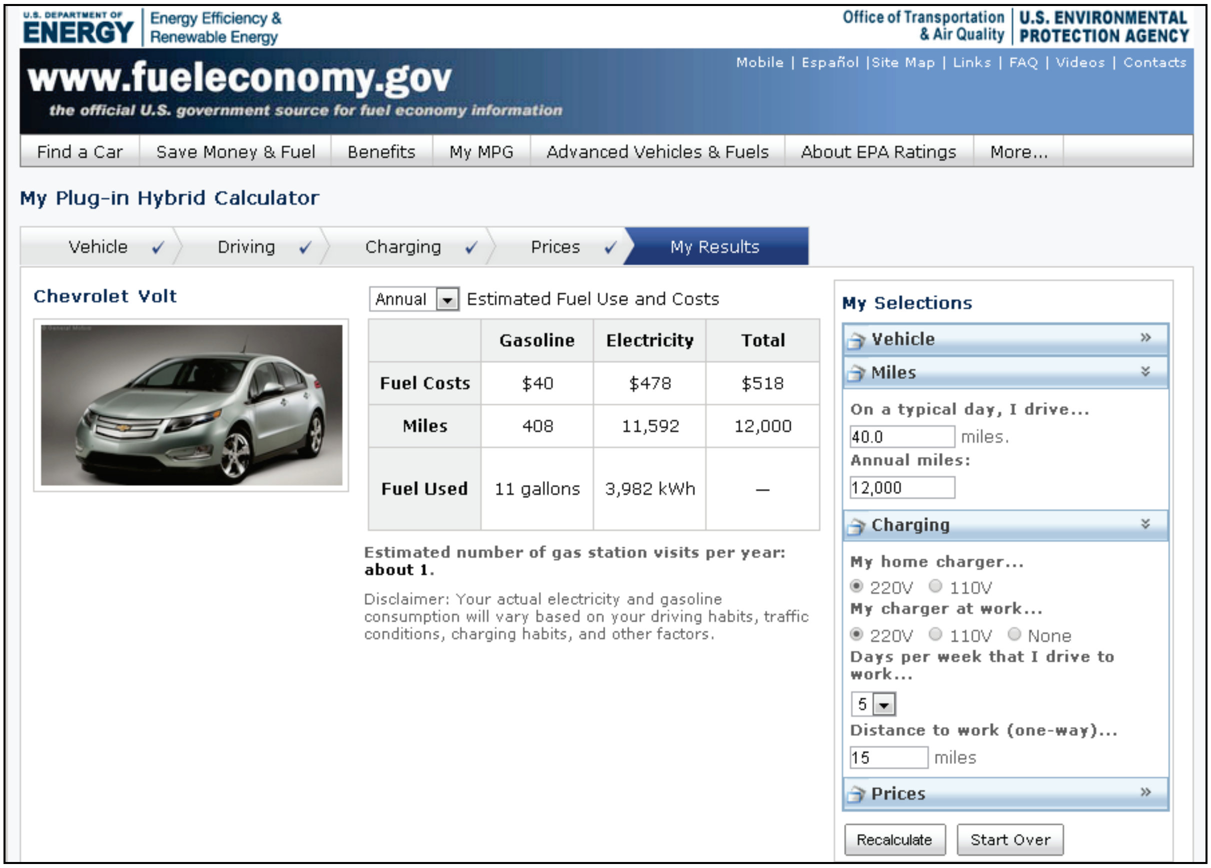
The user picks from a list of PHEV products on the market, and the system automatically reads the efficiency data for a chosen product. The user then picks the Simple Driving form that asks two questions about driving patterns: typical daily distance and annual driving distance. After the user answers a few questions about the availability of home and workplace charging and specifies gasoline and electricity prices, the calculator provides personalized estimates of energy costs, energy consumption, and number of gas station visits.

The user chooses a PHEV product.

Answers two questions about personal driving habits.



Answers brief questions on charging availability.



And receives personalized estimates for PHEV operation.

Publications

1. Z. Lin, J. Dong, C. Liu, and D. Greene, "Estimation of energy use by plug-in hybrid electric vehicles: Validating gamma distribution for representing random daily driving distance," *Transportation Research Record* **2287**(1), 37–43 (2012).

2. Z. Lin, "Optimizing and diversifying the electric range of plug-in hybrid electric vehicles for U.S. drivers," *International Journal of Alternative Powertrains* **1**(1), 108–194 (2012).

Impact of On-Road Wireless Charging on the Electric Vehicle Market

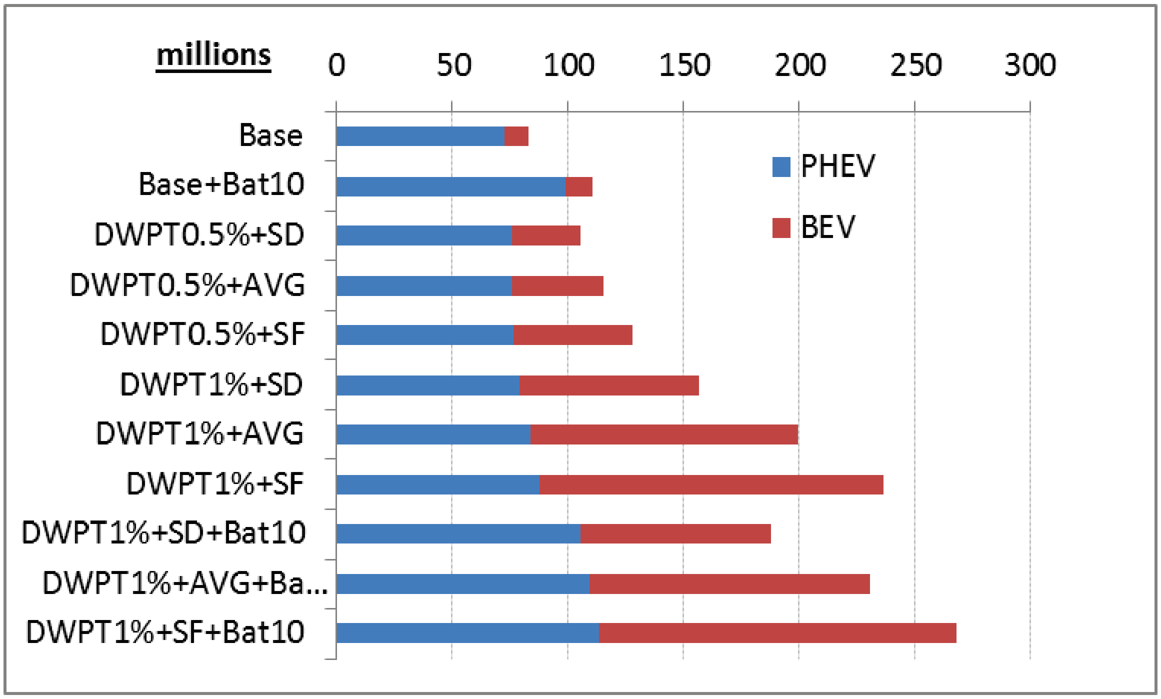
Contact: Zhenhong Lin, linz@ornl.gov, 865-946-1308

Ongoing studies at ORNL find that dynamic wireless power transfer (DWPT), or on-road charging, could significantly increase the market adoption of plug-in electric vehicles (PEVs). The sales impact is predicted to be much greater for battery electric vehicles than for plug-in hybrid electric vehicles.

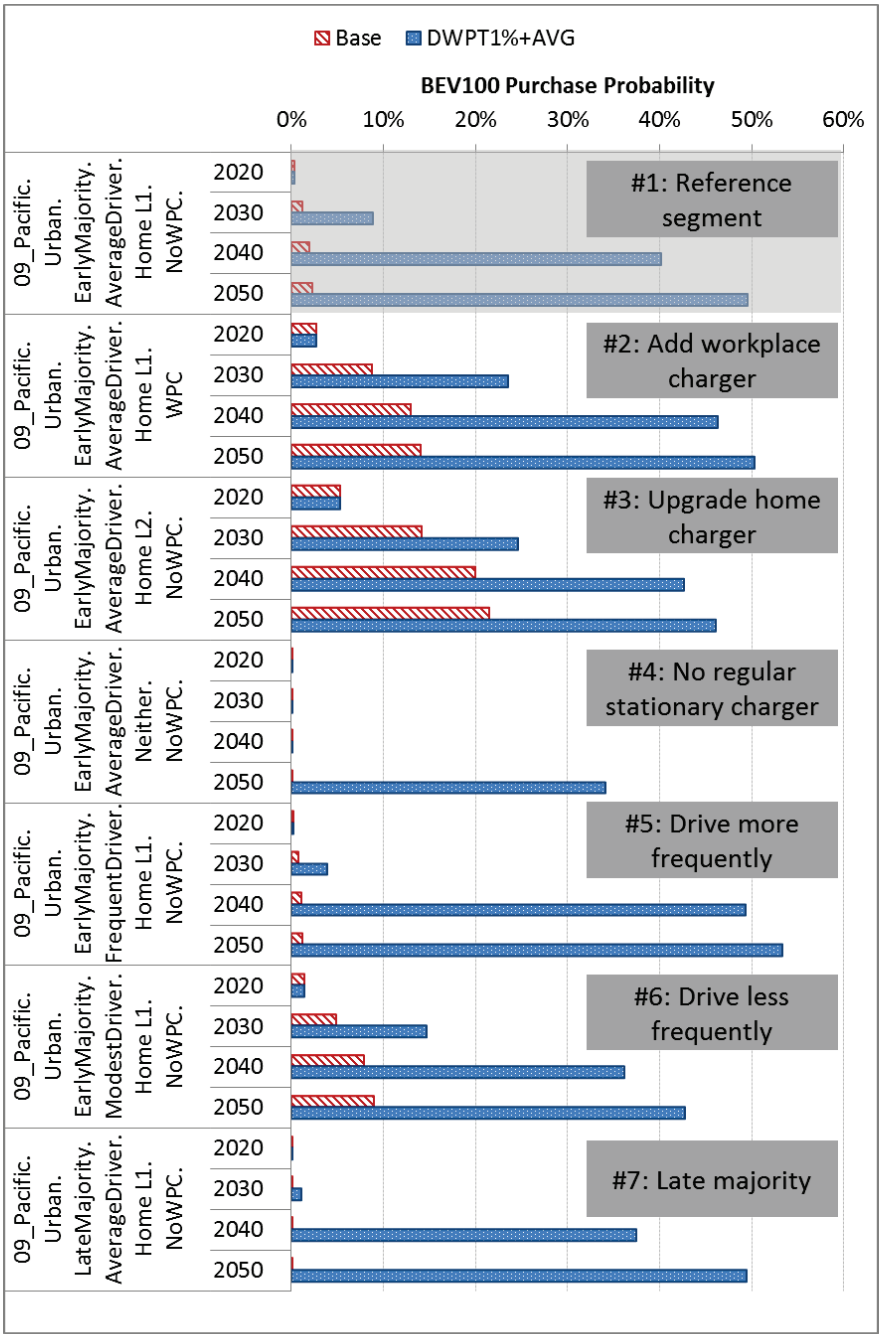
Among consumer segments, the predicted impact varies significantly. Overall, there would be larger effects on consumers who lack adequate charging capability at their homes or workplaces and on consumers with high driving intensity. DWPT could also abruptly expand the PEV consumer base once the availability of on-road charging becomes sufficient

(~0.8% of all roads) and it becomes a viable alternative to home or workplace charging for consumers who do not have access to either.

The research estimates cumulative PEV sales between 2020 and 2050 given different levels of DWPT deployment and improvements in battery technology. It also analyzes the likely effect on sales of two different traffic patterns—highly concentrated traffic volume (San Francisco metropolitan area) or more diffuse traffic (San Diego metropolitan area)—to reveal estimation uncertainty and indicate needs for further spatial analysis.



Estimated cumulative PEV sales during 2020–2050. (DWPT deployment starts in 2020 to 0.5% of all roads [WPT0.5%] or 1.0% [DWPT1%] roads by 2050. The impact varies among scenarios and depends on whether battery technology is accelerated by 10 years [+Bat10] and whether the traffic concentration follows the San Diego pattern [+SD], the San Francisco [+SF] pattern, or the average [+AVG]). Comparing the Base or Base+Bat10 scenarios, the impact is greater on BEV sales than on PHEV sales.



Impact of DWPT by consumer segment. DWPT at 0.8% of roads could significantly increase purchase probabilities across consumer segments, even those who otherwise probably would not consider battery electric vehicles, such as those without home or workplace charging and those who drive frequently.

Publication

1. Z. Lin and J. Li, "Dynamic wireless charging: Potential impact on plug-in electric vehicle adoption," accepted for publication by Society of Automotive Engineers 2014 World Congress.

Costs of Oil Dependence to the US Economy

Contact: Changzheng Liu, liuc2@ornl.gov, 865-946-1306

ORNL continued to develop its Oil Security Metrics Model (OSMM) in 2013 and used it to estimate the costs of US oil dependence from 1970 to 2012 and their economic and other effects. Since the 1970s, oil dependence has been an important national security and economic problem for the United States. To a great extent, national security issues associated with oil dependence are a consequence of its potential damage to the US economy. To inform decisions about national energy policy, it is important to measure those costs.

Oil dependence is not simply a matter of how much oil is imported but is a syndrome, a combination of factors that together create economic, political, and military problems. It consists of the concentration of the world's oil supply in a small group of states with monopoly power, together with the demand-side vulnerability of the US economy to higher oil prices and price shocks. US vulnerability depends on how much oil it consumes, the lack of ready substitutes for oil, and how much oil it imports.

OSMM is built upon linear supply and demand equations. It measures three types of dependence costs: wealth transfer from oil consumers to producers due to monopolistic pricing, loss of potential gross domestic product (GDP) output due to higher than competitive market prices, and costs of adjusting to sudden, large price changes (macroeconomic adjustment costs).

Past estimates showed oil dependence costs peaking at about $350 billion in 1980 and 1981. The ORNL study indicates oil dependence costs reached that level in 2007, soared to approximately $550 billion in 2008, fell back to just over $300 billion in 2009 and 2010, and increased again to $500 billion in 2011–2012. However, US GDP today is more than twice its 1980 GDP. Relative to GDP, oil dependence costs were 3.5% in 2008 and 4.5% in 1980. The cumulative, direct costs of oil dependence to the US economy from 2005 to 2012 are estimated at approximately $3.3 trillion.

Monte Carlo simulations reflecting uncertainties in key parameters produced ranges including 90% of the simulation estimates of $429 billion to $602 billion, with a mean value of $508 billion, for oil dependence costs in 2008 and from $268 billion to $339 billion, with a mean of $302 billion, for 2010. The 5th to 95th percentile range for total costs from 2005 to 2012 is $2.9 trillion to $3.7 trillion.

How much of the cost of oil dependence can be avoided? History suggests reduced demand and increased non-OPEC supply, as was seen between 1990 and 2002, could reduce oil dependence costs by an order of magnitude. A comprehensive strategy of efficiency improvement, substitution of other energy sources for petroleum, and increased domestic energy production could do the same in the future.

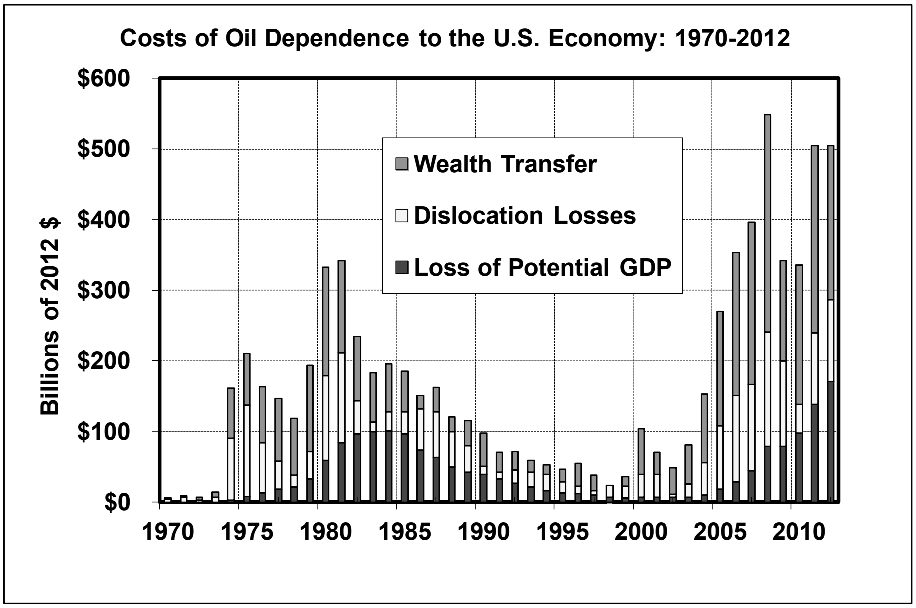
Publications and Presentations

1. D. L. Greene, R. S. Lee and J. L. Hopson, "OPEC and the costs to the U.S. economy of oil dependence: 1970–2010," White Paper 1-13, Howard H. Baker, Jr., Center for Public Policy, University of Tennessee (2013).

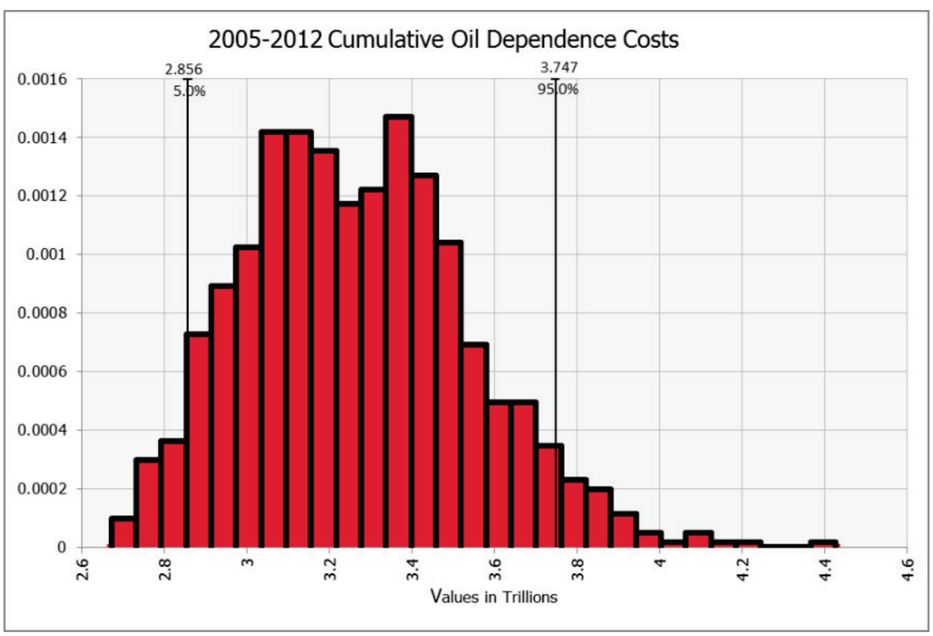
2. D. L. Greene, "The future of the world oil market," presented at the annual meeting of the International Subcommittee of the Energy Committee of the Transportation Research Board, Washington, D.C., January 15, 2013.

3. D. L. Greene, "The economics of US oil dependence and implications for public policy," lecture at The Kennedy School, Harvard University, October 22, 2012.

4. D. L. Greene, "The challenge of energy sustainability in surface transportation," presented at the University Transportation Center Spotlight Conference on Sustainable Transportation, Keck Center, National Academies, Washington, D.C., November 8, 2012.



Annual cost of oil dependence to US economy (1970–2012).



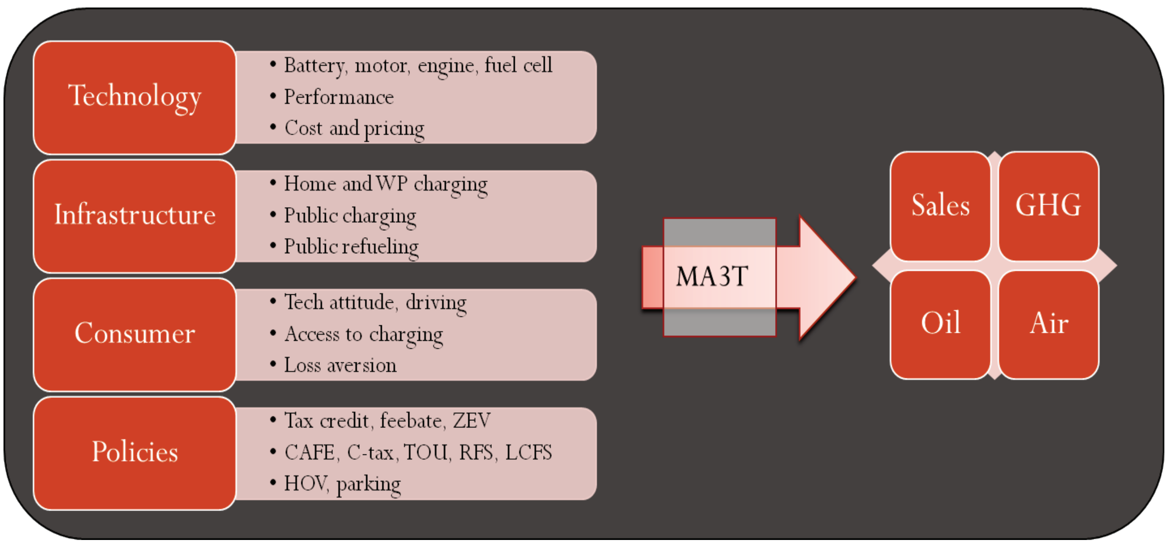
Cumulative oil dependence costs from 2005 to 2012.

Learning-from-History Feature of the MA3T Model

Contact: Zhenhong Lin, linz@ornl.gov

Market Acceptance of Advanced Automotive Technologies (MA3T), a consumer choice model developed by ORNL, endogenously projects sales of competing vehicle technologies among consumer segments. MA3T is a flexible, credible tool for analyzing how technology, behavior, infrastructure, and policy affect sales of new technologies and the resulting societal, environmental, and economic impacts.

During FY 2013, ORNL developers implemented a Learning-from-History (LFH) feature to enhance the prediction accuracy of MA3T. The LFH feature includes two functions—Automatic Calibration and Independent Validation. With Automatic Calibration, MA3T is calibrated with historical sales and prices of vehicle products during 2005–2011. The calibrated MA3T is then independently validated by prices and sales of cars, light-duty trucks, plug-in hybrid electric vehicles, and battery electric vehicles during 2012. With 2013 sales and price data becoming available, LFH calibration and validation will be further improved.



MA3T analyzes how aspects of technology, infrastructure, consumer behavior, and public policies affect sales of vehicle technologies and the social and economic impacts that result from those sales trends.

MA3T forecasts sales of 40 vehicle choices (conventional, natural gas, diesel, plug-in, battery electric, and hydrogen vehicles for both passenger cars and light-duty trucks) among 1,458 consumer segments in response to changes in technologies, infrastructure, consumer preferences, energy prices, and policies.

The consumer segments included represent demand versatility with respect to regions, residential areas, driving patterns, technological attitudes, access to home charging, and access to charging at work. The consumer segmentation, together with the wide range of represented technologies, allows analysis of who buys what technologies, by how many, and when. With comprehensive linkages to market driving forces, MA3T is capable of identifying research and development priorities, infrastructure roll-out strategies, and smart policies for the purpose of promoting a specific vehicle technology, including fuel cell electric vehicles. It can also be used to evaluate and justify any of the previously proposed strategies. MA3T is calibrated and independently validated with historical sales and price data. It can be executed on any personal computer with MS Excel 2010 or later versions.

Publications and Presentations

1. Z. Lin, D. Greene, and C. Liu, *Documentation for the MA3T Model,* working document.

2. Z. Lin, "Modeling market acceptance of plug-in electric vehicles," presented at the Joint Seminar of Vehicle Electrification Group and Climate and Energy Decision Making Center, Carnegie Mellon University, April 9, 2013.

3. Z. Lin, "Updating and enhancing the MA3T vehicle choice model," presented at 2013 DOE Vehicle Technologies Program Annual Merit Review, Washington, D.C., May 13, 2013.

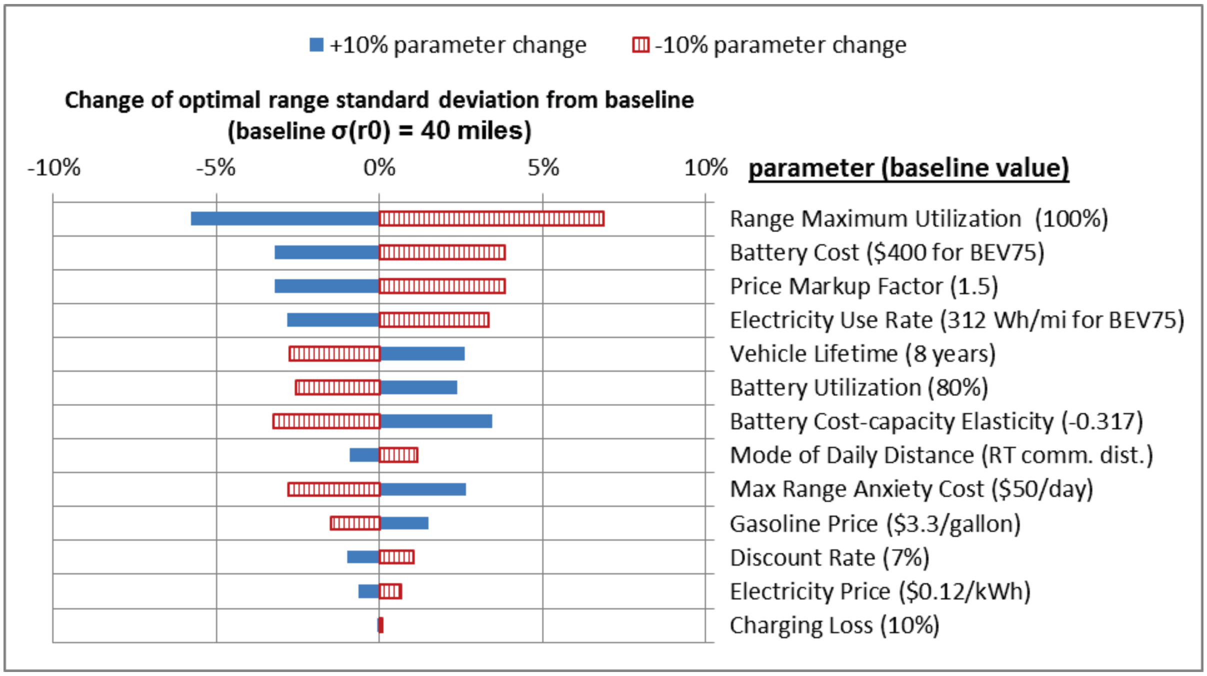
Optimal Market Mix of BEV Ranges for US Consumers

Contact: Zhenhong Lin, linz@ornl.gov

A study by ORNL researchers estimates the optimal market mix of battery electric vehicle (BEV) driving ranges for US consumers. The estimated mix serves as a basis for evaluating the market prospects of BEVs and their impact on petroleum consumption and greenhouse gas emissions.

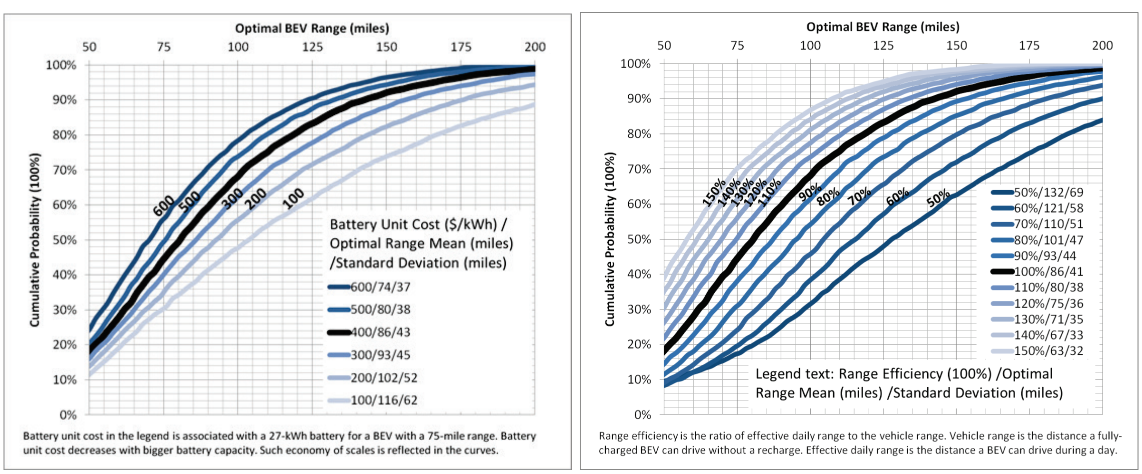
Properly determining the driving range is critical for accurately predicting the sales and social benefits of BEVs. This study proposes a framework for optimizing the driving range by minimizing the sum of battery price, electricity cost, and range limitation cost—referred to as the "range-related cost"—as a measurement of range anxiety. The objective function is linked to policy-relevant parameters, including battery cost and price markup, battery use, charging infrastructure availability, vehicle efficiency, electricity and gasoline prices, household vehicle ownership, daily driving patterns, discount rate, and perceived vehicle lifetime.

Assuming $400/kWh for battery cost and a sample (N=36664) representing new car drivers in the United States, the study estimates optimal BEV ranges among US drivers at 85 miles on average, with a standard deviation of about 40 miles. This suggests a wide dispersion of optimal BEV range among US drivers owing to variations in driving patterns and household vehicle ownership. The average optimal range among US drivers is found to be largely inelastic. The top two influential factors are range maximum utilization, which increases with better charging infrastructure, and battery cost.



Sensitivity of average optimal range.

The quantitative results strongly suggest that ranges of less than 100 miles are likely to be more popular in the BEV market for a long period of time, during which battery costs are expected to decrease and charging infrastructure is expected to improve. These two forces affect optimal ranges in opposite directions: lower battery cost drives BEV demand toward longer ranges, whereas an improved charging infrastructure is found to drive demand toward shorter ranges. The bias of a single range assumption and the effects of range optimization and diversification in reducing such biases are both found to be significant.



(Left) Cumulative share of optimal range by battery cost. (Right) Cumulative share of optimal range by range maximum utilization.

Publications

1. Z. Lin, "Battery electric vehicles: Range optimization and diversification for U.S. drivers," accepted by *Transportation Science* (2013).

2. Z. Lin, "Modeling market acceptance of plug-in electric vehicles," presented at the Joint Seminar of Vehicle Electrification Group and Climate and Energy Decision Making Center, Carnegie Mellon University, April 9, 2013.

Combustion Engines and Fuels

Benefits of High-Octane Ethanol Blends

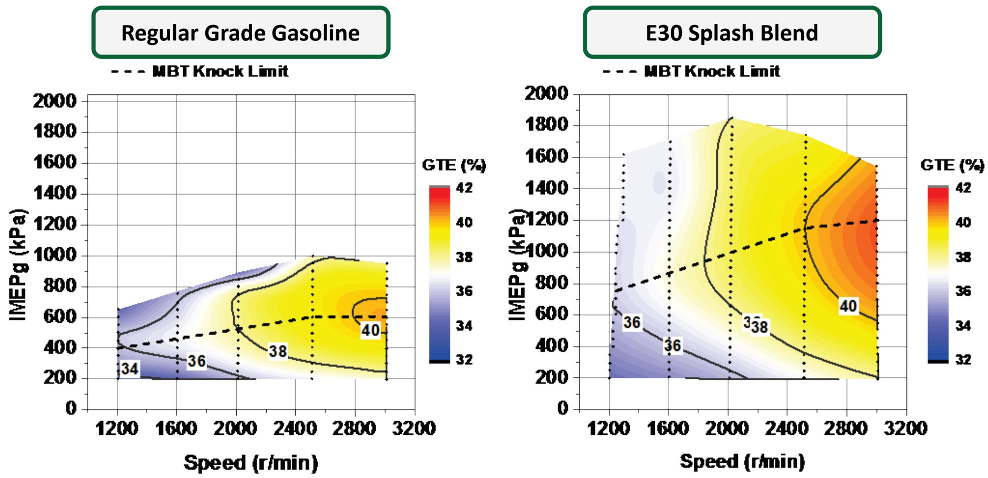
Contact: James Szybist, szybistjp@ornl.gov, 865-946-1248

Ethanol has a number of fuel properties that are advantageous in spark-ignited (SI) engines. Its high octane number and high latent heat of vaporization both contribute to superior anti-knock properties. When engine hardware is configured to take advantage of these properties, ethanol can enable higher thermodynamic efficiency and higher power density than regular or premium grade gasoline.

A number of ORNL studies have illustrated that the superior anti-knock properties of a blend of ethanol and gasoline called E85 can result in higher thermodynamic efficiency even when the fuel blend contains as little as 51% ethanol and is blended with low-octane-number hydrocarbon streams. In FY 2013, ORNL researchers conducted single-cylinder engine experiments illustrating that a 30% splash blend of ethanol with regular grade gasoline can improve fuel quality to such an extent that the power density of the engine is doubled in a high-compression-ratio configuration. The improved performance of the fuel reduces the fraction of the engine map in which the engine is knock-limited, thereby increasing its thermodynamic efficiency over a wide operational envelope. Perhaps more important, the increase in power density enables engine downsizing and downspeeding, which can result in system-level efficiency gains through reduced friction and higher load duty cycles for the same application.

Blends containing 15–30% ethanol improve anti-knock properties with a much smaller penalty in volumetric energy density than E85. Therefore, tank mileage from blends with as much as 30% ethanol in appropriately designed vehicles may be comparable to or better than the tank mileage of conventional gasoline vehicles.

Federal Corporate Average Fuel Economy (CAFE) regulations require higher-efficiency vehicles, and the federal Renewable Fuels Standard (RFS II) requires an increase in the use of bio-derived fuels. ORNL researchers are leading experimental efforts and outreach (via symposiums and conference panels) to automakers, energy companies, fuel distributors, and regulators to determine if it is logistically possible to take advantage of the higher engine efficiency offered by ethanol use to meet both CAFE and RFS II requirements. In addition, a DOE-funded project combining high-octane multi-cylinder engine experiments and drive cycle simulations is being conducted at ORNL in close coordination with industry.



Efficiency contours over the operable speed/load range for regular grade gasoline and an E30 splash blend.

Publications and Presentations

1. J. Szybist and B. West, "The impact of low octane hydrocarbon blending streams on the knock limit of 'E85,'" *SAE International Journal of Fuels and Lubricants* **6**(1), 44–54 (2013).
2. D. Splitter and J. Szybist, "An experimental investigation of spark ignited combustion with high octane bio-fuels and EGR, Part 1 of 2: Engine load range and downsize downspeed opportunity," *Energy & Fuels*, in press.
3. D. Splitter and J. Szybist, "An experimental investigation of spark ignited combustion with high octane bio-fuels and EGR, Part 2 of 2: Fuel and EGR effects on knock limited load and speed," *Energy & Fuels*, in press.
4. D. Splitter and J. Szybist, "Intermediate alcohol–gasoline blends, fuels for enabling increased engine efficiency and powertrain possibilities," SAE Technical Paper 14PFL-0262, to be presented at the 2014 SAE World Congress.

EGR Probe Applications Enable Engine Performance Advances

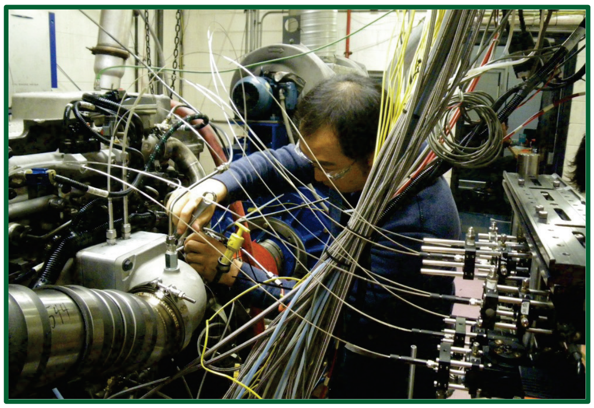
Contact: William Partridge, partridgewp@ornl.gov, 865-946-1234

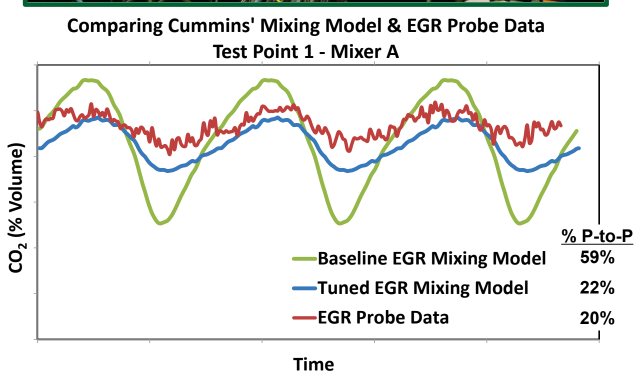
ORNL has developed and applied an exhaust gas recirculation (EGR) probe in a cooperative research and development agreement (CRADA) project with Cummins, Inc. The probe's development provides for crank-angle and spatially resolved CO_2 measurements throughout an engine's intake manifold.

The probe has been used for a wide range of technologies related to developing advanced-efficiency engine systems, including assessment, elucidation, and improvement of intake architectures; mixing physics; control strategies; cylinder-to-cylinder and cycle-to-cycle combustion uniformity; and numerical design tools such as computational fluid dynamics (CFD).

The EGR instrument, based on mid-infrared laser absorption, uses a single-port probe and allows for simultaneous measurement from four separate probes. The physical probe is based on a 3/8 in. outside-diameter tube. Because the probe requires only a single access port to the measurement location, researchers have broad measurement possibilities on developed and advanced packaged engines, in which access often is limited. Minimal modification of the stock hardware is required. EGR distributions can be resolved via multiple access points and probe translation. The spectroscopic approach allows for simultaneous measurement of CO_2 concentration and pressure to differentiate fluctuations associated with mixing and combustion versus density. Four-point multiplex measurements allow for rapid, extensive system mapping. The system is capable of resolving transients not only within individual valve events but also throughout the cycle.

In addition to assessing specific hardware, ORNL researchers can assess and improve the validity of the tools by comparing measured performance with that predicted by CFD design tools. This EGR probe application has enabled a 63% improvement in the baseline EGR mixing model.





An EGR probe allows for on-engine measurements (photo). It has been used to improve the mixing model used for development and design by about 63% (bottom).

Presentation

1. W. Partridge, J. Yoo, R. Connatser, V. Prikhodko, R. Gonzalez, J. Parks, S. Geckler, A. Perfetto, A. Beck, M. Dane, R. Booth, and D. Koeberlein, "Cummins/ORNL FEERC

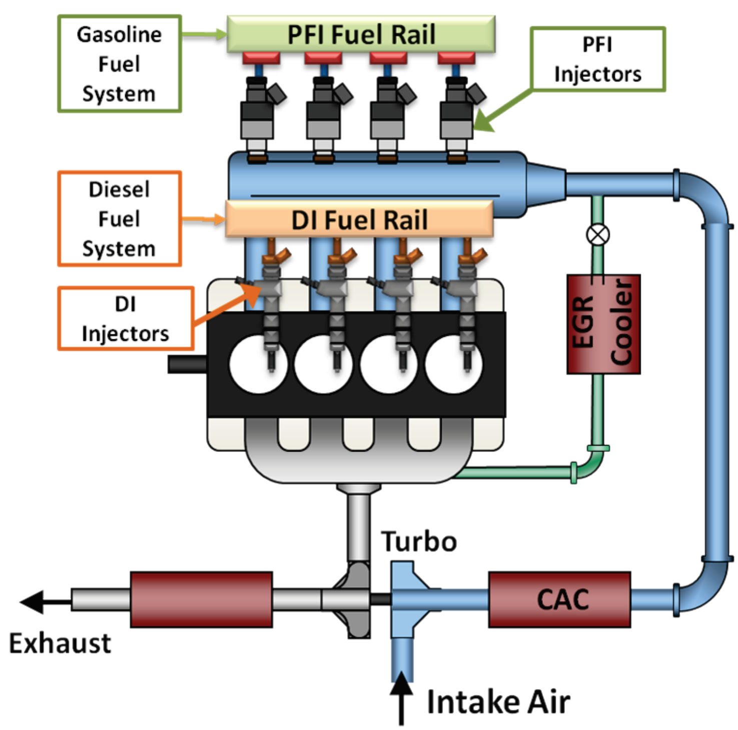
Combustion CRADA: Characterization and reduction of combustion variations," presented at 2013 DOE Vehicle Technologies Program Annual Merit Review, Arlington, Va., May 16, 2013.

High-Efficiency Clean Combustion in Light-Duty Diesel Engines

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

Advanced combustion has shown promise for achieving high thermal efficiencies with ultra-low NO_x and particulate matter (PM) emissions. A reactivity controlled compression ignition (RCCI) engine uses in-cylinder blending of two fuels with different reactivities to improve control of the combustion process. At ORNL, drive cycle modeling of RCCI operation with diesel fuel and a 30% ethanol blend (E30) has demonstrated at least a 20% improvement in fuel economy over a 2009 port fuel injection (PFI) gasoline vehicle baseline.

To model fuel economy and emissions over a variety of drive cycles, ORNL researchers developed and used an experimental RCCI engine map in vehicle system simulations. A 4-cylinder General Motors 1.9 L diesel engine installed at ORNL was modified to include a port fuel injection system using conventional gasoline injectors and pistons that were designed for RCCI operation.



ORNL multi-cylinder RCCI engine.

Experimental steady-state operating points on the modified engine were used to develop a speed/load map consistent with a light-duty drive-cycle and with enough detail for vehicle simulations. The engine map was developed using E30 fuel and certification-grade diesel fuel. The potential fuel economy of RCCI operation was evaluated using vehicle system simulations with experimental steady-state engine maps. Simulations used a multi-mode RCCI/diesel operating strategy by which the engine would operate in RCCI mode whenever possible but, at the highest and lowest engine operating points, would switch to diesel mode.

Multi-mode RCCI/conventional diesel combustion (CDC) operation was shown through vehicle system simulations to have the potential to offer a fuel economy improvement of over 20% compared with a 2009 gasoline PFI baseline. The peak efficiency from the RCCI operating map was within federal light-duty drive cycle speed and load range, whereas CDC peak efficiency was well outside the federal range. However, the current range of the experimental RCCI engine map does not allow full coverage of many light-duty drive cycles. RCCI fuel economy improvements were observed despite lack of complete drive cycle coverage.

Research results showed that NO_x emissions are dependent on the drive cycle coverage of RCCI. Fuel use over the drive cycles showed that nearly equal amounts of gasoline and diesel fuel probably would need to be carried on board for RCCI multi-mode operation. During RCCI-only operation, fuel use was between 57.6% and 66.7% gasoline.

Publications

1. S. Curran, R. Hanson, R. Wagner, and R. Reitz, “Efficiency and emissions mapping of RCCI in a light-duty diesel engine,” SAE Technical Paper 2013-01-0289 (2013).

2. S. Curran, R. Wagner, and R. Hanson, “Reactivity controlled compression ignition (RCCI) combustion on a multi-cylinder light-duty diesel engine,” *International Journal of Engine Research* **13**(3), 216–225 (2012).

3. V. Prikhodko, S. Curran, J. Parks, and R. Wagner, “Effectiveness of diesel oxidation catalyst in reducing HC and CO emissions from reactivity controlled compression ignition,” *SAE International Journal of Fuels and Lubricants* **6**(2), 329–335 (2013).

4. R. Hanson, S. Curran, R. Wagner, and R. Reitz, “Effects of biofuel blends on RCCI combustion in a light-duty, multi-cylinder diesel engine,” *SAE International Journal of Engines* **6**(1), 488–503 (2013).

Novel Bimetallic Catalysts Improve Low-Temperature Oxidation

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

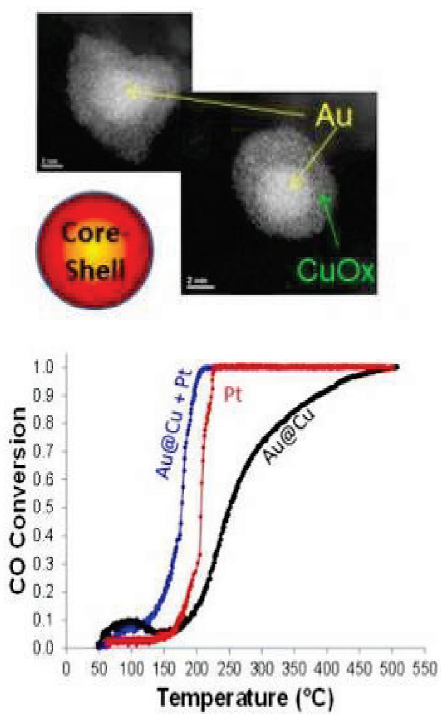
Improvements in the efficiency of advanced combustion engines are creating challenges for emission control systems because greater fuel efficiency is leading to lower exhaust temperatures. Oxidation of CO and other pollutants by catalysts becomes more difficult at lower temperatures, but a new type of catalyst developed at ORNL is enabling improved low-temperature performance.

A bimetallic catalyst composed of gold and copper, discovered through research in ORNL’s Basic Energy Sciences program, has unique properties that vary with exhaust conditions.

Under rich conditions, an intermetallic nanoparticle of gold and copper forms; but under lean conditions, a core-shell particle forms with gold on the inside core surrounded by a copper oxide shell. It is this latter core-shell nanoparticle that exhibits improved low-temperature oxidation.

In studies on a bench flow reactor, the gold–copper catalyst achieves >90% conversion of CO below 100ºC, compared with the typical 190ºC lower limit for platinum-based catalysts. In simulated exhaust gases, NO was found to inhibit CO oxidation more than the gold–copper catalyst. Researchers physically mixed a platinum-based catalyst with the gold–copper catalyst to develop a combined catalyst, which demonstrated synergistic performance benefits and overall improvement in low-temperature oxidation compared with the more common platinum-based catalyst. CO oxidation performance "light-off" was attained at a temperature 30ºC lower than the limit for the platinum catalyst, and NO oxidation efficiency was doubled.

Hydrocarbons currently inhibit catalyst performance, and ongoing research is aimed at addressing hydrocarbon-induced limitations. However, the combination of gold–copper and platinum catalysts shows benefits when hydrocarbon emissions are minimal. The improved catalytic performance will enable advanced combustion engines to meet challenging emission regulation levels.



Micrograph of a gold–copper core-shell catalyst nanoparticle (top) and data showing a lower CO oxidation temperature for a gold–copper and platinum mixed catalyst in the presence of CO and NO (bottom).

First Systematic Study of GDI PM Size, Shape, and Composition

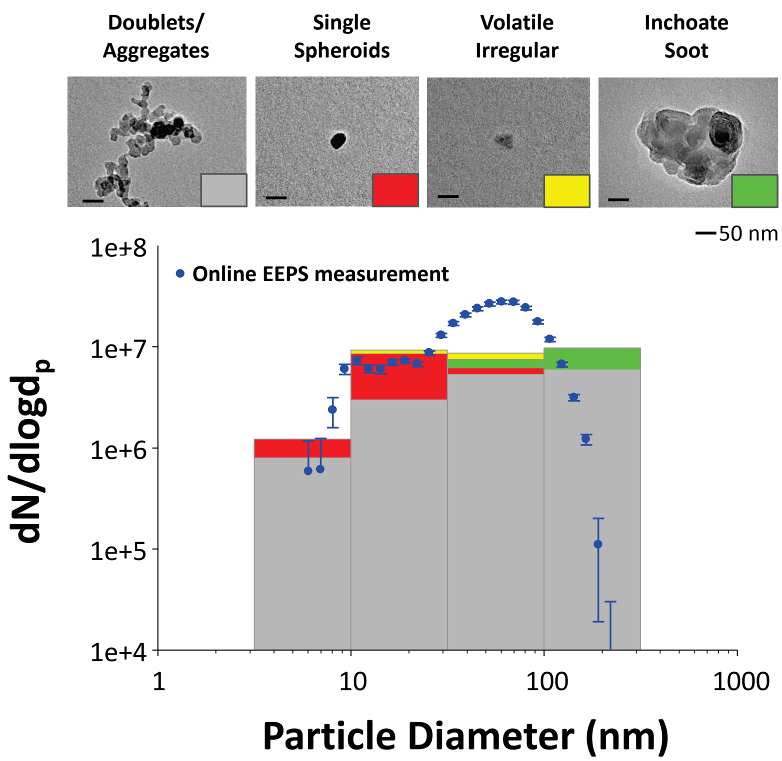
Contact: John Storey, storeyjm@ornl.gov, 865-946-1232

As direct fueling replaces port fuel injection in gasoline engines to boost fuel economy, a rise in particulate matter (PM) emissions has become an environmental challenge. Managing the amount of gasoline direct injection (GDI) PM emissions involves in-cylinder combustion control and/or after treatment with gasoline particulate filters (GPFs). ORNL researchers are seeking a better understanding of the origins of GDI PM emissions to improve in-cylinder control and lessen GPF requirements, thus preserving fuel economy gains while decreasing PM emissions.

Using conventional particle sizing, ORNL researchers studied the soot that results from GDI engines and determined that particles in GDI soot spanned a much wider size range than soot particles produced by diesel engines. Researchers collected a representative sample of GDI soot using a transmission electron microscopy (TEM) grid sampler designed to collect the full spectrum of particle sizes. TEM has been used for two decades to show and describe soot particles; however, ORNL developed a new analysis technique for use with TEM images and was able to quantitatively measure the particle sizes and shapes to arrive at a size distribution.

Soot comprises chain-like structures, called aggregates, of tiny, spherical particles. Modern diesel engines, for example, produce aggregates of uniform primary particles measuring 20–25 nm. Diesel PM uniformity is caused by high injection pressures and uniform atomization. Remarkably, researchers found GDI soot to be mostly aggregates of nanoparticles with a broad size range. The next most abundant particles were single spheroids, and a small fraction were irregular volatile particles that are common in exhaust. Inchoate soot with a thick, low-volatility film made up the remaining 10–20% of the total concentration.

The broad size range of particles indicates that fuel and air are not mixing completely in-cylinder. Fuel impingement on surfaces leads to fuel-rich zones that produce large nanoparticles, as well as areas that have less fuel, resulting in the formation of small particles. Bulk PM analysis determined that soot precursor compounds are present, and film on inchoate soot indicates incomplete formation of the primary soot particle and fuel-rich conditions. As soot builds up on a GPF, packing and pore penetration of small nanoparticles reduces the filter’s porosity and increases backpressure, resulting in a decrease in fuel economy. For this reason, quantitative studies of particle size and shape can guide in-cylinder control of GDI PM to either enhance GPF performance or eliminate the need for GPFs.



Characteristics of GDI soot based on transmission electron microscopy and conventional particle sizing methods. The gray portion of the bars represents aggregates of nanoparticles; red, single spheroids; yellow, irregular volatile particles; and green, inchoate soot.

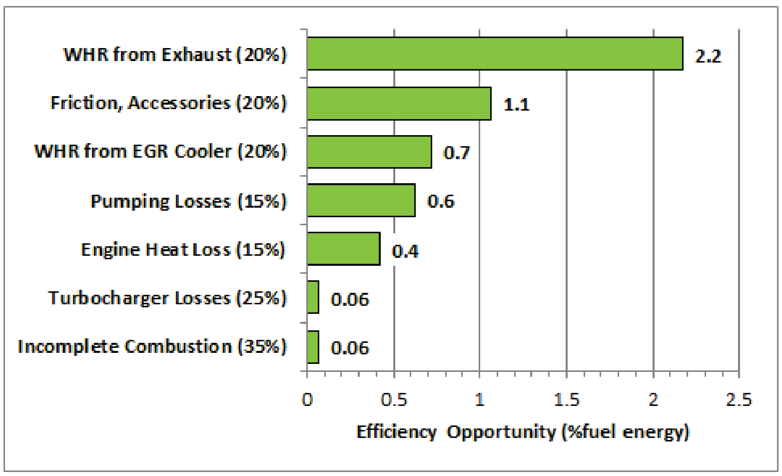
New Method Assesses Engine Efficiency Opportunities

Contact: K. Dean Edwards, edwardskd@ornl.gov, 865-946-1213

Increasingly stringent fuel economy regulations are driving innovative approaches to improving the efficiency of internal combustion engines. Less than half of the energy released during combustion typically produces work with the piston, while the remainder is consumed by inefficient processes including friction, pumping, heat loss, and hot exhaust leaving the tailpipe. The relationships among these processes are so highly interdependent that reducing one area of energy loss often increases another. Achieving a significant increase in engine efficiency requires a thorough understanding of these interdependencies as well as multiple, concurrent approaches to reduce losses and concentrate the remaining energy into pathways (such as the exhaust) where it may be recovered to provide additional work.

Researchers at ORNL have developed a new method to account for the interdependent nature of energy use in an engine and assess the potential benefits of various efficiency improvement strategies. The approach begins with a complete first and second law thermodynamic analysis of experimental and/or simulation data to evaluate how energy is consumed in the engine. The potential efficiency benefits of given strategies are then evaluated by applying thermodynamics-based, multiplicative factors to estimate reductions in energy consumption and predict how the recovered energy may be redistributed among the other energy pathways. The highly interdependent nature of the energy pathways in the engine obviously makes these predictions and the selection of appropriate factors very difficult. However, the mathematical simplicity of this approach allows for extensive sensitivity and uncertainty analyses to be conducted to provide a statistical range of potential benefits for a given efficiency-improvement strategy.

ORNL is working closely with industry stakeholders through the US Council for Automotive Research partnership to apply this new technique to benchmark data from state-of-the-art light-duty engine platforms. Researchers will use the data to develop ways to maximize efficiency for light-duty applications. Potential benefits have been calculated for a light-duty diesel engine for a particular scenario in which reductions in friction, pumping losses, and heat loss provide increased work output with the piston; and energy is concentrated in the exhaust, where additional work can be produced with a waste heat recovery strategy (e.g., a bottoming cycle). This combination of strategies is predicted to potentially provide a combined efficiency gain of approximately five percentage points.



Example scenario for a light-duty diesel engine at part load showing potential opportunity for efficiency gains from reducing or recovering lost energy by the percentages shown on the y-axis.

Impacts of Biodiesel Impurities on Emissions Control System

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

One of the ways the United States can increase energy security is by expanding domestically-produced renewable fuels for transportation. However, each new fuel must be fully investigated for potential incompatibilities because even small changes in composition can have a significant impact on a vehicle's emissions control system and durability. Biodiesel is an emerging, domestically-produced renewable fuel that has great potential but needs to be evaluated to alleviate concerns of the transportation industry.

In a project co-sponsored by Fuels Technologies and Propulsion Materials in conjunction with the National Biodiesel Board, researchers at ORNL and National Renewable Energy

Laboratory (NREL) are studying impurities regulated in biodiesel, giving particular attention to the impacts of sodium, potassium, and calcium impurities.

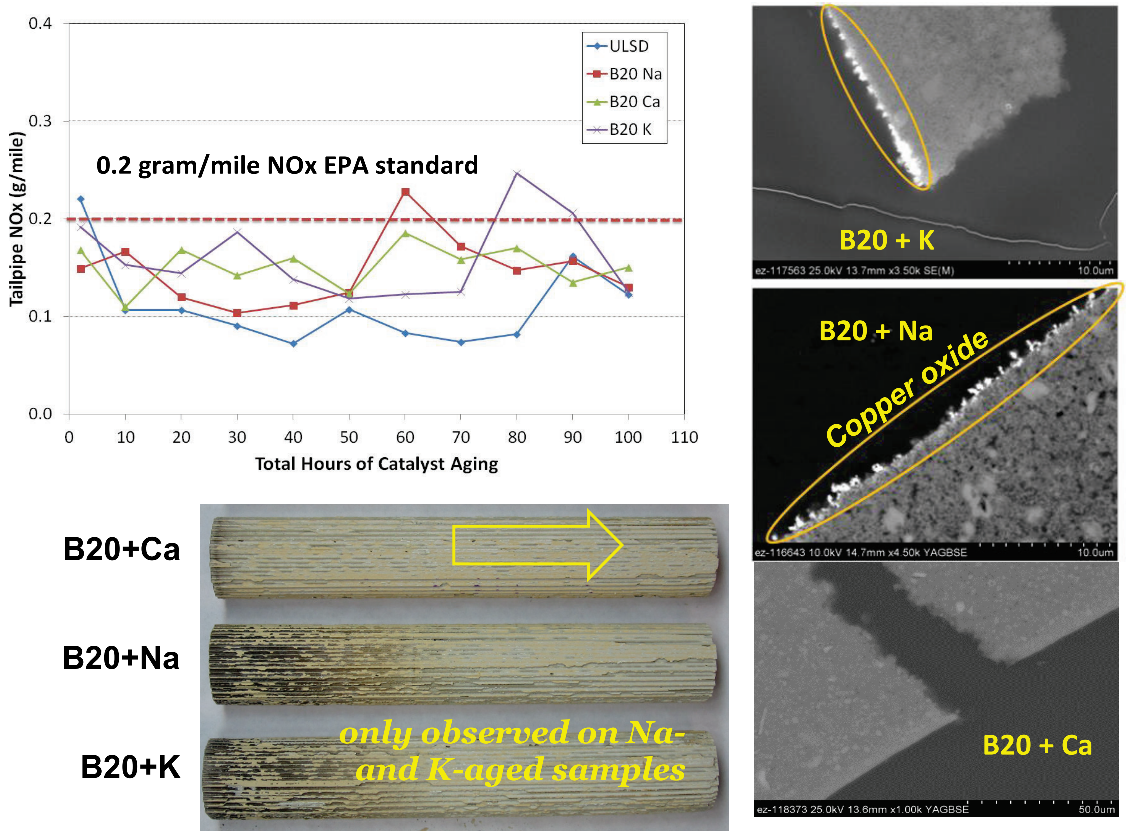
Biodiesel relies on NaOH or KOH in its synthesis process, but these components must be removed. Current specifications require less than 5 ppm Na + K and 5 ppm Ca + Mg in 100% biodiesel (B100) fuel. Diesel fuel is limited to 5% biodiesel, although some vehicles have been certified for up to 20% biodiesel (B20). To study the impact of these metals at a B20 level, NREL and ORNL initiated a collaborative accelerated aging study. Both the full useful life metal exposure and on-vehicle evaluation of the emissions control system were performed at NREL. The vehicle passed the nitrogen oxides (NOx) emissions standards at the end of the test. However, some elevated emissions points with sodium and potassium exposure highlighted the need for further analysis.

Flow bench reactor evaluations at ORNL and Ford Motor Company showed the fronts of the sodium- and potassium-exposed systems had a 10 to 20% decrease in NOx reduction activity on the selective catalytic reduction (SCR) catalyst. At ORNL, the materials characterization illustrated a surprising deactivation mechanism for the sodium and potassium SCR samples: those SCR samples had a thin layer of CuO on the surface of the washcoat. This layer showed that sodium and potassium were displacing copper from the zeolite, and the copper was migrating to the surface. This did not eliminate the overall reactivity of the SCR catalyst but decreased it significantly so that the system would fail emissions tests if the ***entire*** sample were in this state. The dark CuO covered only the front one-third of the front catalyst; the rear catalyst was unaffected.

This research addressed concerns of vehicle manufacturers regarding the introduction of biodiesel at levels up to 20%. The results demonstrated the importance of strict adherence to maintaining metal content standards within the required fuel specification.

Publication

1. J. B. Williams, R. McCormick, T. Toops, A. Wereszczak, E. Fox, M. Lance, G. Cavataio, D. Dobson, J. Warner, R. Brezny, D. Brookshear, and K. Nguyen, “Impact of fuel metal impurities on the durability of a light duty diesel aftertreatment system,” SAE Technical Paper Series 2013-01-0513 (2013).



(Top left) Each of the complete systems met the emissions standard at the end of the full useful life durability evaluation; however, materials characterization showed that the sodium- and potassium-aged samples removed copper from the Cu-zeolite SCR catalyst. The micrographs at right show a thin layer of CuO on the washcoat surface.

Energy Storage

ORNL Produces Lithium-Ion Battery Electrode via Water-Based Process

Contact: Claus Daniel, danielc@ornl.gov, 865-241-9521

ORNL is working to substantially reduce the production cost of lithium-ion batteries (LIBs) while increasing sustainability in the battery manufacturing process. DOE has set a battery cost target for LIB-based electric vehicles (EVs) of $125/kWh by 2020; this target requires a threefold improvement over the current cost of ~$500/kWh.

To meet this ambitious goal, researchers are looking to conventional battery manufacturing to find methods to develop less expensive materials and processing methods, which presently make up more than 80% of the total cost of an EV battery. Conventional electrodes are manufactured by slurry processing with a binder of polyvinylidene fluoride (PVDF) and a solvent of N-methyl-2-pyrrolidone (NMP). NMP is toxic, flammable (it produces vapors during electrode manufacturing), and expensive (it requires costly solvent recovery). ORNL is developing an aqueous processing method for LIB manufacturing in which NMP (at a cost of $1–2/liter) is replaced with deionized water, which costs just $0.015/liter.

The use of deionized water significantly reduces raw materials and processing costs and eliminates the process for recovery and treatment of NMP. The process is also more environmentally benign, an advantage that will be critical in mass production of LIBs. This novel processing route is estimated to reduce the full battery pack cost by up to 20%.

The rate performance of $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ cathodes with various water-soluble binders from aqueous processing was compared with the rate performance of cathodes with a PVDF binder from NMP-based processing. The cathodes produced via aqueous processing demonstrated superior rate performance, an indication that switching from NMP-based to aqueous processing of LIB electrodes offers more than just dramatically reduced costs.

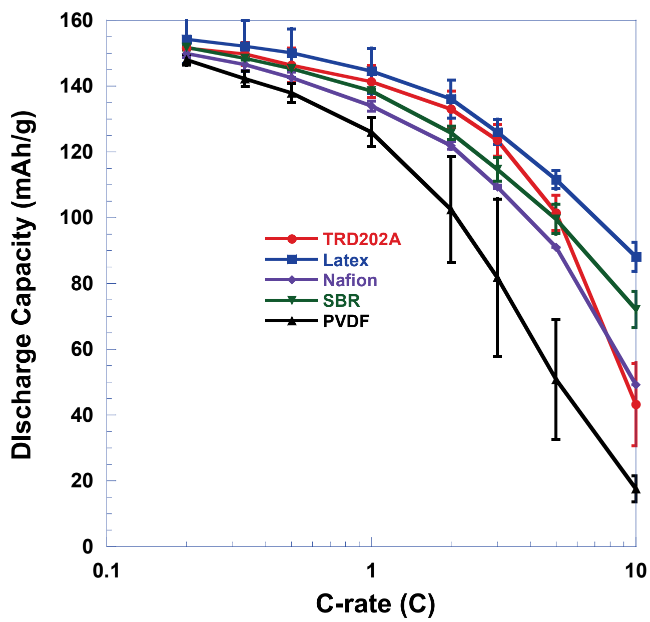
Aqueous processing of the conventional graphite anode is a commonly used, relatively mature technology. However, adapting it to work with the diverse array of LIB cathodes has proved to be a challenge. ORNL is tackling the challenge by understanding the colloidal chemistry of each cathode component for effective dispersion, screening water-soluble binders for superior adhesion and electrode integrity, optimizing mixing protocols for uniform suspensions, improving the surface energy of the aluminum current collector for better wettability of cathode dispersions, developing drying procedures for effective moisture removal, and quantifying the effect of residual moisture on battery performance. During the course of this research, ORNL successfully manufactured DOE's first fully water-processed LIB.

Publications and Patent

1. J. Li, B. Armstrong, J. Kiggans, C. Daniel, and D. Wood, "Optimal polyethyleneimine concentration and mixing sequence for $LiFePO_4$ aqueous nanoparticle dispersions," *Journal of Colloid Interface Science* **405**(1), 118–124 (2013).

2. J. Li, B. L. Armstrong, J. Kiggans, C. Daniel, and D. L. Wood, III, "Lithium ion cell performance enhancement using aqueous $LiFePO_4$ cathode dispersions and polyethyleneimine dispersant." *J. Electrochem. Soc.* **160**(2), A201–A206 (2013).

3. J. Li, B. L. Armstrong, C. Daniel, and D. L. Wood, III, "Aqueous Processing of Composite Lithium Ion Electrode Material," US Patent application 13/651270, filed October 12, 2012.



Comparison of the rate performance of NMC 532 cathodes produced via aqueous processing and NMP-based processing with a PCDF binder. Performance of the cathodes from aqueous processing is superior.

Computer-Aided Engineering for Batteries

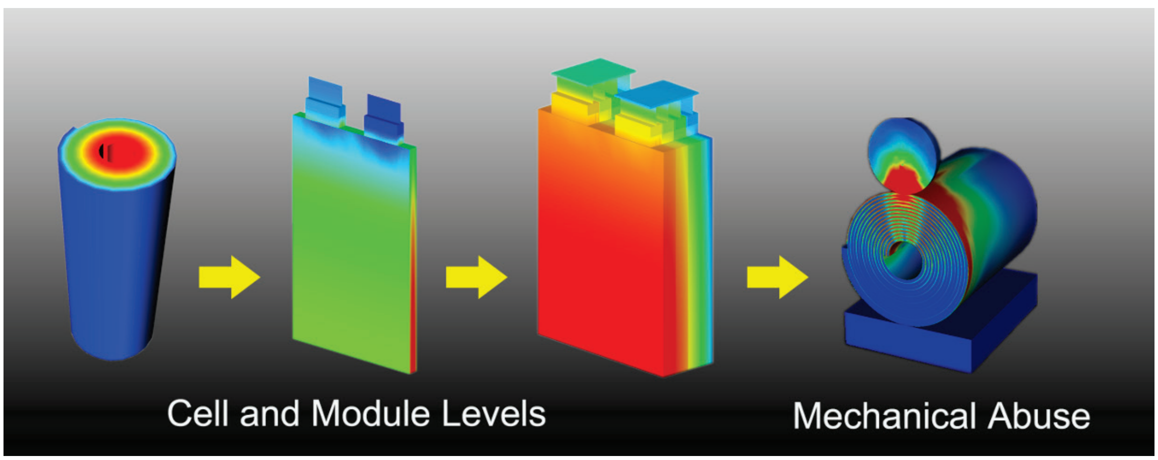
Contact: Sreekanth Pannala, pannalas@ornl.gov, 865-574-3129

In the ongoing complex quest to develop better, longer-lasting batteries for electric and hybrid-electric vehicles, researchers at ORNL are turning to computer-aided engineering and a predictive simulation capability that can guide rapid design by considering performance and safety implications of different chemistry and materials choices. The Computer Aided Engineering for Batteries (CAEBAT) Open Architecture Software (OAS) framework is designed for multiphysics and multiscale battery models. It also enables integration of different components representing physics for charge and thermal transport, electrochemistry, mechanical stresses, and degradation.

This project is the answer to the substantial need for design tools for batteries that can leverage the significant investments in modeling efforts made across DOE and academia. For the first time, researchers are creating an open, flexible computational framework that incorporates diverse existing capabilities as well as new capabilities developed by the vehicle technologies research community. Within this framework, scientists and designers can use decades of development, verification, and validation of modeling tools for individual physics domains and focus on new issues associated with coupling and multi-physics interaction.

The models operate and interact across the porous 3-dimensional structure of the electrodes (cathodes and anodes), the solid or liquid electrolyte system, and the other battery components. Underlying lower-length processes are accounted for through closure equations and submodels based on resolved quantities. Most important, the multi-material interfaces are kept intact.

The computational framework has a modular structure so that components corresponding to particular physical phenomena can be interchanged flexibly and consistently with similar components. Each simulation component in the OAS framework is equipped with coupling interfaces that are wrapped around standalone code. These interfaces convert native data from these components to the data format used by the OAS framework. This enables the components to remain unchanged and yet fully interact with the framework and other components. Extensibility of the framework allows easy integration of new models as they are developed.



The CAEBAT OAS framework approach allows researchers to simulate electrochemical and thermal behavior on the cell, module, and pack levels as well as mechanical response of the battery to a crash or mechanical abuse conditions.

Publication

S. Allu, S. Kalnaus, W. Elwasif, S. Simunovic, J. A. Turner, and S. Pannala, "A new open computational framework for highly-resolved coupled three-dimensional multiphysics simulations of Li-ion cells," *Journal of Power Sources* **246**, 876–886 (2014).

Studying High-Voltage Battery Cathodes for Electric and Hybrid Vehicles

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

Lithium-ion batteries are a leading energy storage technology for electric vehicles (EVs). Lithium- and manganese-rich nickel/manganese/cobalt (LMR-NMC) cathodes deliver higher voltage and energy density in lithium-ion batteries than other candidates, but they experience voltage fade and capacity losses over repeated cycles. To understand the mechanisms underlying these performance issues, researchers are using ORNL's capabilities in materials characterization to explore the structure of LMR-NMC materials.

The project uses several advanced materials characterization tools at ORNL to study LMR-NMC cathodes developed through the Vehicle Technologies Office Applied Battery Research program. Team members are seeking insight into correlations between cation ordering and voltage fade in the cathodes.

Electrochemical experiments compared data collected from pristine TODA HE5050 high-voltage cathode oxides with data from the same material after it was cycled. One cathode was cycled at an upper cutoff voltage (UCV) of 4.2 (2.4–4.2 V voltage window) and the other at a UCV of 4.8 (2.4–4.8 V voltage window). After the battery cells had cycled 125 times, the cathodes were harvested, washed with dimethyl carbonate, and dried. The data revealed voltage fade in the cell with the higher UCV but not in the cell with lower UCV.

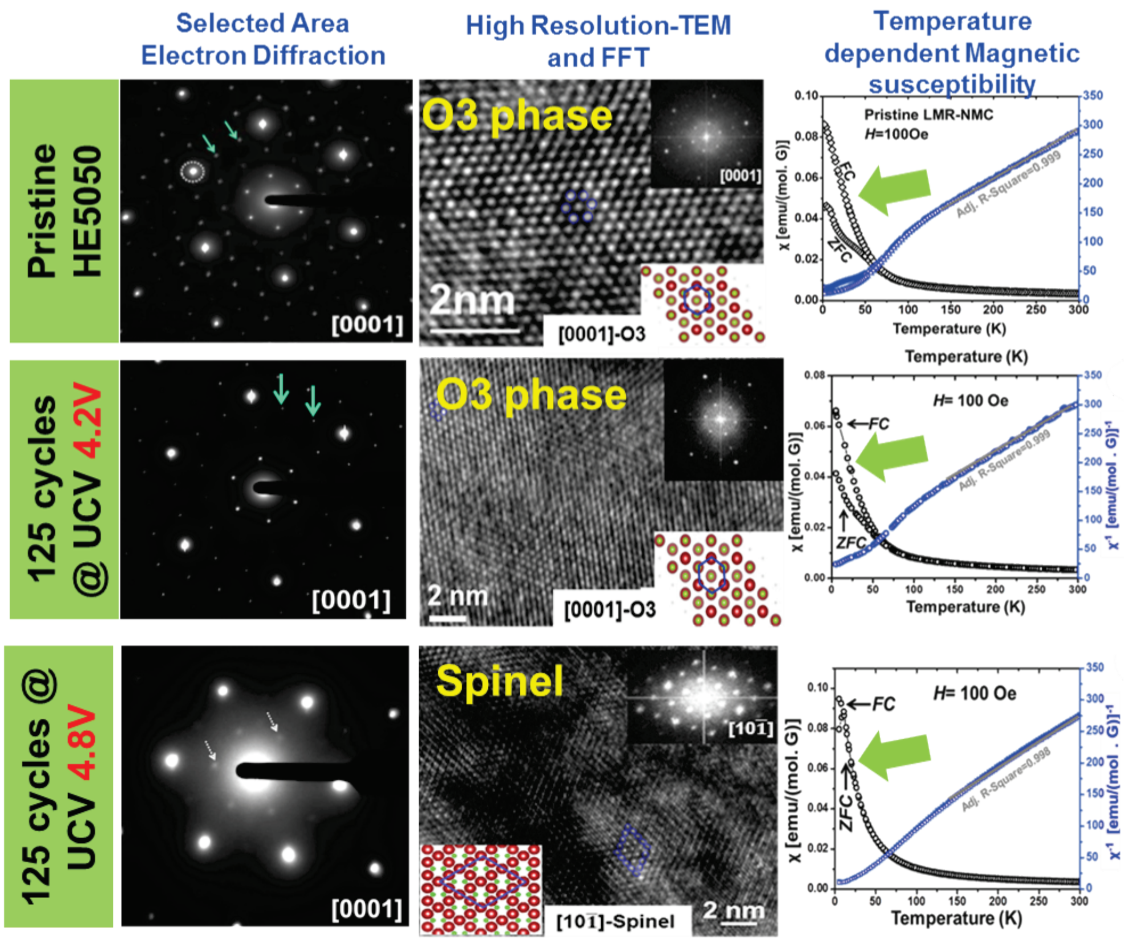
Selected area electron diffraction (SAED) results for pristine HE5050 confirm the presence of cation ordering. High-resolution transmission electron microscopy (TEM) shows a fundamental O3 phase along with the cation-ordering peaks. Magnetic susceptibility data show a divergence of field cooling (FC) and zero field cooling (ZFC) at T=50°C, confirming the cation ordering.

SAED data from HE5050 cycled at 4.2 UCV show it retained cation ordering, and TEM imaging shows the O3 phase. The FC and ZFC divergence is seen in the magnetic susceptibility data, providing further evidence that cation ordering is retained after 125 cycles at 4.2 V UCV.

After 125 cycles at 4.8 V UCV, the SAED pattern shows fundamental O3 reflections, but the cation-ordering reflections have vanished. Instead, extra reflections between two fundamental O3 spots are observed; they indicate the presence of a spinel phase. The SAED data agree with the TEM image showing a spinel-type atomic structure. In the magnetic susceptibility data, the splitting of FC and ZFC (which indicates cation ordering) is not observed. These observations demonstrate that cation ordering is suppressed or vanishes after cycling at 4.8 V UCV and the spinel phase is introduced, which leads to the voltage fade.

After several cycles at a UCV of 4.8 (125 cycles in this study), nucleation and growth of the spinel phase occurs, and the structure may slowly transform to the spinel phase.

These experiments show that structural rearrangement occurs in the LMR–NMC cathode only at higher potentials (e.g., 4.8 V) and indicate a direct correlation between cation ordering and voltage fade.



SAED, high-resolution TEM, and magnetic susceptibility data from pristine TODA HE5050 after 125 cycles charged to UCVs of 4.2 and 4.8 V. Source: Physical Chemistry Chemical Physics *15, 19496, (2013)*

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1. D. Mohanty, A. Huq, E. Andrew Payzant, A. Safa-Sefat, J. Li, D. P. Abraham, D. L. Wood, and C. Daniel, "Neutron diffraction and magnetic susceptibility studies on a high-voltage $Li_{1.2}Mn_{0.55}Ni_{0.15}Co_{0.10}O_2$ lithium-ion battery cathode: Insight into the crystal structure," *Chemistry of Materials* **25**, 4064 (2013).

2. D. Mohanty, A. Sefat, J. Li, R. A. Meisner, R. A. Justine, E. A. Payzant, D. P. Abraham, D. L. Wood, and C. Daniel, "Correlating cation ordering and voltage fade in a lithium-manganese-rich lithium-ion battery cathode oxide: A joint magnetic susceptibility and TEM study," *Physical Chemistry Chemical Physics* **15**, 19496 (2013).

3. D. Mohanty, S. Kalnaus, R. A. Meisner, K. J. Rhodes, E. A. Payzant, D. L. Wood, and C. Daniel, "Structural transformation of a lithium-rich $Li_{1.2}Co_{0.1}Mn_{0.55}Ni_{0.15}O_2$ cathode during high voltage cycling resolved by in situ x-ray diffraction," *Journal of Power Sources* **229**, 239–248 (2013).

4. D. Mohanty, S. Kalnaus, R. A. Meisner, A. Safa-Sefat, J. Li, K. J. Rhodes, E. A. Payzant, D. L. Wood, and C. Daniel, "Structural transformation in a $Li_{1.2}Co_{0.1}Mn_{0.55}Ni_{0.15}O_2$ lithium-ion battery cathode during high-voltage hold," *RSC Advances* **3**, 7479–7485 (2013).

5. D. Mohanty, A. Safa-Sefat, S. Kalnaus, J. Li, R. A. Meisner, E. A. Payzant, D. P. Abraham, D. L. Wood, and C. Daniel, "Investigating phase transformation in $Li_{1.2}Co_{0.1}Mn_{0.55}Ni_{0.15}O_2$ lithium-ion battery cathode during high-voltage hold (4.5 V) via magnetic, x-ray diffraction, and electron microscopy studies," *Journal of Materials Chemistry A* **1**, 6249–6261 (2013).

New Solid State Sulfur-Based Battery

Contact: Claus Daniel, danielc@ornl.gov, 865-241-9521

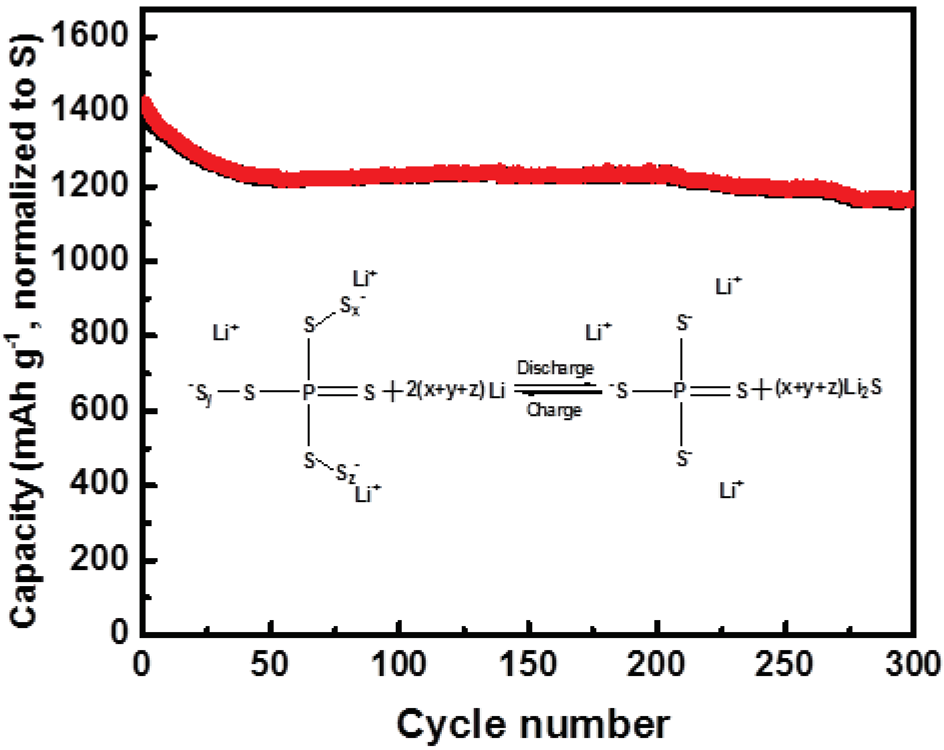
Among known battery chemistries, lithium-sulfur (Li-S) holds the greatest promise for high-energy batteries. However, the development of Li-S batteries has been impeded by the low electronic and ionic conductivities of the sulfur cathode and poor cyclability of the metallic lithium anode. Scientists at ORNL are tackling these barriers to Li-S battery development by designing a battery in an all-solid-state configuration using a new family of sulfur-rich compounds as cathode materials.

These new compounds contain polysulfide bonds that enable reversible energy storage and release and have high ionic conductivity, the key characteristic for improved cycling performance.

To enable cycling of the sulfur cathode in a conventional Li-S battery, a liquid electrolyte with high polysulfide solubility must be used to overcome the poor ionic conductivity of the solid sulfur. This process, however, leads to intrinsically short cycle life. In addition, the growth of lithium metal in liquid electrolytes and the constantly growing solid electrolyte interphase on the anode surface further shorten the Li-S batteries' cycle life and cause safety concerns.

In the ORNL-developed solid-state battery configuration, conventional liquid electrolytes were replaced by a solid electrolyte with two advantages—complete elimination of the polysulfide shuttle and safe cycling of the metallic lithium anode. The key challenges for developing all-solid Li-S batteries are three requirements: (1) electrolytes with high ionic conductivity and excellent electrochemical stability in both the anode and cathode, (2) a cell design that prevents the penetration of lithium dendrites, and (3) a sulfur cathode with high ionic conductivity.

The ORNL group has developed materials such as sulfide-based solid electrolytes and lithium polysulfidophosphate (LPSP) for solid state Li-S batteries. These materials have excellent compatibility with the metallic lithium anode and the sulfur-rich cathode. The key limitation of the sulfur cathode is its low ionic conductivity. The excellent cyclability demonstrated in this research is attributed to the high ionic conductivity of LPSP, which is 10 million times higher than that of lithium sulfide (Li_2S), the most conductive conventional sulfur cathode. A high capacity of 1,200 milliamperes per hour per gram (based on sulfur) was achieved for 300 cycles at 60°C for this all-solid-state battery configuration using these newly developed materials.



Cycling performance of an all-solid-state Li-S battery at C/10 with an LPSP sulfur cathode.

Lightweight Materials

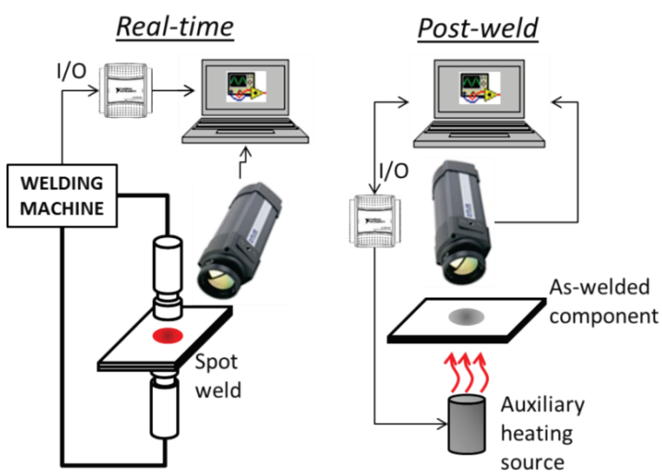
Online Weld Quality Monitor and Control with Infrared Thermography

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

ORNL researchers made significant progress toward development of an infrared (IR) thermography–based system to quantitatively inspect spot weld quality in real time on auto manufacturing lines. A nondestructive weld inspection system will help automakers integrate advanced high-strength steel (AHSS) and other lightweight materials into their products.

Resistance spot welding (RSW) is the most widely used technology for joining auto body components. But variations in welding conditions and part fit that occur in the high-speed assembly process result in imperfect joints that impair vehicle quality and performance. Weld quality is even more critical in joining parts made of lightweight metals. To ensure weld quality, the auto industry needs a nondestructive inspection system that is automated, fast, and low-cost and does not interfere with the automated welding fabrication process. The nonintrusive, noncontact nature of IR thermography makes it especially attractive for highly automated assembly lines.

The project's FY 2013 efforts focused on (1) refining the data analysis algorithm, (2) integrating the automated inspection software with the prototype system, and (3) validating the entire system for various welding conditions.

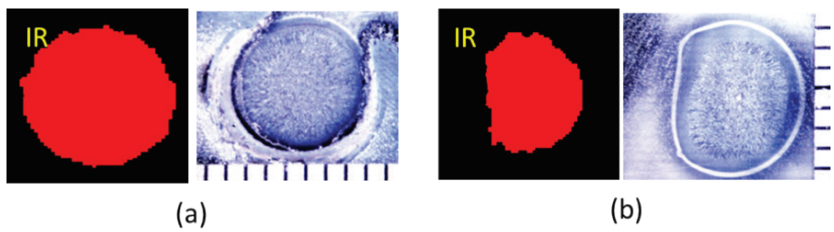


Schematic of the IR thermography–based weld quality inspection system.

Additional real-time and post-weld image data were collected, mostly for boron steels of different grades, thicknesses, coatings, and stack-up configurations. Welding parameters were carefully controlled to produce welds with varying attributes (e.g., nugget size). Real-time IR images of spot welding were acquired, and the resulting welds were further analyzed using the post-weld inspection procedure.

A major technical achievement was the addition of self-learning capability to the software. The system can automatically generate a weld quality database based on destructively measured data and the welding conditions specified by users and then use it to make quantitative predictions of weld attributes.

The research team also further refined image analysis algorithms for real-time IR inspection. The system can collect an image and analyze the data in 1.5–2.5 s and can positively identify weld nugget size, weak stuck welds, and welding expulsion. For post-weld inspection, the system automatically creates a weld quality database with user-provided measurement data. It collects and analyzes an image for each weld in about 3 s. Nugget size, thickness, stuck welds, and excessive indentation are accurately measured, and nondestructive post-weld IR evaluation can measure the weld nugget shape on the faying surface.



Post-weld IR-measured weld shape vs. cross section of destructive measurement (on the faying surface): (a) good weld and (b) weld with irregular shape.

In June 2013, representatives of GM, Ford, Chrysler, and Honda attended an onsite demonstration of the IR prototype system in Detroit. The automakers and their suppliers are interested in working further with ORNL. Further system testing and refinement will be carried out on the production lines of Cosma's Eagle Bend Manufacturing facility in Clinton, Tennessee.

Improving Fatigue Performance of AHSS Welds

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

ORNL and steelmaker ArcelorMittal USA are working to improve the weld fatigue strength and durability of auto body structures made of lightweight materials such as advanced high-strength steel (AHSS), magnesium, and aluminum. Inadequate weld fatigue life hinders widespread use of these materials in vehicles, so improving fatigue life is critical to reducing vehicle weight. Technologies developed in this project are expected to provide cost-effective, practical solutions to the auto industry.

Current weld fatigue improvement methods are based mostly on post-welding steps that are cost-prohibitive in high-volume manufacturing. This project focuses on developing methods that are integral to the welding operation. FY 2013 research focused on developing strategies to mitigate residual stresses in weld start and stop regions; both modeling and observation under test have identified those regions as the critical locations for initiation of fatigue cracking under cyclic loading. Two different approaches showed dramatic improvements in weld fatigue life.

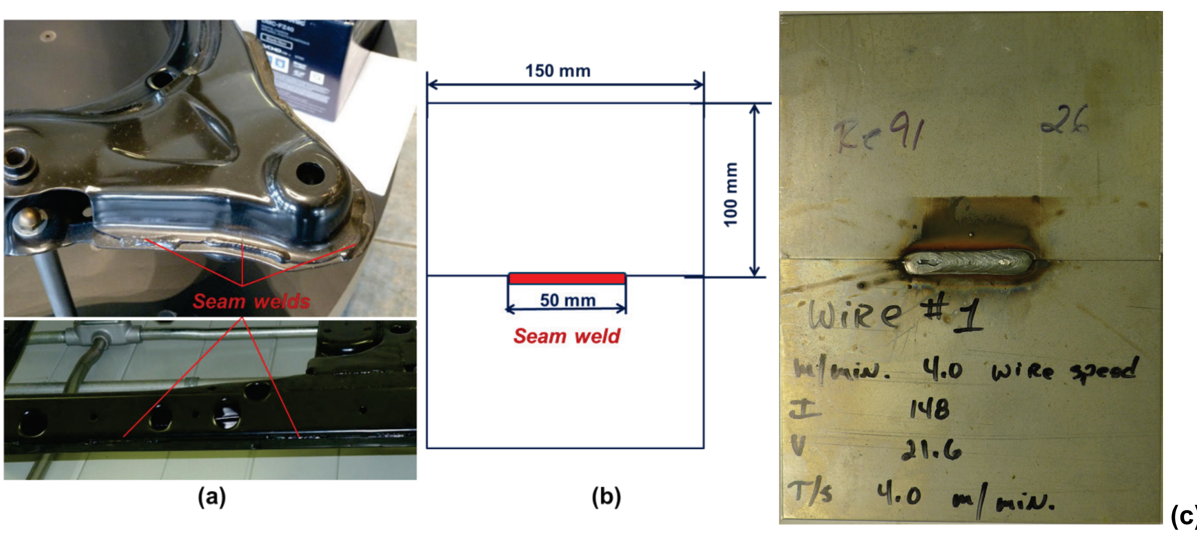
A weld fatigue specimen configuration was designed to mimic the stitch weld pattern typical in auto body and chassis structures. It was fabricated by placing a 50 mm long seam weld on the lap joint of two steel sheets—the most common weld type in vehicles. The configuration contains both weld start and stop. It maintains the weld residual stress field characteristic of actual seam welds and produces stress/strain conditions resembling those that cyclic loading imposes on vehicle structure welds.

The first approach explored a new low transformation temperature (LTT) filler wire design that considered the effect of LTT on weld residual stress and other factors such as weldability, strength, and toughness in the chemical formulation. Preliminary fatigue testing at medium load confirmed 3–5× weld fatigue improvement with the LTT filler wire. The new filler wire is also being tested under other loading levels.

In the second approach, a mechanical stress management technique was developed to mitigate tensile residual stresses in the high-stress-concentration region of the stitch weld. This resulted in 5–10× fatigue life improvement at the low-stress level relevant to the durability of auto body structures, compared with ER70-S filler wire commonly used to weld AHSS body structures. In fact, at 2,000 lb, the weld specimens with stress management did not break after 10 million cycles.

High-energy synchrotron x-ray diffraction was used to determine the weld residual stress and the effect of the mechanical stress management technique. The results showed the technique was indeed able to considerably lower residual stresses, providing a technical basis for the observed improvement in weld fatigue life.

The two approaches will be further refined and optimized and technology commercialization strategies will be formulated in FY 2014.



(a) Representative welding pattern in auto body structures, (b) special weld fatigue specimen configuration, and (c) appearance of actual weld fatigue testing specimen adopted in this project.

Austenite-Ferrite Transformation Details in Carbon Steels

Contact: Zhili Feng, fengz@ornl.gov, 865-574-3797

ORNL researchers combined neutron scattering, x-ray diffraction, and numerical simulation to understand phase transformation behaviors during the annealing of advanced high-strength steel (AHSS) and the mechanisms governing the exceptional combination of high strength and ductility in multilayer composite steels.

Steel is expected to remain a primary auto body structural material for the foreseeable future. First-generation AHSS currently used in vehicles offers excellent crash management and other safety benefits as well as considerable weight reduction. The automotive industry, steel industry, and government are working together to develop third-generation AHSS that will offer even greater potential for weight reduction and safety enhancement, as well as acceptable manufacturability and affordability. These steels would have a strength-to-weight ratio equal to or greater than those of aluminum and magnesium alloys.

Controlling costs will likely require that third-generation AHSSs be no more than modestly alloyed compared with first-generation AHSS and be capable of being produced within existing steel mills.

Researchers used the Spallation Neutron Source (SNS) at ORNL and the Advanced Photon Source at Argonne National Laboratory to characterize in situ austenite–ferrite phase transformation behavior under rapid heating/cooling conditions typical of modern sheet steel production and to analyze the microscopic deformation and failure processes in dual-phase AHSS and multilayered composite steels. In FY 2013, in situ neutron experiments were conducted at SNS for various heating and cooling conditions, focusing on austenite formation and the effects of diffusion and homogenization of alloying elements on the transformation—a key variable in production of first-generation AHSS and in the design of some third-generation AHSS.

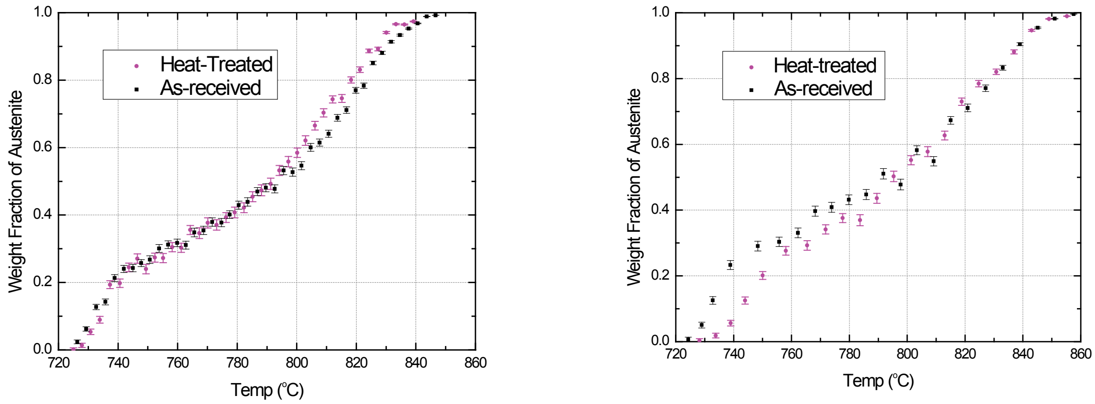
The experimental results suggest that the formation of austenite depends on both the heating rate and the initial microstructure. A phase transformation model was developed and applied to the steel being studied to correlate with the neutron diffraction results to provide a fundamental understanding of the formation of austenite in dual-phase steels.

Publications and Presentations

1. R. Barabash, O. Barabash, M. Ojima, Z. Yu, I. Inoue, S. Nambu, T. Koseki, R. Xu, and Z. Feng, "Interphase strain gradients in multilayered steel composite from microdiffraction," *Metallurgical and Materials Transactions A* **45**(1), 98–108 (2013).

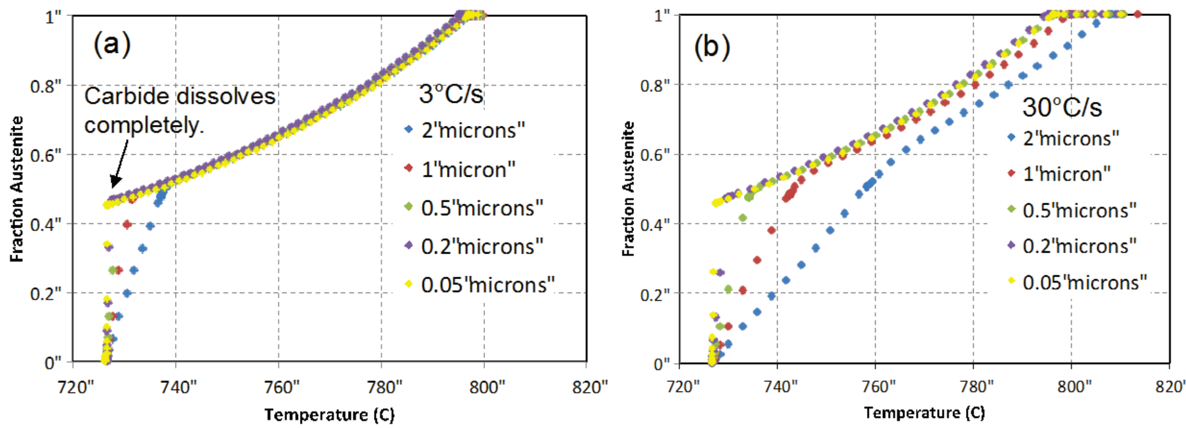
2. Z. Yu, et al. "In situ neutron diffraction study of microscopic deformation processes and the microstructure effect in advanced high-strength steels," invited talk at TMS 142nd Annual Meeting & Exhibition, San Antonio, March 3–7, 2013.

3. Z. Yu, R. Barabash, O. Barabash, W. Liu, and Z. Feng, "In situ probing of microscopic deformation kinetics in advanced high-strength steels," poster presented at TMS 142nd Annual Meeting & Exhibition, San Antonio, March 3–7, 2013. First prize in Young Professional Poster Competition.



(a) (b)

The effect of initial microstructure and heating rate on the nonequilibrium ferrite/martensite (α+α$_M$) to austenite (γ) transformation in a DP980 steel observed by in situ neutron diffraction measurement with (a) a 3°C/s heating rate and (b) a 30°C/s heating rate.



The effect of heating rate on the nonequilibrium phase transformation in tempered martensite predicted by the phase transformation model developed in this project.

IR Heat Treatment and Residual Stress Characterization of Bimetallic Joints

Contact: Tom Watkins, watkinstr@ornl.gov, 865-387-6472

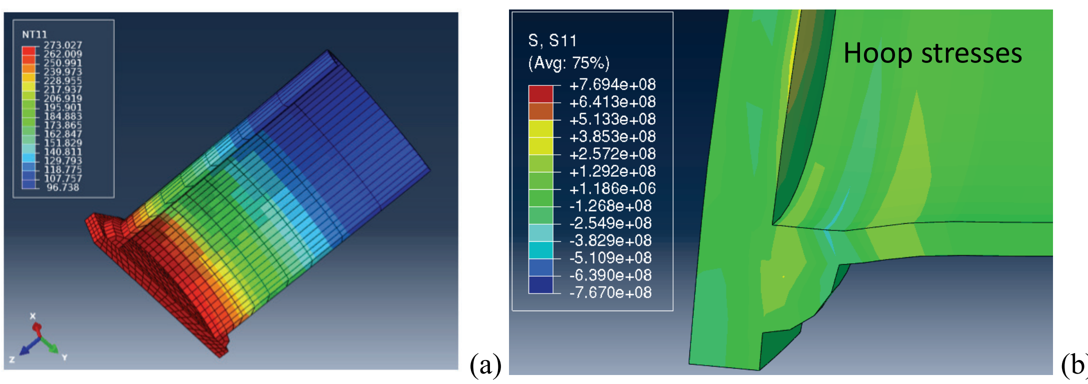
An ORNL project is evaluating the use of infrared (IR) lamps for heat treatment of bimetallic joints to save energy, time, and processing costs in auto manufacturing. In 2014, the ORNL research team treated an aluminum/steel joint in a prototype IR heating furnace and modeled the effects of the heating. The team also used neutron scattering to measure the residual stresses in conventionally treated bimetallic joints.

Aluminum structural components are typically manufactured using a cast AlSiMg alloy and then heat-treated to achieve the desired mechanical properties. The heat treatment processes (T5 and T6) have long thermal cycles that are energy-intensive and costly. The T6 process incorporates a water quench, which imposes corrosion and residual stress concerns for bimetallic components. The ORNL project aims to develop and model an IR heat treatment process for an aluminum casting with a bimetallic joint that produces a T5 temper in less time than conventional processing, and to develop a modified T6 process for improved mechanical properties without any loss of joint integrity. The project focuses on a specific application, but the methods developed are applicable to multiple joints on many vehicle platforms.

ORNL's prototype IR electric furnace was used to heat an AlSiMg alloy component with an AlSiMg/steel joint. The furnace contains tungsten–halogen lamps located above and below the aluminum component to equalize the temperature distribution within it. A CAD model was used to study the effect of IR heating on temperature and stress distributions within the part. A heat transfer model of the part was completed and a stress analysis model developed in ABAQUS. The temperature distribution in the steel portion of the joint during heating was simulated. The thermomechanical model to predict residual stress used a rate-independent isotropic hardening plasticity model for the steel. Temperature-dependent property data were used for properties for both materials.

As residual stresses play an important role in these joints, the team used neutron diffraction at ORNL's High Flux Isotope Reactor to measure and map residual stresses in a series of conventionally heat-treated joints. Residual stresses were measured in both the steel and aluminum in the radial, hoop, and axial directions.

The results of the ORNL research indicate that IR heat treatment can significantly improve the mechanical properties of bimetallic components and maintain the necessary residual stresses without water quenching. It also reduces process time and cost.



Temperature (°C) distribution for the steel portion of the joint. (a) The front surface is the symmetry plane; the top surface is shown facing the IR heat source. (b) Stress distribution (Pa) through a vertical cross-section of the steel near the edge for the hoop stress component (deformation magnification 3 times).

Presentations

1. T. R. Watkins, A. S. Sabau, H. Yin, D. L. Erdman III, W. Zhang, T. W. Skszek, and X. Niu, "Residual stress determination in cast bi-metallic joints," presented at TMS 2013 Annual Meeting, San Antonio, March 6, 2013.

2. H. Yin, A. S. Sabau, G. M. Ludtka, T. W. Skszek, and X. Niu, "Yield strength prediction for rapid age-hardening heat treatment of aluminum alloys," presented at TMS 2013 Annual Meeting, San Antonio, March 5, 2013.

3. H. Yin, A. S. Sabau, T. W. Skszek, and X. Niu, "Microstructure evolution modeling for solution treatment of aluminum alloys," presented at TMS 2013 Annual Meeting, San Antonio, March 5, 2013.

ORNL Commissions Carbon Fiber Technology Facility

Contact: Lee McGetrick, ORNL, mcgetricklb@ornl.gov, 865-574-6549

The Carbon Fiber Technology Facility (CFTF) at ORNL was commissioned for operations in March 2013, 6 months ahead of schedule and almost $2 million under budget. DOE selected ORNL to build and operate the CFTF under a competitive call for proposals for a highly flexible pilot-scale low-cost carbon fiber facility to demonstrate and evaluate affordable new manufacturing technologies. Construction began in March 2011.

CFTF has a unique carbon fiber line for demonstrating advanced technology scale-up and producing market-development volumes of prototypical carbon fibers. It has the capability and flexibility—unmatched anywhere in the world—to process a range of feed stocks and product forms. CFTF bridges the gap between laboratory research and commercial-scale deployment of low-cost carbon fiber technologies, filling a critical need to promote industrial competitiveness for the manufacture of carbon fiber in the United States.

Co-funded by VTP and the Advanced Manufacturing Office, the project supports EERE efforts to transition technologies to industry—specifically cost-effective carbon fiber for composite materials in high-volume energy applications.

Since beginning operation, CFTF has met or exceeded goals for safe, efficient, compliant operation and production of low-cost carbon fibers. During its first year, the facility exhibited a perfect record of safety and environmental compliance. A process was implemented in June 2013 by which these lower-cost carbon fibers and other products such as oxidized polyacrylonitrile fibers can be placed in the hands of industry for the development of prototypical composite applications to prove value of the fibers.

Successful commercialization of low-cost carbon fiber technology for energy and economic benefits to the United States is the overarching CFTF objective. Notable progress is being made in converting textile acrylic fibers supplied by the Kaltex Group, a large textile fiber producer in northern Mexico. Between July 8 and September 20, 2013, eight production lots of oxidized acrylic and carbon fibers were produced from the Kaltex precursor material. Results from these production runs indicate increasingly improved properties in tensile strength and modulus, suggesting the material may be a good candidate for full-scale production of lower-cost carbon fibers. The project shows that a low-cost carbon fiber can be produced from a textile-grade acrylic fiber and has resulted in many inquiries from industry partners.

Plans are to scale up the use of other alternative precursor materials, including lignin-based carbon fibers, cellulosic paper carbon materials, and polyolefin-based carbon fibers.

Large carbon fiber tow in production at the Carbon Fiber Technology Facility using a textile-grade acrylic fiber.

Presentations

1. L. B. McGetrick and C. D. Jackson, "The human factor in carbon fiber manufacturing," presented at Carbon Fibers 2012 Conference, San Diego, December 5, 2012.

ORNL Team Pursues Energy-Efficient Advanced Carbonization Technology

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

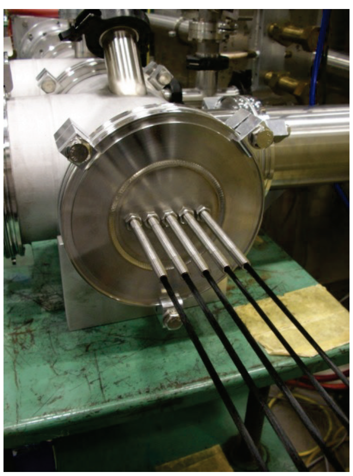
A project at ORNL'S Carbon Fiber Technology Facility (CFTF) seeks to demonstrate and eventually commercialize a revolutionary energy-efficient advanced conversion technology. Co-funded by VTP and the Advanced Manufacturing Office, this technology enables the manufacturing of carbon fiber that is technically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

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

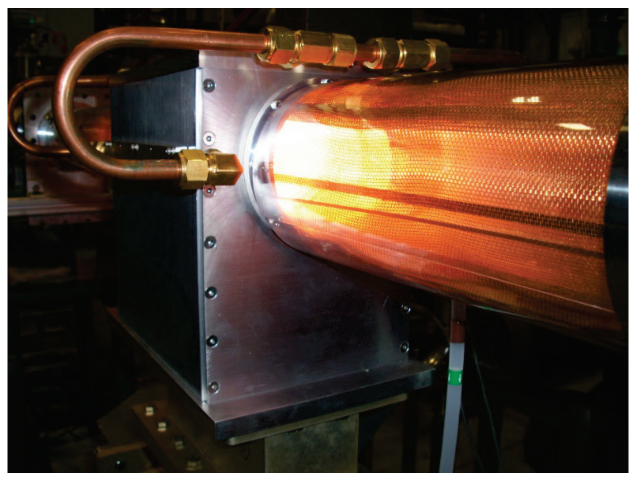
The technology development team recently completed modifications and upgrades to the MAP line that enable it to process five tows continuously and demonstrate a >2-hour stable run. Mechanical properties meeting program requirements (250 KSI strength, 25 MSI modulus) have been achieved, but uniformity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

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

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



The MAP line exit feedthroughs are fully strung with five tows in the horizontal configuration.



Improved microwave energy and enhanced plasma hardware. This approach, demonstrated here with a single unit, should allow improved energy deposition control for industrial scale-up.

Advanced Oxidative Stabilization of Carbon Fiber Precursors

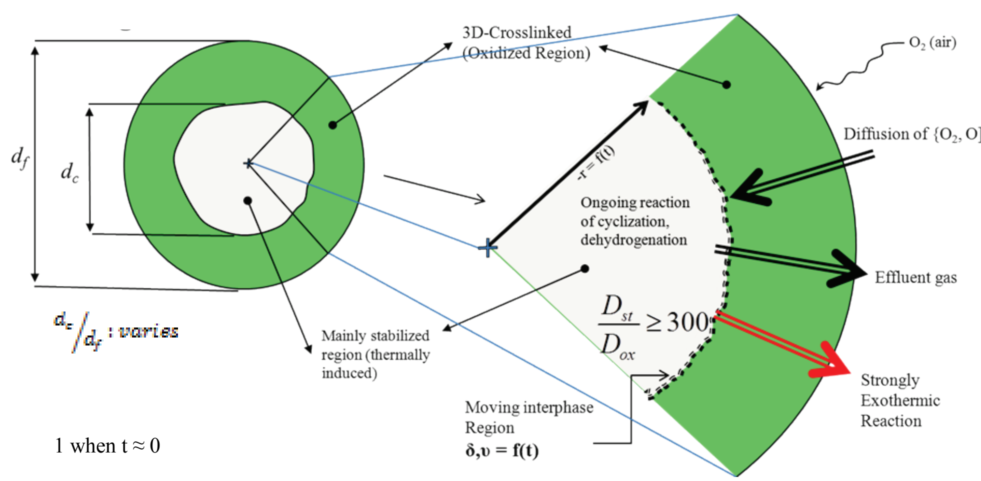
Contact: Felix Paulauskas, paulauskasfl@ornl.gov, 865-576-3785

The cost of producing carbon fiber (CF) is the single most important factor controlling its incorporation in future automotive systems. Significant effort is being expended to develop enhanced production technologies, such as a higher-speed, lower-cost oxidative stabilization process and a higher-speed microwave-assisted plasma (MAP) process carbonization method.

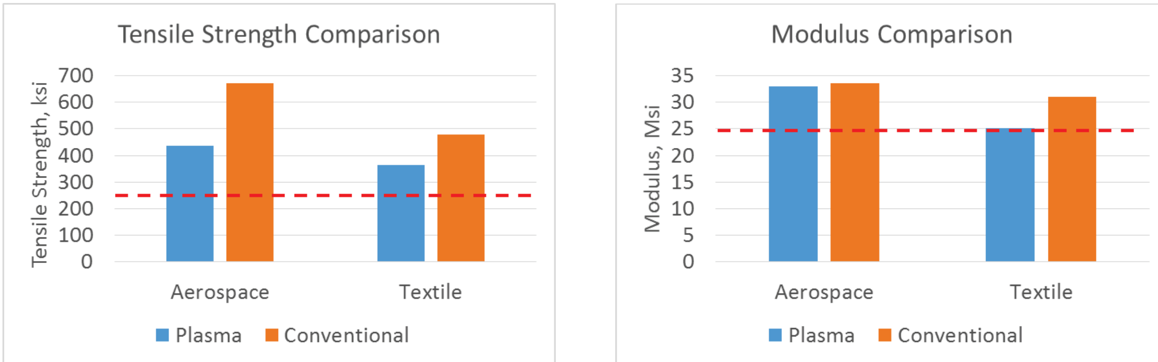
Conventional oxidation is a slow thermal process that typically consumes more than 80% of the processing time in a conventional CF conversion line. A rapid oxidation process could dramatically increase conversion line throughput and appreciably lower the fiber cost, so researchers are working to develop an atmospheric plasma processing technique to rapidly and inexpensively oxidize polyacrylonitrile (PAN) fibers.

Atmospheric pressure plasma is a new high-rate technology for use in industrial processes. A related project has already demonstrated the potential for significantly accelerating carbonization. The oxidation residence time must be greatly reduced to effect fast conversion and match the speed of the advanced carbonization technology. This project is developing an atmospheric plasma oxidation technology that could be used in line with conventional conversion equipment or integrated with other advanced fiber conversion processes to produce low-cost CF for the automobile industry. This effort is aimed at further developing those technologies to be able to continuously process multiple 12–50K tows of fiber and achieve properties meeting minimum property requirements with tow-to-tow and along-the-tow property variation within ±15%. The goals also include significantly reducing the time required for oxidative stabilization by 2–3 times (conventionally 90–120 min), which will permit greater fiber production rates and improved economics.

The technology has been proved at the laboratory scale and is now being scaled to the pilot scale. Later it will be scaled to the pre-production scale in collaboration with industrial partners. The research team is working to establish a clear path of technology transfer to industry by the end of FY 2014. By the end of FY 2015, researchers project that they will be ready to procure, install, test, and operate a pilot-scale (25 ton/year) plasma oxidation module in an advanced technology pilot line. The next step will be the design and construction of an advanced technology pilot line installed at ORNL's Carbon Fiber Technology Facility. It will be used to validate system performance and scalability as well as produce the required quantities of advanced-technology CFs to support the Lightweight Materials Program's advanced development activities.



Single-filament cross section during conventional oxidative stabilization process.



Mechanical properties of plasma oxidation vs. conventionally carbonized PAN fiber. Oxidation residence time was 30 min for aerospace, 33 min for textile-grade PAN.

Understanding Protective Film Formation by Magnesium Alloys in Automotive Applications

Contact: Kinga A. Unocic, unocicka@ornl.gov, 865-574-0996

ORNL is using advanced characterization methods to gain insight into the formation of protective films on magnesium (Mg) alloys, with the ultimate goal of permitting more widespread use of these alloys in vehicles.

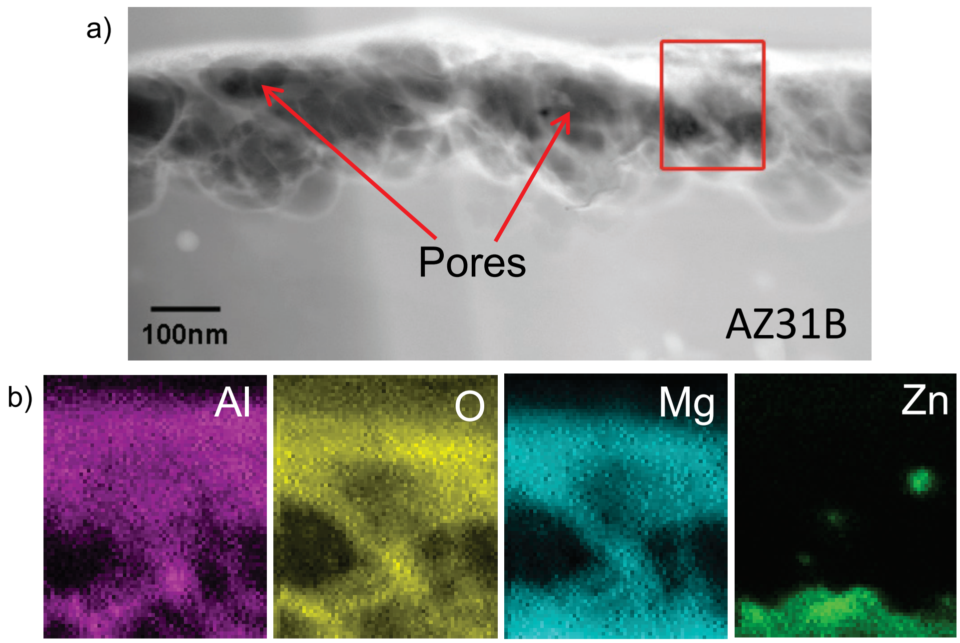
Mg alloys offer low density, good strength, amenability to casting, and ease of recycling, but their high susceptibility to corrosion is a barrier to widespread adoption in auto manufacturing. A key factor in the lack of corrosion resistance is that Mg alloys do not establish a continuous, fully protective surface film under many exposure conditions. Alloying and/or conversion coatings have been shown to modify surface film performance; however, a detailed understanding of how and why is currently lacking.

This project seeks to provide a detailed nanoscale picture of the structure and composition of corrosion films on Mg alloys as a function of alloy content and exposure conditions. Mg alloys are notoriously difficult to work with because of their high reactivity, so development of appropriate sample preparation and characterization techniques is essential.

Techniques being evaluated include (1) in-situ focused ion beam (FIB) milling as a sample preparation method and transmission electron microscopy (TEM) analysis of the surface film cross-section to determine film morphology and nanoscale segregation of alloy additions, (2) secondary ion mass spectrometry (SIMS) tracer studies of Mg alloys/coatings to understand growth mechanism(s) and hydrogen and oxygen uptake into corrosion films, (3) neutron scattering of Mg alloy surface film nanoporosity and hydrogen species incorporation, and (4) atom probe tomography (APT) to provide 3-dimensional quantification of chemistry at the atomic scale at the film and alloy–film interface.

Advanced TEM sample preparation and characterization methods developed in FY 2012 were successfully applied in FY 2013 to study aqueous film formation on Mg alloys as a function of exposure time and alloying additions. After a sample of the widely used commercial alloy AZ31B was immersed in water for 24 h, a partially hydrated MgO base film several hundred nanometers thick was formed on its surface. Some porosity was evident, and an underlying thin area at the film–metal interface indicated heavier element segregation. Energy-dispersive spectroscopy x-ray analysis (maps and line profiles) showed aluminum presence throughout the entire film thickness and zinc enrichment at the metal–film interface.

Compared with film formation and corrosion on high-purity Mg controls, the nanoscale segregation of aluminum and zinc into the film and the metal–film interface regions on AZ31B is believed to slow the film growth rate and improve corrosion resistance. The baseline water film growth behavior will be used for SIMS isotopic tracer studies, neutron scattering, and APT in FY 2014, and as a baseline condition to analyze the effects of varying alloy additions and exposure conditions.



(a) High angle annular dark-field scanning TEM image of the film cross-section formed on AZ31B after 24 h immersion in water. (b) EDS x-ray maps of Al, O, Mg, and Zn acquired from the region marked with the box in (a).

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1. K. A. Unocic, H. H. Elsentriecy, M. P. Brady, H. M. Meyer III, G.-L. Song, M. Fayek, R. A. Meisner, and B. Davis, "Transmission electron microscopy study of aqueous film formation and its evolution with time on magnesium alloys," submitted to *Corrosion Science* in 2013.

2. K. A. Unocic, H. H. Elsentriecy, M. P. Brady, G.-L. Song, H. M. Meyer III, J.R. Keiser, L.M. Anovitz, G. Rother, J.K. Thomson M. Fayek and B. Davis, "Characterization of film formation on commercial and model magnesium alloys," presented at Magnesium Technology 2013 Symposium at 2013 TMS Annual Meeting, San Antonio, March 4, 2013.

3. H. H. Elsentriecy, K. A. Unocic, M. P. Brady, G.-L. Song, H. M. Meyer III, J.R. Keiser, L.M. Anovitz, G. Rother, J.K. Thomson M. Fayek and B. Davis, "Characterization of film formation on commercial and model magnesium alloys," presented at Meet the candidate Poster Session Symposium at 2013 TMS Annual Meeting, San Antonio, March 4, 2013.

Power Electronics and Electric Motors

10 kW Wide Bandgap Device-Based Inverter

Contact: Madhu Chinthavali, chinthavalim@ornl.gov, 865-946-1411

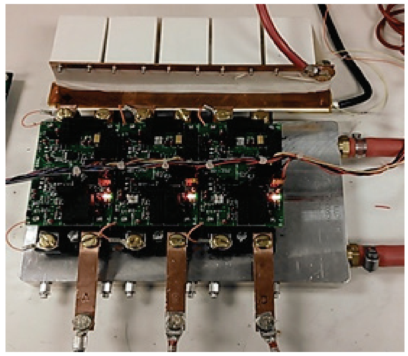
ORNL researchers have developed a highly efficient silicon carbide inverter for use in electric vehicles that offers protection against high temperatures and operating frequencies while reducing system costs.

Power electronics systems on hybrid, plug-in hybrid, and all-electric vehicles impose harsh environmental requirements on electrical components. Costly thermal management systems are necessary to avoid device failures, because these vehicles operate at high temperatures. At the same time, the pressure to keep costs reasonable for such vehicles is resulting in designs that use less hardware. These design changes offer the added benefits of lighter weight and greater efficiency.

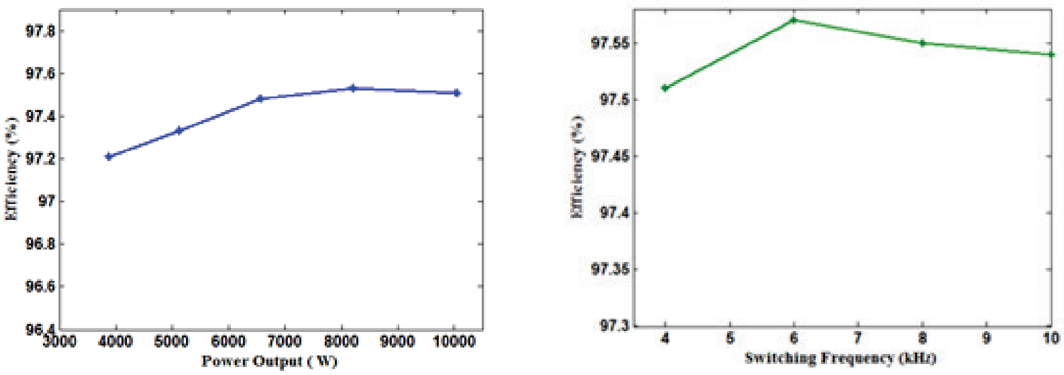
Emerging wide bandgap (WBG) devices are poised to offer significant improvements in power electronics for hybrid, plug-in hybrid, and electric vehicles. WBG devices can operate with enhanced efficiency over higher temperatures and operational frequencies. These characteristics lead to reduced cooling requirements and minimized passive component requirements, providing vehicle designers with opportunities for revolutionary strides in power electronics. The characteristics of two particular compounds—silicon carbide and gallium nitride—enable the development of smaller, more efficient, robust power electronics in a multitude of clean energy applications.

Following a review of a third-party analysis of WBG devices from multiple vendors, researchers at ORNL developed a 10 kW all-silicon carbide inverter using commercially available modules. Gate drivers from Rohm were used in the inverter, which measures 226 × 224 × 73 mm. The gate driver is equipped with galvanic isolation up to 3,000 V_{rms} and features integrated overcurrent protection, undervoltage lockout, and temperature feedback. The modules are mounted on a commercial heat sink with thermal grease as the medium of heat transfer from the lower side of the power modules. This prototype model will be packaged so that controls and capacitors are close to the heat sink. The small individual capacitors used in a series will ensure better cooling and reduced costs.

Inverter test results indicate the overall inverter efficiency is about 98% under various operating conditions. These results will be used as a benchmark for development of a next-generation inverter that will be built using an ORNL-developed WBG package. The results indicate that the inverter will meet DOE's 2020 inverter targets if it is scaled to 30 kW. In addition, WBG technology will aid developers in achieving targets for volume, efficiency, power density, and system costs established through U.S. DRIVE, a government–industry partnership focusing on research and innovation for vehicle efficiency and energy sustainability.



Prototype of a 10 kW silicon carbide inverter.



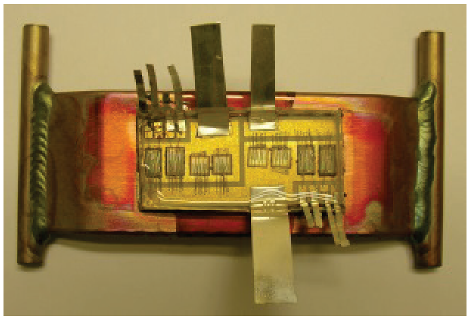
(Left) Inverter efficiency vs. output power at 325 Vdc, 4 kHz switching, and 60 ℃ coolant with a flow rate of 1.5 gal per min. (Right) Inverter efficiency changes only slightly as switching frequency increases.

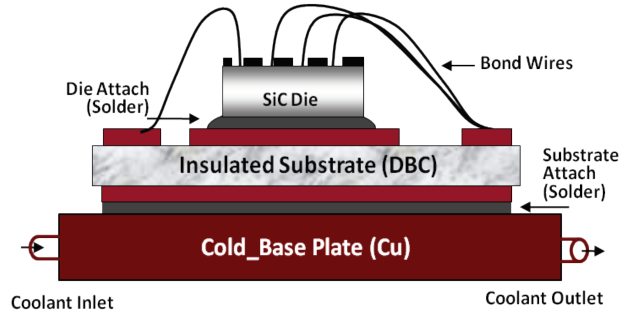
Advanced All-SiC Automotive Power Electronics Module

Contact: Zhenxian Liang, liangz@ornl.gov, 865-946-1467

ORNL is developing advanced wide bandgap (WBG) automotive power electronics technologies to help achieve DOE Advanced Power Electronics and Electric Motor Program targets. This effort involves multidisciplinary capabilities including packaging development and characterization; thermal, electrical, and thermomechanical expertise; and reliability, process and manufacturing considerations.

A prototype of an all-silicon carbide (SiC) 100 A/1,200 V phase-leg power module was fabricated in-house at the ORNL Packaging Laboratory. The module is composed of the latest industrial SiC power devices, a metal oxide semiconductor field effect transistor (MOSFET), and a junction barrier Schottky diode. It also features second-generation thermal packaging, allowing integrated direct cooling. Combining the superior attributes of SiC and packaging advancements, this module allows much higher efficiency and higher-density power conversion.





Prototype of all-SiC 100 A/1200 V phase-leg power module with integrated mini-cooler (left). Schematic of its thermal package (right).

The module was comprehensively characterized and compared with its silicon (Si) counterparts in an insulated gate bipolar transistor (IGBT)/PiN diode module with the same rating. The SiC MOSFET allowed reductions of 45% in die area, 25% in voltage drop (at 40 A), and 78% in switching power losses. The specific thermal resistivity of the integrated cooling package is more than 33% lower than that of a conventional (first-generation) package.

The allowed current density for a 100°C temperature increase is 66 A/cm^2 to 185 A/cm^2 for the different packages. The die area can be reduced by from 1.9 to 2.2 times by changing from Si IGBTs to SiC MOSFETs and by 1.3 to 1.5 times by using the second-generation cooling configuration rather than the conventional design.

The module's performance improvements enable system operation at efficiencies and frequencies beyond the Si limits. This module is a significant stride toward achieving DOE's power density and cost targets for power electronics systems.

Publications and Presentations

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Development of Low-Loss Motor Lamination Steel

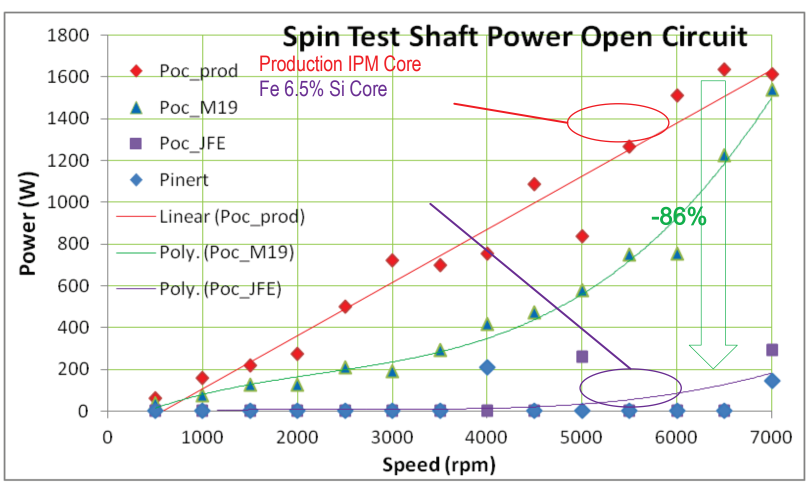
Contact: Burak Ozpineci, burak@ornl.gov, 865-946-1329

Electric traction drive systems (ETDSs) account for 16% of overall losses in all-electric vehicles over an Urban Dynamometer Driving Schedule drive cycle. Most of these losses are accumulated in the traction motor. For example, the 2012 Nissan LEAF ETDS has a line-averaged efficiency of 92.5%, the combined result of 95.2% traction motor efficiency and 97.2% inverter efficiency. Therefore, ETDS efficiency improvements are focused on motor materials that have the potential to significantly reduce core losses. ORNL has developed a novel processing method for a high-silicon steel that exhibits both low losses and reduced cost.

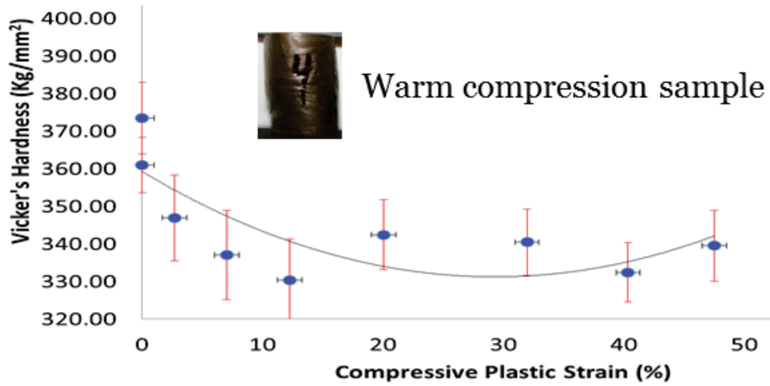
Static and dynamic tests comparing a high-silicon steel with a production lamination core steel confirmed the low-core-loss benefits of high-silicon blends. A grade 29M19C5 steel, which contains 2.67% silicon (per ASTM A677 36F155 for 0.36 mm M19), was compared with JFE 10JNEX900 (JFE Supercore™), which contains 6.5% silicon, the highest percentage of silicon used in steel.

The commercial 6.5% silicon steel is produced by chemical vapor deposition (CVD). It has low core losses but is very expensive. ORNL has pursued a novel processing technique based on strain softening during warm deformation (first reported by Chinese researchers) that effectively destroys lattice ordering (the B2 phase), leading to restoration of ductility and subsequent ease of cold formability. The ORNL process leads to low-cost Fe-6.5% Si steel sheet for motor laminations with magnetic properties equal to or better than those of the JFE 10JNEX90 produced by CVD.

Scaleup and commercialization of the alternative process is important to industry and motor manufacturing because of the major cost reduction. More development of the alternative production process is needed, specifically in the optimization of boron content and the thermomechanical process parameters. ORNL is exploring superimposed ultrasonic vibration during deformation as a means of eliminating the need for warm rolling.



Comparison of core-only losses for the various materials at full rotor flux vs. speed.



Work softening at ORNL of Fe–6 wt % Si–500 ppm B during warm compression at 400 °C.

Multiple Isolated Flux Path Switched Reluctance Motor

Contact: Timothy Burress, burressta@ornl.gov, 865-946-1216

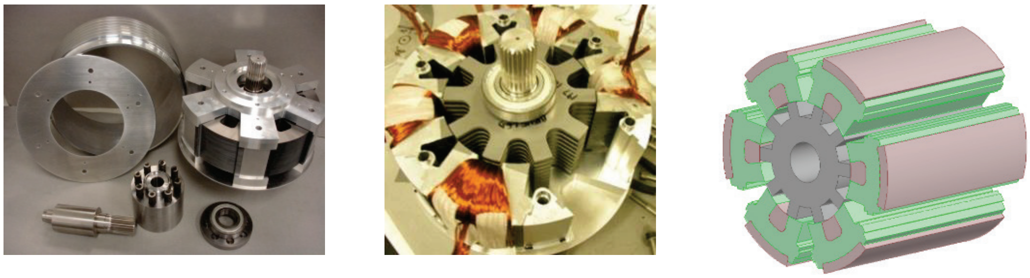
The simplicity of switched reluctance (SR) motors results in many benefits related to cost, reliability, and manufacturability. A novel SR motor design developed at ORNL addresses issues with these motors and offers a cost-effective, competitive alternative to permanent magnet motors made with rare earth materials, which have incurred significant price volatility in recent years.

Torque ripple and acoustic noise are the primary negative characteristics of SR motors, particularly when they are considered as an alternative to permanent magnet motors in passenger vehicles. Therefore, reluctance motors with multiple isolated flux paths (MIFPs) were developed by ORNL to facilitate better control over torque ripple and acoustic noise and achieve a secondary goal of improving power density and specific power. The segmented MIFP SR motor design introduces the potential to locate teeth within closer proximity to each other, thereby facilitating torque ripple reduction while maintaining magnetic saliency, which is the fundamental method of producing torque in SR motors.

Many MIFP variants were researched. The first-generation SR motor design consists of six segmented stator pieces forming 12 stator teeth with a conventional SR rotor with 10 teeth. The use of segmented stator pieces opens up many design opportunities that can lead to increased power density and/or reduced torque ripple and acoustic noise. One primary advantage is the capability to use yoke-wound stator coils. Although the use of this winding technique may seem insignificant, a closer look reveals the following benefits:

- Winding manufacturability—Stator pieces can be wound before installation.
- Improved heat transfer—Copper, which transfers heat about 40 times better than steel, is located on the outer perimeter of the motor and is well suited for interfacing with a heat exchanger. This will increase continuous operation capabilities.
- Broad teeth—Increased overlap of torque production among phases can reduce torque ripple and acoustic noise.

- Increased fill factor—Slots contain only one coil instead of two, thereby eliminating issues with interference between coils.
- Noise damping—Voids between stator pieces can be filled with damping material.



Hardware for ORNL's first MIFP SR motor prototype (left) and nearly assembled motor with yoke-wound stator coils (center). Finite element analysis model of second generation MIFP SR motor (right).

A second-generation MIFP SR motor design is under way, using custom design optimization and simulation tools (developed during first-generation design) to produce a motor suitable for electric vehicle applications. So far, simulations indicate that a Nissan LEAF–sized MIFP SR motor can produce a peak power of 95 kW, which satisfies DOE's 2015 targets and is higher than the published peak power of 80 kW for the LEAF. Efforts to improve continuous power capability and further reduce acoustic noise are ongoing.

Propulsion Materials

Studies Confirm Catalytically Active Single Platinum Atoms

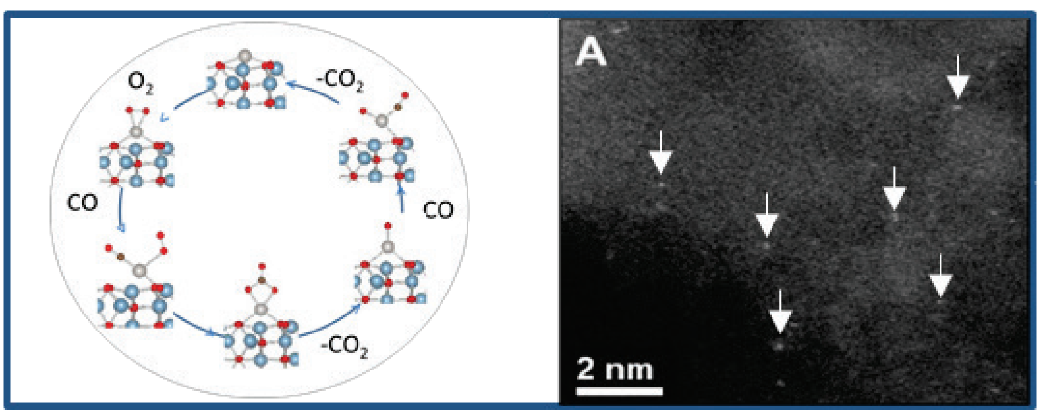
Contact: C. K. Narula, narulack@ornl.gov, 865-574-8445

Modern characterization tools have confirmed the presence of a significant fraction of active metal as single atoms and 10–20 atom rafts in a fully formulated supported noble metal catalyst. The catalytic activity of single atoms was only recently confirmed in studies at ORNL.

Because supported single atoms cannot engage in catalysis via a conventional Langmuir-Hinshelwood (L-H) pathway, their participation in catalysis was uncertain. Recent literature showed that single supported atoms are indeed catalytically active, provided the support can participate in catalysis (e.g., CeO_x and FeO_x as oxygen sources) to enable L-H pathway.

An automotive emission treatment catalyst generally contains single supported platinum (Pt) atoms, 10–20 atom rafts, and fully formed Pt particles supported on γ-alumina, an inert substrate that cannot participate in the catalytic process. In first principles theoretical modeling work at ORNL, researchers showed that single atoms of Pt group metals (Ni, Pd, and Pt) supported on θ-alumina are in zero oxidation state. Researchers also proposed that these single supported atoms will be catalytically active because the metal atoms in these systems are isoelectronic with $(Ph_3P)_2M$, a catalytically active organometallic compound.

Characterization by aberration-corrected electron microscopy, extended x-ray absorption fine structure, and x-ray near edge structure shows that the ORNL sample contains mono-disperse single supported Pt atoms on θ-alumina. The CO oxidation occurs on this catalyst with a turnover frequency of 18.7×10^2 (s^{-1}) measured at 20% CO conversion at 251°C, suggesting it is a highly active catalyst.



A CO oxidation pathway on single supported platinum atoms (left) and aberration-corrected electron microscopy images of 0.18% platinum on θ-alumina (right).

Since an L-H pathway is not possible on a single supported Pt atom, researchers proposed a CO oxidation pathway inspired by organometallic chemistry of isoelectronic $(Ph_3P)_2Pt$ species. The first principles study showed that CO oxidation occurs via formation of carbonate species whose decomposition is endothermic. This suggested that the catalyst surface will become covered with CO_3 during oxidation, and the reaction will stop unless external energy is supplied to decompose the CO_3 species. Diffuse reflectance infra-red spectroscopic monitoring of species of the catalyst surface during CO oxidation reaction (as a function of temperature) provided evidence for the formation of CO_3 at room temperature.

This research shows that single supported Pt atoms are indeed catalytically active species that can participate in emission treatment rather than being spectators to the catalytic process while waiting to become part of a fully formed Pt particle via sintering. These results also suggest that Pt rafts, which are accumulations of single Pt atoms bonded via oxygen, can participate in catalytic processes.

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2. C.K. Narula, et al., "CO oxidation on supported single Pt atoms: Experimental and ab initio density functional studies of CO interaction with Pt atom on θ-Al_2O_3 (010) surface," *J. Am. Chem. Soc.* **135**, 12634 (2013). This paper was highlighted in *Nature Chemistry* **5**, 809 (2013).

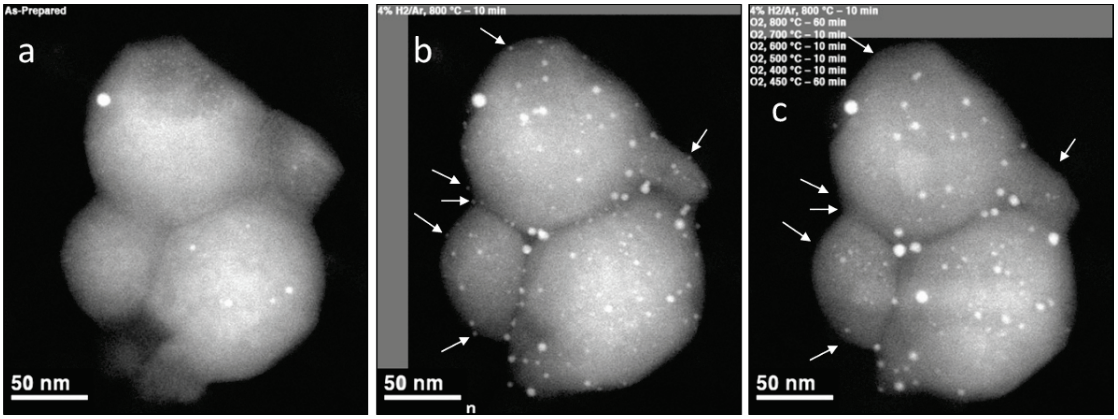
Electron Microscopy for Characterization of Catalyst Microstructure

Contact: Larry Allard, ORNL, allardlfjr@ornl.gov, 865-607-1144

Researchers at ORNL are exploring new in situ electron microscopy techniques for ultra-high-resolution imaging of catalytic materials in gaseous environments to study the reduction of NOx automotive emissions.

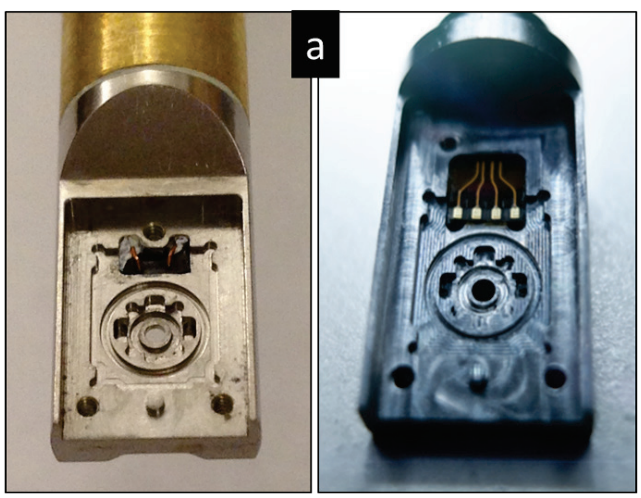
ORNL partnered with the microscopy company Protochips to expand its capabilities for in situ reaction studies with a unique gas-cell reactor system for ORNL's aberration-corrected electron microscope. The ORNL team is using a generation 3 (Gen 3) gas-cell holder for atomic imaging of catalysts at elevated temperatures and at gas pressures up to a full atmosphere. These are being used to study "self-regenerating" catalysts for emission reduction in partnership with Ford Research Laboratory and the University of Michigan. The researchers are also developing and using a Gen 4 holder and computer-controlled gas manifold, the basis for a commercial in situ gas reaction system for Protochips.

Microscopy gas-reaction experiments on catalyst powder materials were used to study redox reaction dynamics at conditions that mimicked ex situ studies conducted at the University of Michigan on model single-crystal perovskites with deposited precious metals. The reaction in the platinum-based catalytic trap oxidizer system proved to be asymmetric: metal extruded from the oxide within several seconds upon reduction but dissolved back into the support only after hours of aggressive oxidation. Finer particles dissolved more readily than larger particles. Many of the particles that formed during the reduction cycle were located in the interior of the crystal support and were not available for the catalytic process.



Example of in situ reaction sequence from the platinum–catalytic trap oxidizer work. (a) As-prepared (oxidized condition) sample shows only a few nascent platinum particles. (b) First reduction condition (800°C, 10 min) shows more particles, including some clearly on the surface (arrows). (c) After several oxidation cycles from 450 to 800°C for more than 2 h, many larger particles remain, but the original surface particles are apparently redissolved.

ORNL's experience with the Gen 3 reactor holder, and gradual development and modification of the ORNL gas manifold system to allow precise control of gas pressure and flow conditions, enabled Protochips to produce the Gen 4 gas cell holder and gas manifold. It offers four electrical leads rather than two, and the leads are specially fabricated with a proprietary "flexicable" design for proper electrical insulation and contact pads. These ensure easy loading of the heater and lower window devices when the cell is built for in situ experiments.



Comparison of interior geometry of Gen 3 (left) and Gen 4 gas cell holders with four-contact "flexicables."

The Gen 4 gas cell will be interfaced with a Protochips-fabricated gas manifold operated via computer control that allows remote programming and operational control capabilities for all valves, pumps, gas supply, gauges, and heater power. The system will be delivered and tested at ORNL during FY 2014.

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1. L. Allard, S. Overbury, W. Bigelow, M. Katz, D. Nackashi, and J. Damiano, “Novel MEMS-based gas-cell/heating specimen holder provides advanced imaging capabilities for in situ reaction studies,” *Microsc. Microanal.* **18**, 656–666 (2012).

2. L. Allard, J. Wittig, M. Chi, K. More, W. Bigelow, J. Damiano, and D. Nackashi, “Novel closed-cell gas-reaction holder allows characterization of behavior of bimetallic nanoparticles under elevated temperatures and gas pressures,” *Micros. Microanal. (Suppl. 2)* August (2013).

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Computational Modeling Assists Development of New Valve Alloys

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

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

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

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

Using the microstructures of these alloys as a target, researchers used computational thermodynamics to design new alloys with microstructures that resulted in high-temperature tensile and fatigue properties similar to or better than those of the commercial alloy used currently in exhaust valve applications. In contrast to the commercially available alloy with Ni+Co contents above 66 wt %, the Ni+Co content in these newly identified candidate alloys was lower than 50 wt %, resulting in reduced materials cost. These new alloys not only will enable the development of exhaust valves that can operate at much higher temperatures, but also will do so at potentially lower cost, facilitating the deployment of higher-efficiency vehicles.

Thermally Conductive Epoxy Molding Compound

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ORNL is exploring ways of improving the thermal conductivity of epoxy molding compounds (EMCs) used to package and insulate electronic components in automotive applications. Research in this project demonstrated the effectiveness of low-cost magnesium oxide filler in improving the thermal management capability of EMCs.

Desired EMC characteristics include electrical insulation, a low thermal expansion coefficient (to avoid damage from thermal cycling to internal parts encapsulated with the EMC), mechanical robustness and resistance to moisture absorption to protect from exterior environments, resistance to degradation on exposure to high temperatures, and insusceptibility to electric and magnetic fields.

An important limiting factor of traditional (composite) EMCs is their low thermal conductivity (κ), which limits options for thermal management for the electronic components they protect. Because the epoxy is the continuous phase in the EMC composite structure, it also has a low κ (typically κ ~ 0.2–0.3 W/mK). However, EMCs can be engineered for higher κ with an appropriate choice of filler material and control of its content. Doing so with a low-cost filler was the focus of this project.

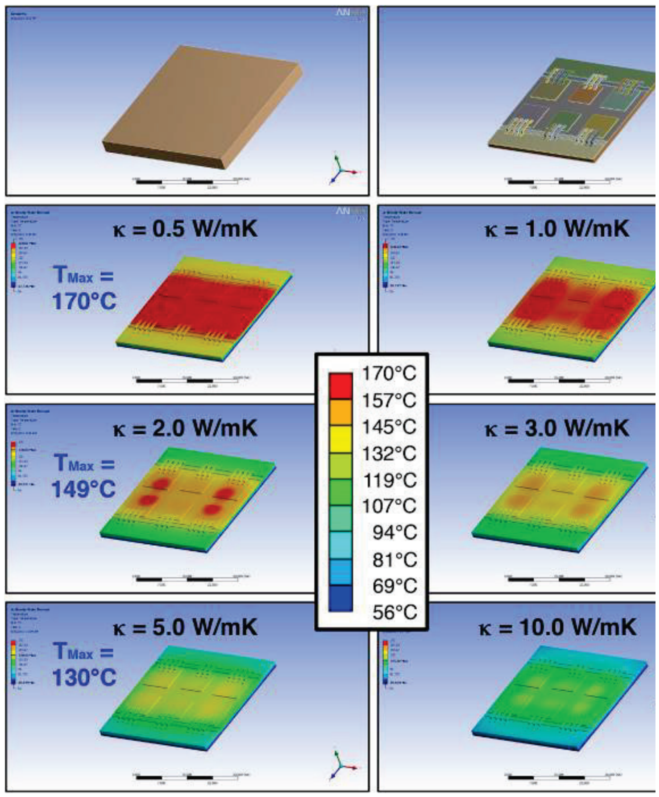
For example, the use of a hypothetical EMC with a thermal conductivity of 3–5 W/mK in combination with active cooling can substantially lower the maximum temperature of the constituent packaged in the material. Using an EMC with 3–5 W/mK can lower junction temperature by tens of degrees. Such a temperature reduction can improve device longevity and performance and enable the use of additional means of cooling and potentially more space- and weight-efficient redesigns of electronic and motor components.

Magnesium oxide has an attractive combination of characteristics as a filler in epoxy. It is an inexpensive compound with a relatively high bulk thermal conductivity. Another unique and attractive characteristic is it has low hardness and abrasiveness, which reduce mold fixture wear during EMC molding.

The significant outcome of this study was the demonstration that a bulk thermal conductivity of up to 3 W/mK can be achieved at low cost if MgO is used as a filler in an

EMC. This is a tenfold increase in thermal conductivity compared with unfilled epoxy and about two times the κ of traditional (SiO_2-filled) EMCs. The results signify that MgO-EMCs would be much more effective than traditional EMCs at lowering the maximum temperature of encapsulated components while having equivalent cost.

Because of the attractive performance of this new MgO-EMC, a potential large-scale EMC manufacturer is considering it as a commercial product, and engineers are considering its use in new power electronic and electric motor applications.



Temperature distribution and maximum temperature modeled in a hypothetical power module encapsulated by an EMC material with different thermal conductivities. A larger thermal conductivity decreases the maximum temperature of the module.

Publication and Invention Disclosure

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Surface Microengineering Lowers Friction to Improve Fuel Economy

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

Reducing friction on pistons, bearings, and other contacting parts in internal combustion engines can substantially increase vehicle fuel efficiency. Studies show that under typical operating conditions, friction at the piston ring-cylinder bore is responsible for as much as 50% of an engine's total mechanical friction losses; losses in crankshaft bearings and valve train components raise the total to more than 70%. Even slight friction reductions in key subsystems—multiplied by millions of vehicles on the road—can have a significant impact on energy efficiency.

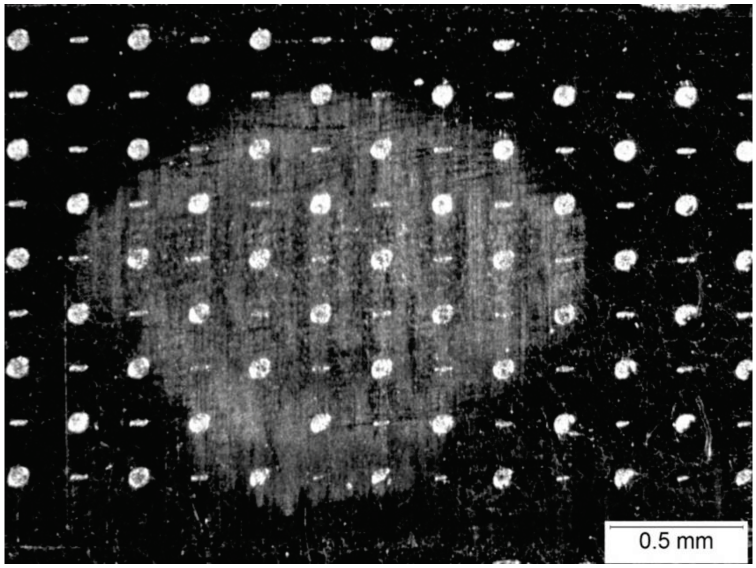
ORNL researchers are exploring the use of microengineered surfaces to enable engine makers to apply new friction-reducing strategies in their designs. Micro-texturing is an aspect of surface engineering that can control wear debris particles and allow surfaces to operate under efficient lubrication. In a collaboration with George Washington University (GWU), ORNL investigated micro-geometrically patterned surfaces (textures) and their effects on friction reduction. Developments included creating textures on curved surfaces like those of engine parts. Laboratory-scale friction testing methods were chosen to simulate a range of sliding conditions, such as unidirectional motion, reciprocating motion, elevated temperature operation, and operation under a time-varying spectrum of bearing loads similar to those in pistons, cam lobes, and connecting rod bearings. One of the tests used in this evaluation is an ASTM standard for engine friction (ASTM G181), development of which was led by ORNL. A custom-built, variable load/speed testing rig has generated valuable information on the ability of textures to reduce bearing friction.

Historically, coarse spiral grooves were sometimes machined into journal bearing bores to help replenish the lubricant and remove harmful wear particles. Newer microscale geometric patterns use advanced manufacturing and surface treatment methods to control lubricant flow at the microscale; this project builds on such work. Low-viscosity engine oils can reduce viscous losses, but they also reduce the ability of engine bearings to form a thick fluid film that separates surfaces. Thinner films tend to be less effective in protecting surfaces from wear. Surface microengineering is a promising approach to overcoming some of the negative aspects of using low-viscosity oils.

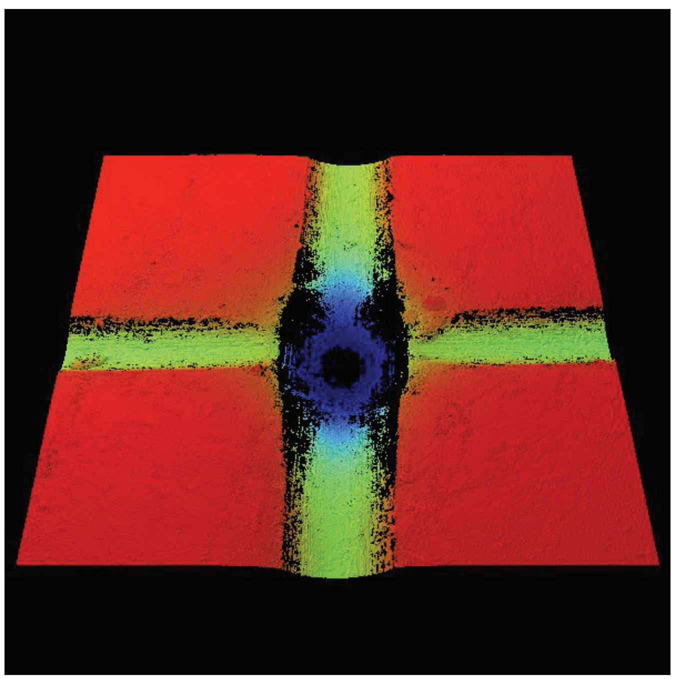
Chemical and mechanical methods are being evaluated to produce functional textures on surfaces like convex piston rings and concave engine bearing bores. GWU is using micro-lithography, and ORNL is using mechanical methods such as indentation arrays and compression of hard wire meshes. GWU research has shown that combinations of features like circles and ellipses can be more effective than a single shape to decrease lubricated friction. Using the shape combination principle, ORNL's wire compression texturing approach produces grooves and oval depressions. Upcoming work will investigate methods of preserving the functionality of micro-textured surfaces using thin films and coatings.

Publication

1. P. J. Blau, *Use of Textured Surfaces to Mitigate Sliding Friction and Wear of Lubricated and Non-Lubricated Contacts*, ORNL/TM-2012/20, Oak Ridge National Laboratory, 2012.



The surface of a commercial diesel engine piston ring, after friction testing, has a mixed pattern of circles and ellipses to reduce friction. The gray area is the site of contact with the opposing surface.



Topographic image of a bronze surface patterned by compression texturing with grooves and valleys.

Vehicle Systems

Wireless Charging for Electric Vehicles

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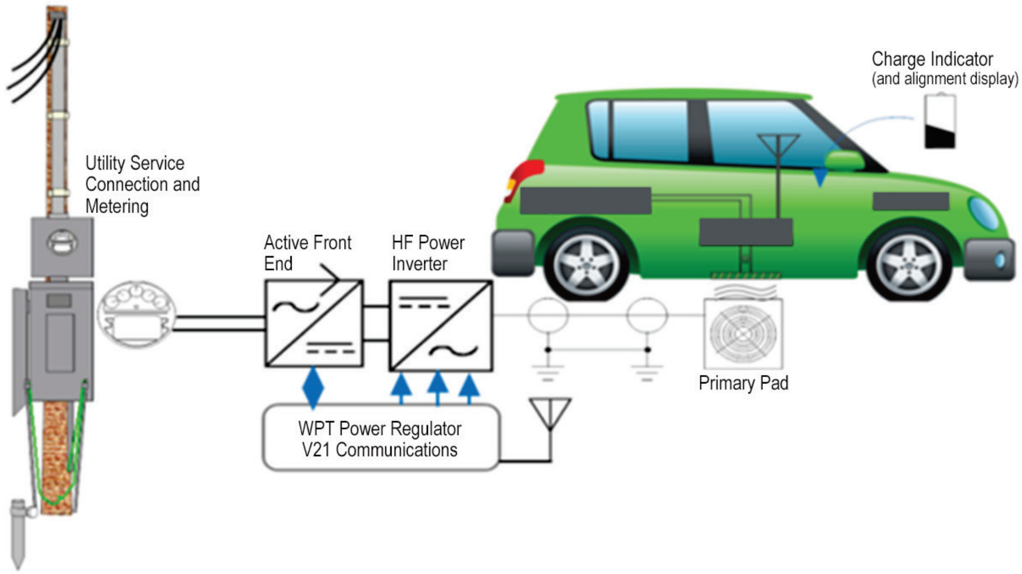
Wireless charging of electric vehicles, wireless power transfer (WPT), has the potential to eclipse conductive vehicle charging because of its autonomy, safety, and convenience to the customer. The use of private, secure, standardized radio communication, especially vehicle-to-infrastructure, means any vehicle can charge at any location. The complete charging process can in effect be totally transparent to the customer. ORNL researchers are working to develop a deep understanding of WPT—to identify the challenges and issues through analytical and experimental work so that technology gaps can be addressed.

Major accomplishments during FY 2013 included these:

- Achieved >10 kW power transfer at >85% utility input to WPT dc output (battery input) using laboratory bench demonstration hardware and software.
- Demonstrated an active front end for ORNL's WPT base station that uses commercial wide bandgap silicon carbide metal oxide semiconductor field effect transistors as the grid-input power factor corrector (PFC) stage.
- Developed and demonstrated a high-frequency (HF) power transformer for isolation of WPT base station electronics from HF feed cable and primary pad.
- Accessed the controller area network (CAN) in a Prius Hymotion plug-in hybrid test vehicle to demonstrate that battery management system messages needed for power flow regulation are available.
- Developed primary-side control strategy to manage the PFC voltage used as power flow regulation and HF power inverter frequency control to track variations in vehicle to ground pad gap.
- Demonstrated DOT standard dedicated short-range communications radio in the feedback loop.
- Developed and delivered all WPT schematics and bill of materials to a commercialization partner.

Other significant findings include assessment of WPT versus the four center-frequency bands available, showing that operation in the 20 kHz band is preferable for efficiency and misalignment tolerance. ORNL shared testing results for WPT operation in the four frequency band allocations for automotive wireless charging with the SAE J2954 wireless charging task force and frequency selection subcommittee. It was also found that a fully functional WPT installation will consist of a cascade of five major functional subsystems to provide grid power quality, electrical isolation, and low harmonic frequency generation.

Technology innovations also occurred during year one of this program. Specifically, we incorporated wide bandgap semiconductor devices operating at HF in the WPT PFC stage, and low-loss soft ferrites in magnetic components. One innovative material yet to be evaluated is a nanocomposite ferrite developed by Ageis Technologies that shows promise of



Wireless charging: utility pole to vehicle battery.

dramatic bulk and mass reduction of magnetic components. Areas of application for nano-composite ferrites include the PFC stage input inductors, the HF isolation transformer, and the coupler flux guides. The flux guides in particular tend to be thin and long, making them susceptible to fracturing under flexure. ORNL's material scientists devised a coating process and material that significantly increases their flexure strength.

Publications, Presentations, and Patent

1. O. C. Onar, J. M. Miller, M. S. Chinthavali, L. Tang, and S. Campbell, "SiC MOSFET based single phase active boost rectifier with power factor correction for wireless power transfer applications," presented at IEEE Applied Power Electronics Conference, APEC2014, Fort Worth, Texas, March 16–20, 2014.

2. M. S. Chinthavali, J. M. Miller, and O. C. Onar, "A comprehensive analytical and circuit level model development for wireless power transfer systems," presented at IEEE Applied Power Electronics Conference, APEC2014, Fort Worth, Texas, March 16–20, 2014.

3. J. M. Miller, O. C. Onar. And P. T. Jones, "ORNL developments in stationary and dynamic wireless charging," presented at Special Session: Advances in Wireless Power for Electric Vehicles, IEEE 5th Energy Conversion Congress & Exposition, ECCE2013, Denver, September 16–20, 2013.

4. O. C. Onar, J. M. Miller, S. L. Campbell, C. Coomer, C. P. White, and L. E. Seiber, "A novel wireless power transfer for in-motion EV/PHEV charging," presented at IEEE Applied Power Electronics Conference, APEC2013, Long Beach, Calif., March 17–21, 2013.

5. O. Onar and J. M. Miller, "Buffering Energy Storage Systems for Reduced Grid and Vehicle Battery Stress for Wireless In-motion Wireless Power Transfer Systems," DOE S-Number S-124,533, ID Number 201202956, October 2012.

Vehicle Systems Integration Laboratory Advances Powertrain Research

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Growing transportation costs and upcoming regulations have increased the focus on vehicle fuel efficiency and emissions control, highlighting a need for more aggressive research addressing the complex interactions of advanced powertrain technologies. ORNL's Vehicle Systems Integration (VSI) Laboratory is accelerating the pace of powertrain development by performing prototype research and characterization of advanced systems within a controlled environment, while exposing the systems to real-world conditions. VSI Lab capabilities range from advanced light-duty vehicles to hybridized Class 8 powertrains.

The ability to test a complete "power pack," consisting of an engine plus a transmission, for a fully loaded Class 8 truck is the focus of the VSI Lab. The test cell can handle both conventional and hybrid powertrains for a variety of architectures. The battery emulation system provides a flexible environment for subjecting the powertrain under test to a variety of possible energy storage solutions.

To exercise the system and demonstrate performance, a dual dyno configuration was used to characterize the maximum torque curve for a conventional powertrain. The maximum torque generated by this powertrain was found to be just over 18,000 N·m, demonstrating the full range capability of the VSI powertrain test cell.

More tests were conducted on the conventional powertrain coupled to the twin dynamometer configuration to evaluate the hardware-in-the-loop and virtual vehicle capabilities. The GEM model from the Environmental Protection Agency was incorporated into the system to demonstrate the flexibility to integrate a variety of vehicle models. The powertrain test cell monitors and records a wide variety of data and can accommodate more sensors as future tests dictate.

VSI Powertrain Test Cell "power pack" test configuration for heavy duty applications.

Major equipment upgrades in 2013:

- The AVL Powertrain Dynamometer Test System was procured and installed. Full functionality was demonstrated using a conventional Class 8 heavy duty powertrain consisting of a Cummins ISX.
- The AVL eStorage System (battery emulator) was procured and installed in the powertrain test cell.
- The hardware-in-the-loop system was procured, installed, and commissioned for both engine-in-the-loop and powertrain-in-the-loop configurations. Both conventional and hybrid powertrain architectures were successfully demonstrated.
- Two complete sets of emissions analyzers were procured, installed, and commissioned to measure raw, engine-out emissions and post-aftertreatment (tail-pipe) emissions.
- An AVL 250 kW high-speed (12,000 rpm) dynamometer was ordered for the component test cell. It features a through shaft to support two separate experimental setups in the laboratory.
- A modular, cross-hatch designed bed plate was ordered for the component test cell to provide adequate space to support two experimental setups simultaneously.