Sustainable Transportation Program

2011 Annual Report

ORNL/TM-2012/196

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

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Sustainable Transportation Program

2011

Annual Report

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ORNL's Sustainable Transportation Program performs research and development leading to new vehicle and transportation system technologies. Highway transportation—light-, medium-, and heavy-duty vehicles—accounted for approximately 23% of U.S. greenhouse gas emissions and about 64% of all petroleum used in the United States in 2009[1]. Energy use in highway transportation is expected to increase almost 21% by 2035—from 11.1 to 13.4 million barrels per day oil equivalent[2]. ORNL researchers are focusing on clean, efficient, and intelligent paths to reducing transportation fuel consumption and emissions, and achieving improved energy security. The research and development portfolio includes alternative fuels, more efficient vehicle components, lightweight materials, transportation electrification, and intelligent transportation systems and operations.

The Program's primary support comes from the Department of Energy, Office of Energy Efficiency and Renewable Energy, through three technology development programs: Vehicle Technologies, Fuel Cell Technologies, and Biomass Programs. Support also comes from the Department of Transportation, other federal agencies, and the private sector.

Support of the Vehicle Technologies Program was highlighted by achievement of the U.S. DRIVE Partnership[3] engine efficiency goal, use of neutron imaging techniques to study emission control devices and lithium distribution in battery electrodes, and advancing electric vehicle charging technologies including solar-assisted charging and wireless charging. Researchers are investigating innovative electric motor designs that reduce or eliminate the need for rare-earth permanent magnets, which are subject to market fluctuations in availability and cost.

ORNL has worked with the Fuel Cell Technologies Program for several years on a nitrided material for use in fuel cell bipolar plates. In FY 2011, a collaborative effort with General Motors to explore manufacturability of the material by GM's exist-

1 Davis, S. C., S. W. Diegel and R. W. Boundy. 2011. Tables 1.12, 1.13, 11.3, 11.7 in *Transportation Energy Data Book, Edition 30*. ORNL-6986, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

2 U.S. Energy Information Administration. 2011. Table A7 in *Annual Energy Outlook 2011 With Projections to 2035*. U.S. Department of Energy, Washington, D.C.

3 Formerly the FreedomCAR and Fuel Partnership, U.S. DRIVE is a non-binding and voluntary government-industry partnership focused on advanced automotive and related infrastructure technology research and development.

ing stamping and welding practices was successful. A new multiyear project began to develop a stationary hydrogen storage system; preliminary engineering design has demonstrated that the integrated steel and prestressed concrete storage vessel can sustain 5,000 psi pressure based on industry codes and standards.

In Biomass Program support, researchers launched the Bioenergy Knowledge Discovery Framework, a computational tool for data visualization and analysis. Staff completed and issued an update to the 2005 "Billion Ton Study" that confirmed the technical feasibility of U.S. lands supplying a billion tons of dry biomass annually, while giving increased attention to environmental sustainability and land-use change[4]. A widely cited study[5] using empirical data found that indirect land use change resulting from expanded corn ethanol production over the past decade has been minimal. ORNL completed a three-year study measuring critical property changes for classes of fuel dispenser materials exposed to ethanol-blended fluids[6]. The test results are intended to identify potential issues and guide the selection and development of materials compatible for use in E15 dispensers.

The Sustainable Transportation Program continued to provide outstanding support to the Department of Transportation, enhancing data quality and developing on-line analysis tools for the 2009 National Household Travel Survey data and Freight Analysis Framework, the most comprehensive publicly available data sets on personal and freight movement in the United States. The Federal Motor Carrier Safety Administration reaffirmed their multi-year commitment to the Commercial Motor Vehicle Roadside Testing Corridor, stating that ORNL had demonstrated the capability to take care of all their roadside-based testing needs.

Highlights of selected Program research and development efforts begin on page 23.

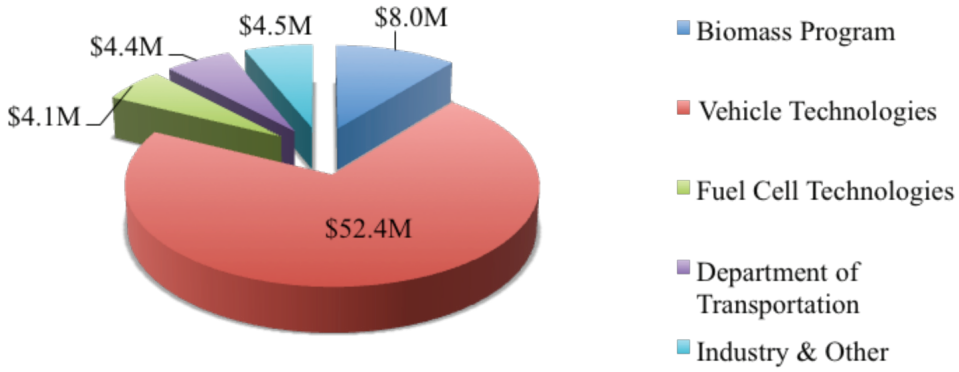
4 U. S. Department of Energy. 2011. *U.S. Billion-Ton Update: Biomass Supply for a Bioenergy and Bioproducts Industry*. R.D. Perlack and B.J. Stokes (Study Leads), ORNL/TM-2011/224. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

5 Oladosu, G., and K. L. Klein. 2010. "Decomposition analysis of U.S. corn use for ethanol production from 2001-2008." Presented at California Air Resources Board (CARB) Low Carbon Fuel Standard Expert Workgroup Meeting, Sacramento, Calif., October 14–15.

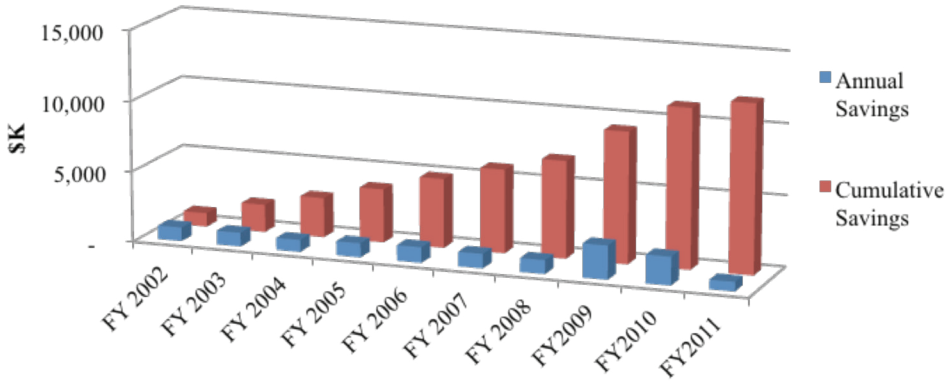
6 Kass, M., et al. 2011. *Intermediate Ethanol Blends Infrastructure Materials and Compatibility Study: Elastomers, Metals, and Sealants.* ORNL/TM-2010/326. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Program Support

The Program received $73.4M in new funding in FY 2011 with the largest portion being from the Vehicle Technologies Program.



About half of the Program's R&D is conducted at the National Transportation Research Center (NTRC) located in Knoxville, Tennessee. Since 2002, the NTRC has benefited from a reduced overhead rate by virtue of being located off the ORNL main campus. The figure below shows the approximate annual and cumulative cost savings resulting from NTRC's off-site location. In FY 2012, the ORNL cost model will change and NTRC will no longer be considered "off site" for overhead purposes.

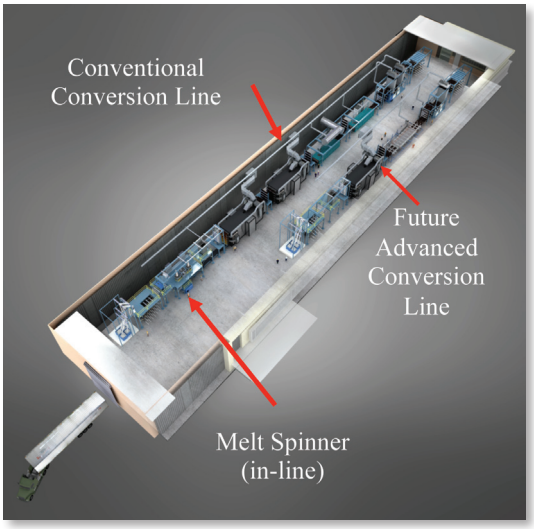


From FY 2002 through FY 2011, cumulative overhead savings of $11.9M have been applied to research and development projects at the NTRC due to its off-campus location.

Facilities

Establishing, upgrading, and maintaining facilities and experimental capabilities is a key element of the Program's support for its sponsors. In FY 2011, the Program expanded capabilities and launched new facilities to support R&D programs in materials, advanced combustion, energy storage, vehicle systems, power electronics, hydrogen, and analysis.

Lightweight Materials. The Program's largest infrastructure project is the Carbon Fiber Technology Facility, funded in late 2009 as part of the American Recovery and Reinvestment Act. This $34,700,000 facility will house systems capable of producing semi-production quantities (up to 25 tons per year) of low-cost carbon fiber sufficient to make large-scale material and process evaluations. The highly flexible facility will be capable of handling multiple precursor chemistries and material formats. It will house a melt spun precursor fiber semi-production line and conventional fiber conversion technologies, and will accommodate advanced conversion technologies as they mature. The Carbon Fiber Technology Facility is scheduled to be operational in 2013.
A critical link in scaling technologies from lab scale to the Carbon Fiber Technology Facility, ORNL's conventional Carbon Fiber Pilot Line is getting a significant upgrade to enhance throughput, controls, and flexibility, and integrate carbonization and oxidation capabilities with the Precursor Evaluation System. The upgraded Pilot Line will be capable of producing 12 pounds of fiber per day as compared to the current 2 pounds per day. Tension control will be significantly enhanced, as will surface treatment, sizing, control system, and data acquisition capabilities.



Layout of the Carbon Fiber Technology Facility production area.

NTRC-2. ORNL has leased a newly constructed building adjacent to the NTRC to provide additional office space and laboratories for the Sustainable Transportation Program. New capabilities housed in NTRC-2 include the Vehicle Systems Integration Laboratory, Battery Cell Manufacturing Facility, and Transportation Analysis and Visualization Laboratory.

Vehicle Systems Integration Laboratory. The Vehicle Systems Integration Laboratory will enable fully integrated, system-level research on advanced combustion, electric drivetrain, controls, and fuel technologies. It will allow researchers to study complex interactions of advanced prototype technologies to achieve maximum efficiency with lowest possible emissions. Equipped for light-, medium-, and heavy-duty powertrain architectures, the VSI lab will facilitate understanding of advanced transportation technologies operating under real-world conditions. The laboratory is scheduled to be operational in summer 2012.

Battery Cell Manufacturing Facility. A battery cell manufacturing facility will focus on developing and refining new technologies for materials processing and battery assembly to reduce scrap rate, increase production speeds, and improve battery performance. This facility is scheduled to be operational in spring 2012.

Transportation Analysis and Visualization Laboratory (TRAVL). TRAVL features a 15-panel high-definition video wall that accommodates simultaneous display of up to 30 high-definition video content sources. With processing power for multi-HD 3D graphics, the system supports the most advanced real-time simulation and modeling collaborations. Future TRAVL projects will include visualizing freight on highway, rail and waterways systems; large scale truck tracking to assess energy efficiency and safety; and integrating geo-visualization with human factors research.

Power Electronics and Electric Machines. A state-of-the-art laboratory was created to support investigation of innovative materials, structures, and processing of the power electronics module, or PEM. The PEM plays a large role in the operation of electric vehicles. Advanced PEMs can offer superior performance, thermal management, and power density.

The automated test facility for performance characterization of wide bandgap semiconductors was upgraded: throughput and detail have been improved, characterization costs have been lowered, and high switching frequency of gallium nitride devices is now accommodated.

Advanced Combustion and Fuels. The air handling system was upgraded on the flexible single-cylinder research engine. The upgraded air handling system will allow research to expand the high load limits of advanced combustion, and will support research into pre-ignition phenomena in boosted spark ignition conditions (for example, superknock).

High Temperature Materials Laboratory. A specialized in situ gas flow holder was developed for the aberration-corrected scanning transmission electron microscope. The holder allows for the observation of catalysts in the presence of a gas at pressures up to 1 atmosphere and temperatures up to 1200°C with sub-nanometer-scale spatial resolution. This new technology will enable a number of unique experiments involving real-time observation of catalyst sintering, coarsening, phase transformations, and so forth.

Fuel Cell Technologies. An electron energy loss spectrometer was installed on an ORNL transmission/scanning transmission electron microscope, which has been used to characterize carbon corrosion mechanisms in polymer electrolyte membrane (PEM) fuel cell membrane electrode assemblies, and ionomer structure and chemistry in PEM fuel cell electrodes. The energy dispersive spectroscopy system on the microscope was upgraded with a silicon drift detector for rapid elemental data acquisition for compositional analysis.

A new hydrogen charging system capable of maintaining or varying hydrogen pressure up to 10,000 psi has been designed and is being assembled. Combining the existing tensile and fracture toughness testing load-frames with a new fatigue testing load-frame under development in a collaborative project sponsored by the Department of Transportation, the upgraded testing facility will enable the comprehensive study of the effect of hydrogen on material properties under very high pressures that are relevant to hydrogen production, delivery, and storage infrastructure.

Patents and Invention Disclosures

Sustainable Transportation Program researchers submitted 44 invention disclosures resulting from efforts funded by the Vehicle Technologies Program and the Fuel Cell Technologies Program. Another 17 invention disclosures were filed in related efforts leveraged by funding from other federal agencies, industry, and ORNL strategic investments such as the Laboratory Directed Research and Development Program. Of these 61 invention disclosures, 18 were elected for patent filings, and 38 are still under consideration.

During FY 2011, six patents were awarded based on previous filings.

Lightweight, Durable Lead-Acid Batteries. U.S. Patent No. 8,017,273. Inventors: Edgar Lara-Curzio, Ke An, James O. Kiggans, Jr., Nancy Dudney, Cristian Contescu, Frederick S. Baker, and Beth L. Armstrong.

Utilization of Rotor Kinetic Energy Storage for Hybrid Vehicles. U.S. Patent No. 7,936,076. Inventor: John S. Hsu.

Self-Learning Control System For Plug-In Hybrid Vehicles. U.S. Patent No. 7,849,944. Inventor: Robert C. DeVault.

Laser-Induced Fluorescence Fiber Optic Probe Measurement Of Oil Dilution By Fuel. U.S. Patent No. 7,839,492. Inventors: James E. Parks, II and William P. Partridge, Jr.

System To Continuously Produce Carbon Fiber Via Microwave Assisted Plasma Processing. U.S. Patent No. 7,824,495. Inventors: Terry L. White, Felix L. Paulauskas, and Timothy S. Bigelow.

Iron-Based Alloy And Nitridation Treatment For PEM Fuel Cell Bipolar Plates. U.S. Patent No. 7,829,194. Inventors: Michael P. Brady, Bing Yang, and Philip J. Maziasz.

Awards and Professional Honors

Research staff members received numerous awards and professional recognitions, reflecting significant contributions to research and technology development. Hydrogen sensor R&D funded by the Fuel Cell Technologies program won an R&D 100 award. A fuel-in-oil diagnostic technique developed under a Cooperative Research and Development Agreement with Cummins won a Federal Laboratory Consortium Excellence in Technology Transfer award. Four researchers received Outstanding Mentor Awards from the DOE Office of Science in recognition of outstanding contributions and dedication in mentoring. Program researchers made significant contributions to Operation Tectonic Fury, winner of the 2011 CODiE Award for Best Science or Health Instructional Solution, awarded by the Software and Information industry Association. A selection of the most notable awards and recognitions is shown in Table 1.

Table 1. Awards and professional honors received in FY 2011 by ORNL Sustainable Transportation Program researchers

Lawrence F. Allard, Jr.	Best Paper in the materials applications field from *Microscopy and Microanalysis Journal*
Nina Balke	DOE Office of Science Early Career Award
Teresa L. Barone	DOE Office of Science Outstanding Mentor Award
Gary J. Capps	DOE Office of Science Outstanding Mentor Award
Gary J. Capps	Appointed to the Federal Motor Carrier Safety Administration's Smart Roadside Initiative Technical Advisory Committee
Madhu S. Chinthavali	Outstanding Presentation, Applied Power Electronics Conference and Exhibition
Virginia H. Dale, Michael R. Hilliard, Esther S. Parish, Deanne J. Brice, Charles T. Garten, Jr., Alexandre Sorokine, and Robert M. Whitten	Mission 2 of Operation Tectonic Fury, winner of the 2011 CODiE Award for Best Science Instructional Solution, awarded by the Software and Information industry Association; and the 2011 Award of Excellence from *Technology & Learning Magazine*
Claus Daniel	U.S. co-chair for the energy storage session, National Academy of Engineering German-American Frontiers of Engineering Symposium

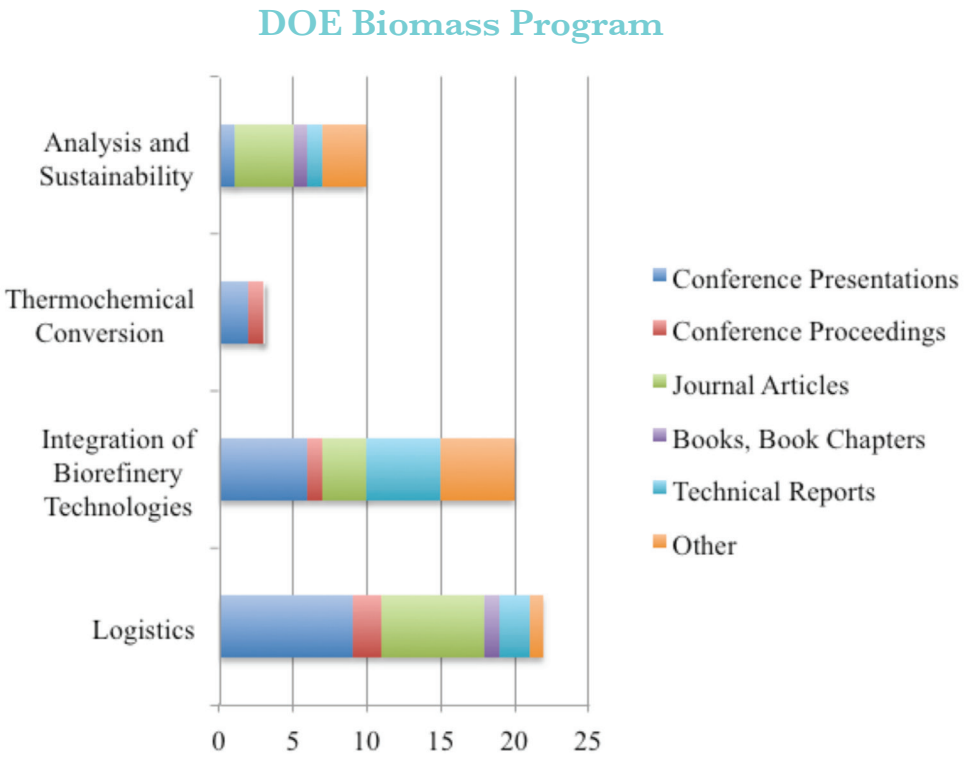
Sujit Das	Appointed to the Transportation Research Board Committee on Transportation Economics
Sujit Das	Appointed to the Transportation Research Board Committee on Alternative Transportation Fuels and Technologies
Diane Davidson	Board of Directors, Intelligent Transportation Society of Tennessee
Diane Davidson	Appointed to the Transportation Research Board Committee on Critical Transportation Infrastructure Protection
Diane Davidson	Chair, Federal Transit Authority's Transit Rail Advisory Committee for Safety
Stacy C. Davis	Appointed to the Transportation Research Board Committee on Alternative Transportation Fuels and Technologies
Rebecca A. Efroymson	Peer reviewer for the Environmental Protection Agency report, *Biofuels and the Environment: First Triennial Report to Congress.*
Rebecca A. Efroymson	Appointed to the National Research Council Committee on Sustainable Development of Algal Biofuels
Oscar Franzese	DOE Office of Science Outstanding Mentor Award
Rick Goeltz	Chair, Transportation Research Board Technical Expert Task Group to Design and Implement a System for Archiving and Disseminating Data from Strategic Highway Research Program 2 Reliability and Related Studies
David L. Greene	Appointed to the Board of Directors of the American Council for an Energy Efficient Economy
David L. Greene	Edward L. Ullman Award from the Transportation Geography Specialty Group of the Association of American Geographers
David L. Greene and Zhenhong Lin	2011 Department of Energy Vehicle Technologies Program Research and Development Award
Camden R. Hubbard	Fellow, ASM International
Ho-Ling Hwang	Appointed to the Transportation Research Board Committee on Travel Survey Methods
Keith L. Kline	Invited to participate in the Roundtable for Sustainable Biofuels Expert Group on Indirect Impacts
H. E. (Bill) Knee and Oscar Franzese	Transportation Research Board 2011 Pyke Johnson Award for the outstanding paper published in the field of transportation systems planning and administration

Michael J. Lance	Excellence in Oral Presentation at the SAE Powertrains, Fuels & Lubricants Meeting
Michael J. Lance	Selected to be published in the *SAE International Journal of Engines*, "Characterization of Field-Aged Exhaust Gas Recirculation Cooler Deposits", 2010-01-2091
Nickolay V. Lavrik, Panos G. Datskos, Scott R. Hunter, and Barton Smith, ORNL; Michael J. Sepaniak and James F. Patton, University of Tennessee	R&D 100 Award, Nano-Optomechanical Hydrogen Safety Sensor Based on Nanostructured Palladium Layers
Jan-Mou Li	Appointed to the Transportation Research Board Committee ABJ30 on Urban Transportation Data and Information Systems
Zhenxian Liang	Guest editor, *Journal of Advances in Power Electronics*, for a special issue on "EMI/EMC, Passive Components and Power Electronics Integration Techniques"
Zhenhong Lin	Appointed to the Transportation Research Board Committee on Transportation Energy
Philip J. Maziasz	Battelle Distinguished Inventor
Mitchell Olszewski	Appointed to a multinational North Atlantic Treaty Organization working group charged with assessing the rare earth materials situation relative to electric motive power systems
James E. Parks and William P. Partridge, Jr.	Federal Laboratory Consortium Excellence in Technology Transfer Award for "Laser-induced Fluorescence Fiber-optic Measurement of Fuel in Oil"
William P. Partridge, Jr.	DOE Office of Science Outstanding Mentor Award
Duminda I. Randeniya	Member, Professional Advisory Committee for "Improving Log Transportation with Data Based Monitoring and Analysis in Northern Wisconsin and Upper Peninsula of Michigan," a study by the Michigan Technological University and University of Wisconsin- Superior
Kevin J. Rhodes	Featured researcher in the *Pacific Acoustic Corporation Spring Newsletter* for his acoustic emission work on battery materials
Kevin J. Rhodes	2011 Margaret C. Ettner Student Lecturer Award from the American Crystallographic Association

Kevin J. Rhodes, Melanie J. Kirkham, Roberta A. Meisner, E. Andrew Payzant, Nancy J. Dudney, and Claus Daniel	60th Annual Conference on Applications of X-ray Analysis Best Poster Award for "In situ XRD Characterization of Thin Film Electrodes for Electrochemical Energy Storage Devices"
David J. Singh	Elected to the Executive Committee of the American Physical Society, Division of Computational Physics
Scott Sluder	Vice Chair, SAE Land & Sea Group
Gui-Jia Su and Lixin Tang	Best Paper at the 7th IEEE Vehicle Power and Propulsion Conference
Erin Webb	Member, Biomass Research and Development Initiative Inter-agency Working Group for Bioenergy Logistics
Andrew A. Wereszczak	Fellow, American Ceramic Society

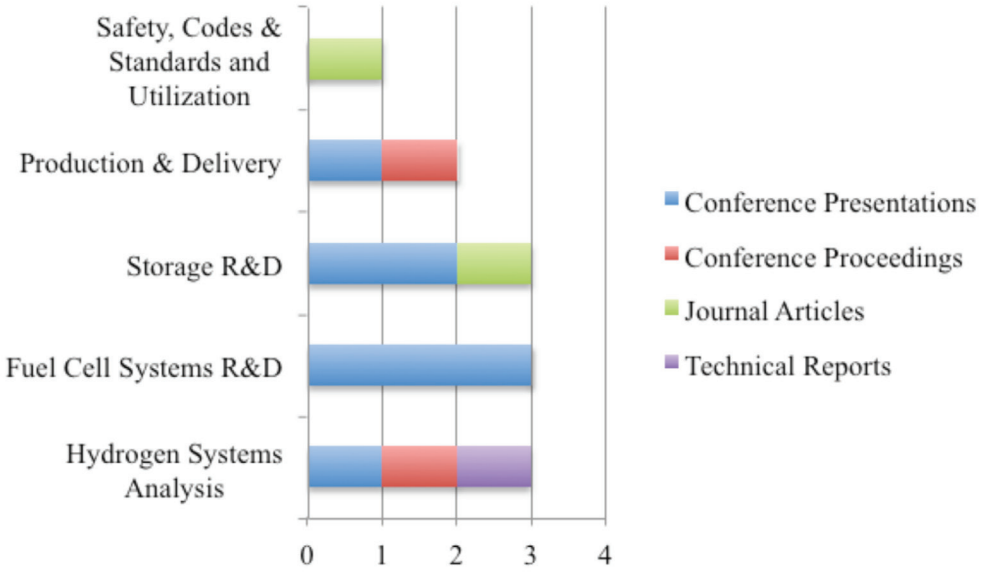
Publications and Presentations

Sustainable Transportation Program staff produced more than 300 journal articles, technical reports, presentations, and papers in conference proceedings. A breakdown by sponsor and type of publication is presented below.



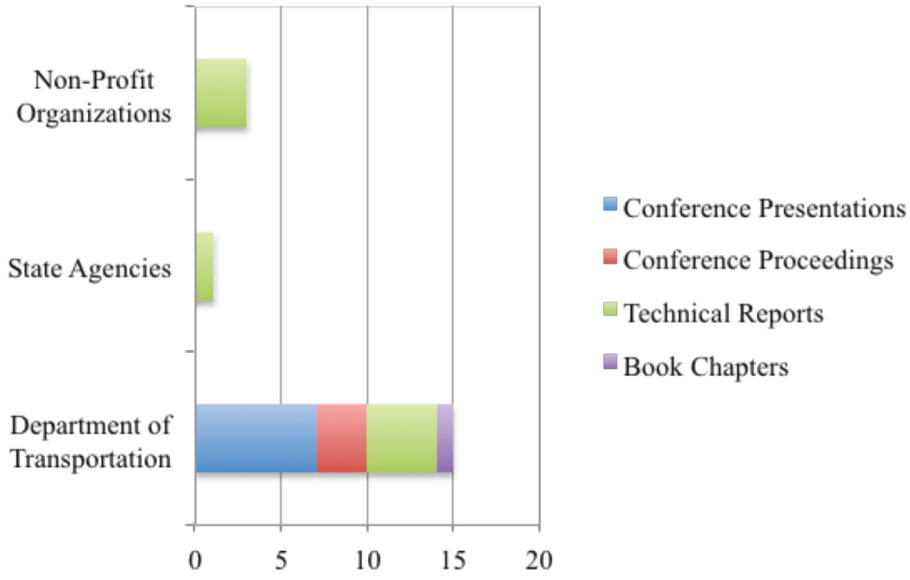
Research sponsored by the Biomass Program resulted in 55 publications and presentations in FY 2011. Source: ORNL Publication Tracking System.

DOE Fuel Cell Technologies Program



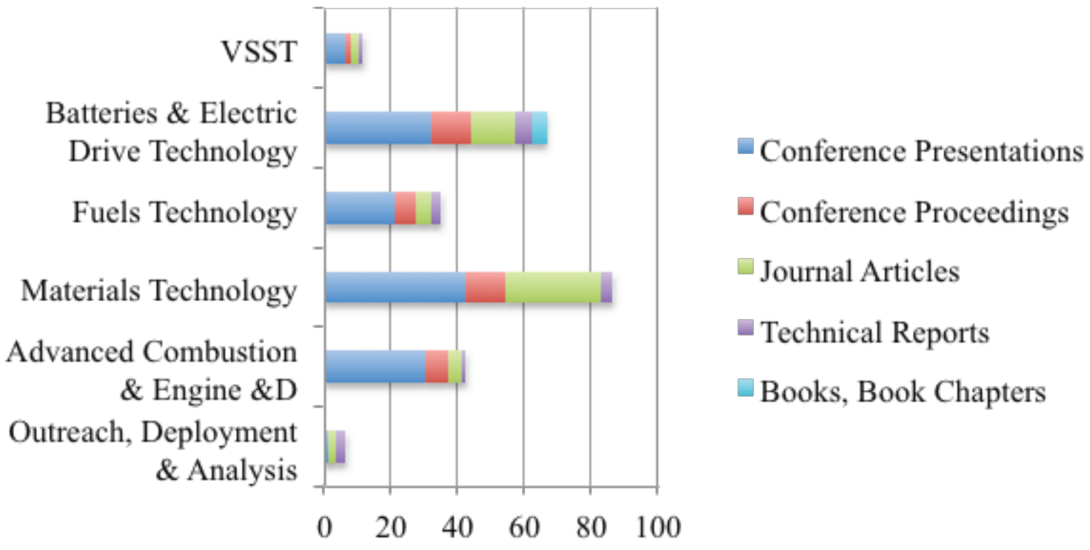
Research sponsored by the DOE/EE Fuel Cell Technologies Program resulted in 12 publications and presentations in FY 2011. Source: ORNL Publication Tracking System.

DOT and Other Sponsors



Research sponsored by the Department of Transportation, state agencies, and non-profit organizations performed by staff in ORNL's Center for Transportation Research resulted in 18 publications and presentations in FY 2011. Source: ORNL Publication Tracking System.

DOE Vehicle Technologies Program



Research sponsored by the DOE/EE Vehicle Technologies Program resulted in 247 presentations and publications in FY 2011. Source: ORNL Publication Tracking System.

Biomass R&D

Billion Ton Update

Bioenergy Knowledge Discovery Framework

Ethanol Blends Materials Compatibility

Biomass Supply Chain Modeling & Analysis

Sustainability of Biomass Production

Billion Ton Update

In 2005, ORNL led the Billion-Ton Study for the U.S. Departments of Energy and Agriculture. The resulting landmark report, *Biomass as Feedstock for a Bioenergy and Bioproducts Industry: The Technical Feasibility of a Billion-Ton Annual Supply*, played a pivotal role in the development of the Energy Independence and Security Act of 2007 with findings confirming the technical feasibility of U.S. lands supplying a billion dry tons of biomass annually. Now in another groundbreaking study, ORNL, leading a team of researchers from seven universities, two national laboratories (ORNL and the Idaho National Laboratory) and four U.S. Department of Agriculture (USDA) offices, has updated the original study. The main findings remain the same: the ambitious goals the United States has set for biofuels use are not only achievable but sustainable. The 2011 report, however, goes beyond merely updating the previous report to provide a comprehensive resource assessment and address many of the issues raised since 2005. The update is remarkable in its detailed temporal and spatial resolution (annual supply curves at the county level for almost 20 different feedstocks) and attention to environmental sustainability, not only providing information on the potential quantities of feedstocks and their cost, but also addressing the resulting land use changes. The study also sets a new standard for transparency and data accessibility as all the county-level results were made available to the public, researchers, and industry through the Bioenergy Knowledge Discovery Framework, a web-based application developed at ORNL that allows visualization of the data as maps and selective downloading of any and all of the data generated by the study.

Released in August 2011 by DOE, the Billion-Ton Update can be found online at eere.energy.gov/biomass/pdfs/billion_ton_update.pdf or on the Bioenergy Knowledge Discovery Framework at www.bioenergykdf.net.

One season's growth of potential cellulosic biomass feedstock.

Key Differences Between the 2005 Billion-Ton Study and the 2011 Billion-Ton Update

2005 Billion-Ton Study	2011 Billion-Ton Update
National estimates—no spatial information	County-level with aggregation to state, regional, and national levels
No cost analyses	County supply curves for major primary feedstocks
Environmental sustainability addressed from national perspective	Environmental sustainability modeled for residue removal
No explicit land-use change modeling	Land-use change modeled for energy crops
Long-term time horizon (2025–2050)	2012–2030 timeline
2005 USDA agricultural projections; 2000 forestry Resource Planning Act (RPA)/Timber Production Output (TPO)	2009 USDA agricultural projections; 2007 forestry RPA/TPO
Estimates of current availability	Annual projections based on a continuation of baseline trends (USDA projection)
Long-term projections involving changes in crop productivity, crop tillage, residue collection efficiency, and land-use change	Annual projections based on changes in crop productivity, tillage, and land use

Publications

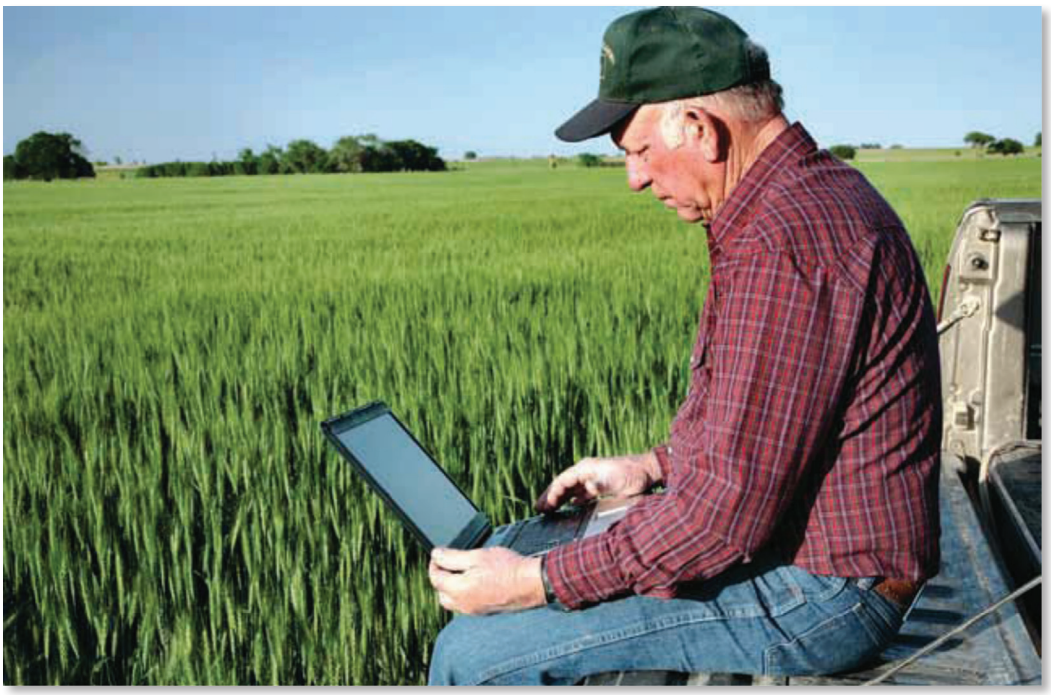
- U.S. Department of Energy. 2011. *U.S. Billion-Ton Update: Biomass Supply for a Bioenergy and Bioproducts Industry*. R. D. Perlack and B. J. Stokes (study leads). ORNL/TM-2011/224. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

- Perlack, R. D., et al. 2005. *Biomass as Feedstock for a Bioenergy and Bioproducts Industry: The Technical Feasibility of a Billion-Ton Annual Supply.* DOE/GO-102995-2135 or ORNL/TM- 2005/66. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

The Bioenergy Knowledge Discovery Framework

Meeting the challenging goals the United States has set for bioenergy use requires new ways of accessing, evaluating, synthesizing, and visualizing information. The DOE Office of Biomass Program (OBP) tapped ORNL in 2008 to develop a framework to promote sharing and integration of bioenergy resource information; engage various stakeholder communities; offer guidance and access to comprehensive data, modeling, and visualization resources; and incorporate OBP- and partner-funded research. The result is the Bioenergy Knowledge Discovery Framework (KDF), a web-based platform that provides access to the latest data, models, and analysis tools. The Bioenergy KDF seeks to harmonize data from different sources and provide integrated decision-making capabilities using Web 2.0 and social networking technologies. Unique among such resources, the Bioenergy KDF allows users to pose questions to be referred to experts for answers. The website (www.bioenergykdf.net/) was released in January 2011 and has experienced consistent growth, accumulating nearly 700 registered users as of January 2012, with an average of 150 unique site visits per day.

The Bioenergy KDF contains approximately 1,400 curated spatial data sources, more than 1,200 downloadable data sets, more than 1,100 map services at different scales, hundreds of curated resources describing models and important journal articles, and links to many web resources. Data from the Billion Ton Update; the Biofuel Infrastructure, Logistics, and Transportation (BILT) model; and the National Bioenergy Routing Model were successfully integrated in 2011. In conjunction with



publication of the Billion Ton Update report in August 2011, the Bioenergy KDF provided the main source of access to the report, data, and basic analysis capabilities. Feedstock data can be downloaded in either raw form or in a spreadsheet format based on user-supplied criteria. Data can also be visualized within a map interface to allow examination of biomass resource distribution based on scenario, year, and estimated biomass crop prices. The BILT model, released in November 2011, allows users to explore the biofuel supply chain for a state by displaying where biomass resources can be drawn from, sent for refining, and distributed for end use. The National Bioenergy Routing Model is a multimodal transportation model that provides an easy user interface for analysis of basic routing results for transporting biomass and bioenergy products.

In 2012, updates to the Bioenergy KDF will provide additional avenues for collaboration, new tools and models for web-based bioenergy analysis, and a subject matter expert database to connect researchers and experts from across the bioenergy research community.

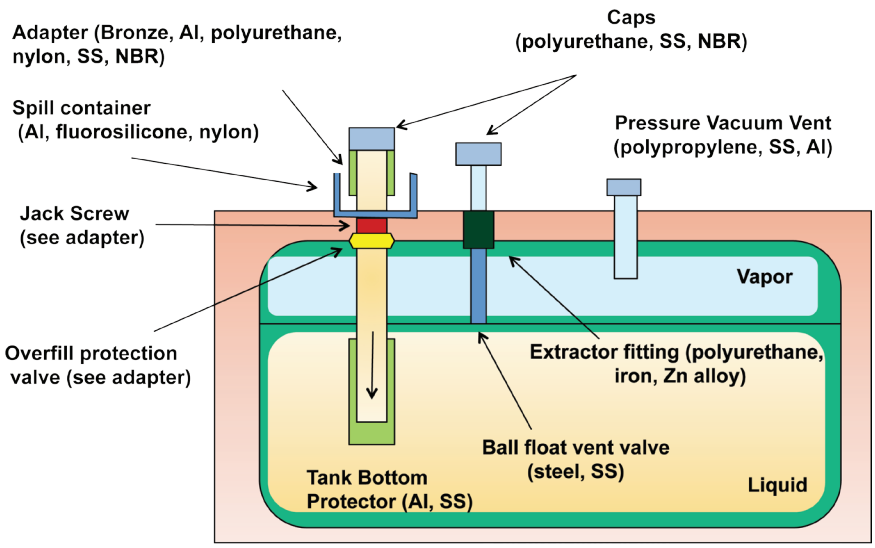
Ethanol Blends Materials Compatibility Study Released

ORNL, in collaboration with the National Renewable Energy Laboratory and Underwriters Laboratories, has been conducting a study of the compatibility of intermediate ethanol blends and automotive fuel dispenser materials. The first report on project results was released in 2011 to assist industry in assessing potential material compatibility issues, and to support development of new materials for fuel dispenser applications.

The study looked at the metals, elastomers, sealants, cork, and plastics that are used in the gasoline fueling infrastructure. Many of these systems have been in service for years and were not designed for ethanol concentrations greater than 10%. "Before E15, E20, or intermediate blends of gasoline with higher levels of ethanol are introduced into the nation's fueling infrastructure, their effects on the fueling infrastructure must be determined," said Mike Kass of the ORNL Energy and Transportation Science Division. To do this, Kass explained, the team conducts controlled tests under accelerated conditions to determine potential damage over a lifetime of component use in ethanol-blended gasoline. Previous efforts centered on intermediate ethanol levels ranging from 10 to 25% ethanol, while recent activities have focused on blends of 50 and and 85% ethanol.

During the project, ORNL developed a unique stir tank facility to expose material samples to various test fuels, allowing many materials to be screened in a relatively short time. The test tanks are sealed, held at elevated temperature, and continuously stirred for 4–16 weeks. Some of the samples are immersed in the test fluid, while others are tested in the vapor space to determine whether the fuel vapors are also damaging to the materials. Samples are removed periodically and analyzed for corrosion, sealability, durability, and leakage.

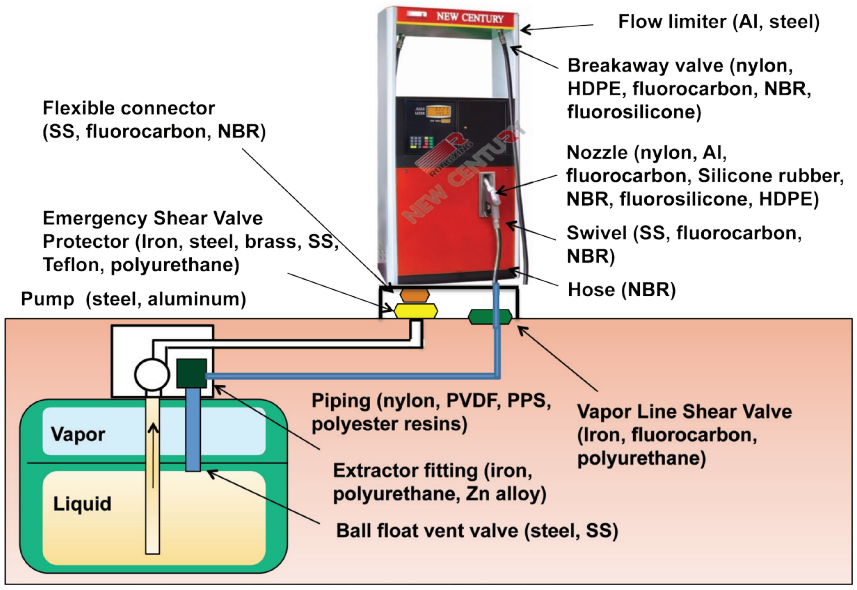
Typical Components and Materials from Truck to Tank



The results showed metals exhibited little to no measureable corrosion in intermediate blend fuels. Different classes of elastomer materials (fluorocarbons, and so forth) exhibited generally consistent behavior, with some showing very little change when exposed to intermediate ethanol blends and others changing substantially. The researchers found that newer sealants passed the leakage tests; older sealants not designed for ethanol did not. Study results for plastics and cork are still pending and will be reported when available.

This information will play a critical role in designing new infrastructure systems to handle intermediate levels of ethanol-blended gasoline. In addition, according to Kass, the data will help to advance development of adequate retrofit kits for existing infrastructure, which will enable higher levels of ethanol to be sold.

Typical Components and Materials from Tank to Nozzle



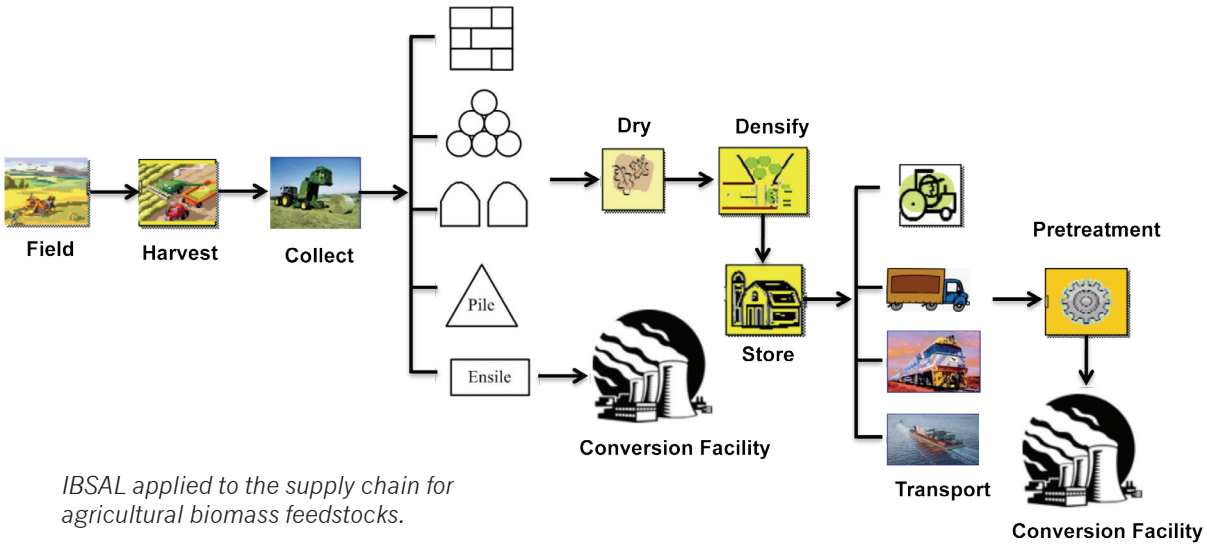
Publications

- Kass, M. J., T. J. Theiss, C. J. Janke, S. J. Pawel, and S. A. Lewis. 2011. *Intermediate Ethanol Blends Infrastructure Materials Compatibility Study: Elastomers, Metals, and Sealants.* ORNL/TM-2010/326. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Biomass Supply Chain Modeling and Analysis

A key challenge in achieving U.S. energy independence goals is synchronizing all the steps in the biomass-to-biofuels supply chain. Integrated analysis of the entire supply chain is needed to identify bottlenecks and alleviate them before major costs are incurred. ORNL took a major step in this direction this year with the release of a new version of its Integrated Biomass Supply Analysis and Logistics Model (IBSAL). Originally released in 2008, IBSAL simulates the flow of biomass through collection, transport, storage, and preprocessing and estimates energy consumption and costs. The new version, IBSAL-MC (MC stands for multi-crop), is a hybrid push-pull model. The farm side of operations pushes biomass during a harvest season to ensure all available biomass is collected. The conversion side pulls adequate feedstock to meet biorefinery needs at the other end. The multi-crop feature of the model ensures that the push and pull requirements are met from every available cellulosic biomass feedstock that meets a biorefinery's specifications.

Unlike conventional models used to analyze the cost of logistics, IBSAL considers conditions such as changes in moisture due to rain or snow; crop maturity; and potential losses of dry matter during field operations or in storage. IBSAL uses core functions and specific data to create unique logistics modules for different crop types and biomass growing regions. The model also calculates energy inputs



IBSAL applied to the supply chain for agricultural biomass feedstocks.

and carbon emissions to identify ways to minimize the environmental impacts of bioenergy feedstock supply chains. These capabilities make IBSAL a unique tool for minimizing risks associated with the flow of high-quality, cost-effective feedstock to a biorefinery.

In a recent application, the model was used to simulate a proposed cellulosic ethanol plant requiring 750 dry metric tons of straw per day to produce 70 ML of ethanol per year. The model showed that despite the abundance of straw in the region—more than 5 times the annual demand of the plant—the daily demand of the plant would be fully met for only 104 days. Only 92% of the total annual demand would be met. Approximately 530 farms were required within a radius of 64 miles to meet the daily demand of 750 tons. Several managerial insights were given to improve the biomass logistics system in terms of demand fulfillment, logistics costs, and resource utilization, including reconfiguring on-farm and at-plant storage to increase daily demand fulfillment.

IBSAL can be accessed through the Bioenergy Knowledge Discovery Framework at www.bioenergykdf.net.

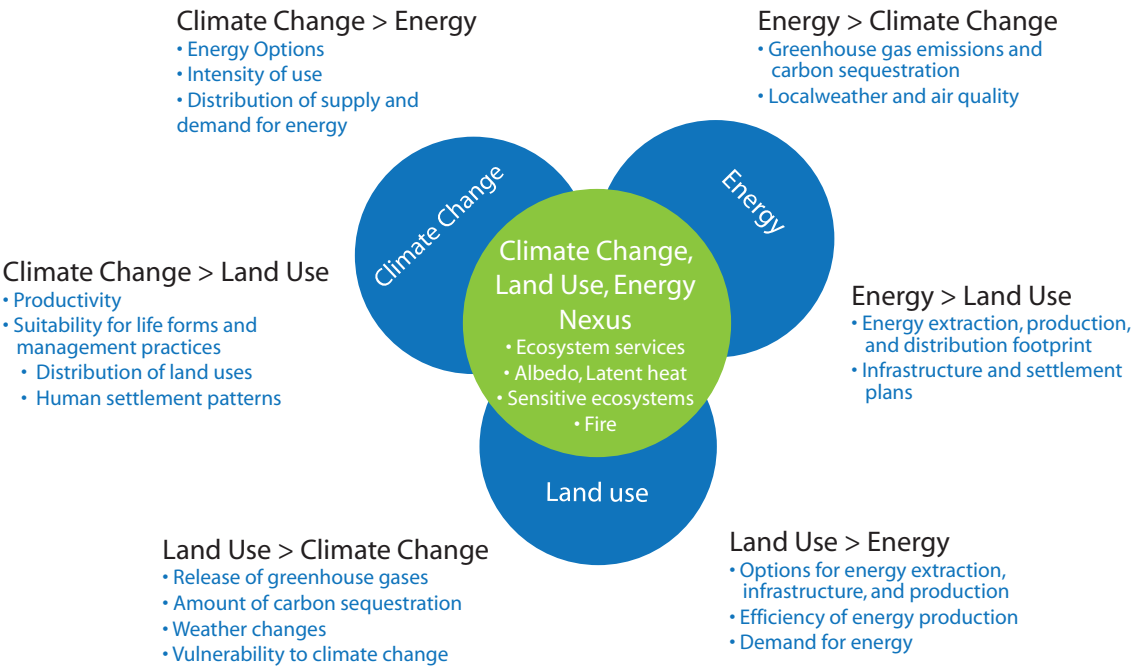
Publications

- Ebadian, Mahmood, Taraneh Sowlati, Shahab Sokhansanj, Mark Stumborg, and Lawrence Townley-Smith. November 2011. "A new simulation model for multi-agricultural biomass logistics system in bioenergy production." *Biosystems Engineering* 110(3):280–290.

Sustainability of Biomass Production

Concerns about the social, economic, and environmental impacts of ambitious goals to displace large portions of petroleum and other traditional sources of energy with biofuels/bioenergy in a relatively short time are not unique to the United States; similar concerns have been raised in other countries that have other goals, potential feedstocks, and cropping and conversion systems. A worldwide need exists for high quality data on the impacts and sustainability of biofeedstock production and for comprehensive analyses of the production, use, and sustainability of biofuels. The ORNL Center for BioEnergy Sustainability (CBES), a leading resource for dealing with the environmental impacts and ultimate sustainability of biomass production for conversion to biofuels and bio-based products, provides those data and analyses—not just for the burgeoning U.S. bioenergy industry but, through global partnerships and outreach, for the entire world.

In 2011, CBES research focused on issues related to land-use change and how to define and measure characteristics of bioenergy sustainability. A cross-disciplinary CBES team identified a suite of 19 indicators in 6 categories that can be used to characterize the environmental sustainability of bioenergy systems. The suite is intended to be a practical toolset for characterizing key environmental effects of a range of bioenergy systems, including different pathways, locations, and management practices. In other research, the landscape implications of bioenergy feedstock choices were shown to be significant and to depend on site-



Relationships among energy, land use, and climate change. Arrows indicate influence of one factor on another.

specific land use practices and their environmental impacts. Although land-use changes and carbon emissions associated with bioenergy feedstock production are dynamic and complicated, lignocellulosic feedstocks offer opportunities that enhance sustainability when compared to other transportation fuel alternatives. Furthermore, contrary to concerns that have been raised about land-use change and diversion of corn exports because of ethanol production in the United States, a decomposition analysis of the empirical data on the sources of corn found little support for the argument that either of those phenomena played a significant role as U.S. ethanol production increased over the past decade. This and related research highlighted the need for additional scientific analysis to correct key assumptions and support more realistic modeling of land-use change compared to current efforts. Finally, research demonstrated how tightly land use, climate change, and energy choices are linked, something previous studies have failed to address in an integrated fashion. For the future, decision makers will need integrated approaches that consider all of these elements and their interactions, as well as other anthropogenic forces, when making policy decisions.

Publications

- Dale, V.H., R. A. Efroymson, and K. L. Kline. 2011. "The land use – climate change – energy nexus." *Landscape Ecology* 26(6):755–773.
- McBride, A. C., V. H. Dale, L. Baskaran, M. Downing, L. Eaton, R. A. Efroymson, C. Garten, K. L. Kline, H. Jager, P. Mulholland, E. Parish, P. Schweizer, and J. Storey. 2011. "Indicators to support environmental sustainability of bioenergy systems." *Ecological Indicators* 11(5):1277–1289.
- Oladosu, G. A., K. Kline, R. Martinez and L. Eaton. 2011. "Sources of Corn for Ethanol Production in the United States: A Review and Decomposition Analysis of the Empirical Data." *Biofuels, Bioprod. Bioref.* 5:640–653.

Department of Transportation

R&D

Wireless Roadside Inspection

Fuel Tax Evasion Detection System

Intelligent Transportation Systems Deployment Survey

New Method for Estimating Fuel Economy by Vehicle Class

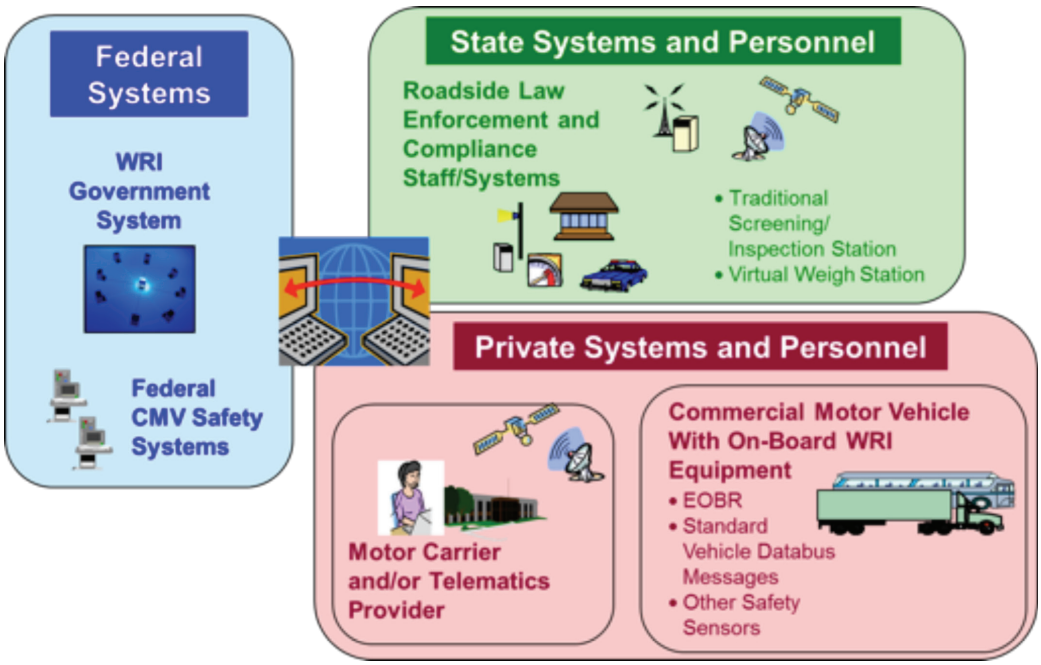
Smart Roadside Initiative for Commercial Vehicle Operations—Wireless Roadside Inspection

In early 2011 ORNL successfully completed phase 2 of the Wireless Roadside Inspection (WRI) Program, the WRI Pilot Test. WRI is part of the Federal Motor Carrier Safety Administration (FMCSA) Smart Roadside Initiative, whose goal is to leverage technology to create an environment in which information can be shared among the various parts of the transportation system (commercial vehicles, motor carriers, enforcement resources, highway facilities, and so forth) to improve motor carrier safety, security, operational efficiency, and freight mobility.

Each year both the number of commercial vehicles on the road and the number of miles they travel increase, but inspection resources tend to remain constant and in some cases have actually decreased. WRI holds the promise of increased inspections—including on the fly—and thus greater safety for everyone on our nation's roadways.

The goal of the pilot test was to determine the viability and effectiveness of wireless commercial motor vehicle inspections using current telematics techniques and systems. Additionally, the pilot was used to further refine the WRI concept of operations and the WRI systems architecture. An important part of the pilot was establishing gratis partnerships with commercial carriers, commercial motor vehicle and safety sensor technology manufacturers, and telematics service providers.

During the pilot test, safety data messag-



Wireless roadside inspection system overview.

es, which included vehicle identification information, driver identification information, and driver status information, were successfully transmitted to a government back office system using commercial mobile radio services, demonstrating end-to-end system functionality. During the pilot, 1,200 safety data messages were successfully transmitted in real time, many of them from vehicles traveling at highway speeds. As a follow-on to this effort, FMCSA has tasked ORNL with conducting a Field Operational Test that will include a complete end-to-end system with multiple fleets, multiple vehicles, and multiple technology partners, leveraging what was accomplished in the pilot test and similar projects at ORNL to streamline the complexity of the effort and explore and abate risk areas.

The Field Operational Test total system scope (consisting of partners, hardware, software, and vehicles) is small enough to be manageable but large enough (1,000 vehicles) to yield statistically meaningful test data that will answer the go/no-go question for the deployment of the WRI system nationally.

Publications

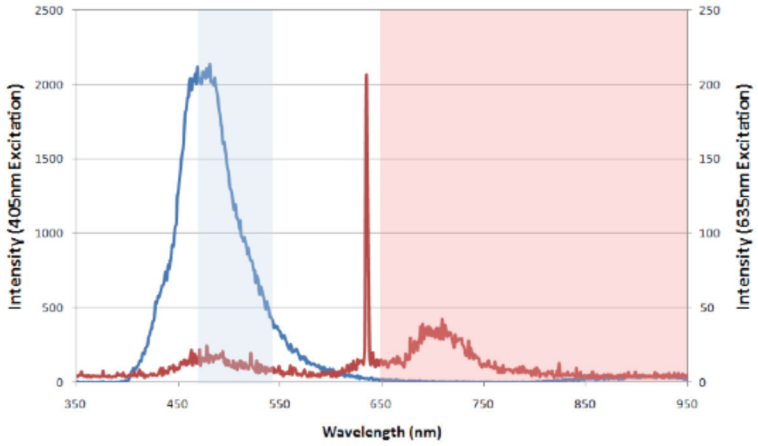
- Franzese, O., et al. 2011. *Wireless Roadside Inspection Phase II Tennessee WRI CMRS Pilot Test Final Report.* ORNL/TM-2012/40, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Development of a Supply Chain–Based Fuel Tax Evasion Detection System

A multidisciplinary team at ORNL has successfully completed proof of concept testing of a novel system to detect fuel tax evasion.

Fuel taxes provide the major source of funding for the U.S. highway system. While ensuring that motor fuel and other highway use taxes are properly collected is a priority for the Federal Highway Administration (FHWA), the complexity of the fuel supply chain in the United States creates numerous opportunities to evade fuel taxes—amounting to $3 billion in lost revenues by one estimate[1]. Hence, FHWA sponsored an Exploratory Advanced Research Project at ORNL to provide a comprehensive system aimed at reducing or eliminating fuel tax evasion schemes involving fuel tanker trucks.

The approach taken by ORNL included a number of innovations such as integration of multiple measures tailored for specific diversion schemes, development and evaluation of chemical marking agents and in-line sensors to detect the presence and concentration of marked fuels, and integration of advances in sensor technology, data acquisition, wireless communications, vehicle tracking, and information analysis. In addition, because most existing approaches are reactive, one of the goals of the ORNL approach was to provide a system that would proactively monitor and determine the legitimacy of individual loads, offloads, and movements of petroleum products in near real time.

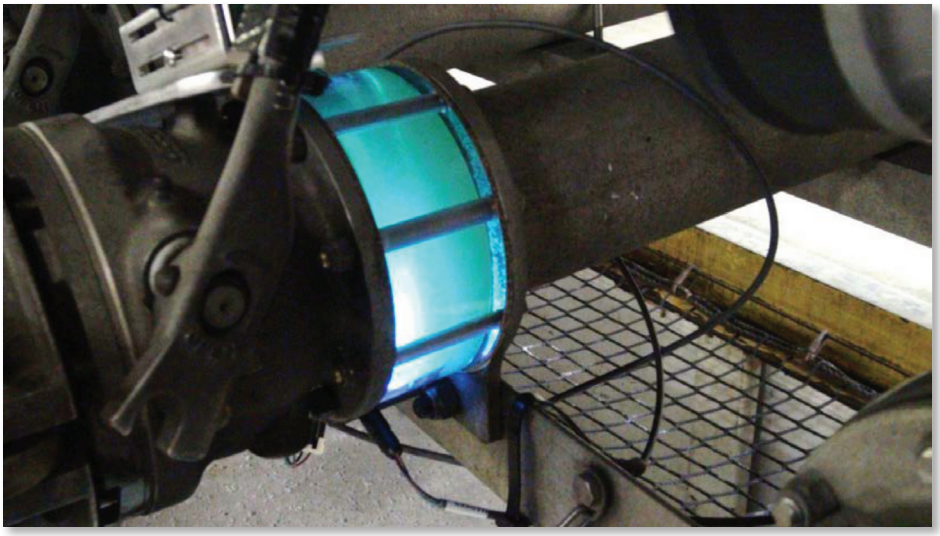


Spectral response of marked diesel at two different excitation wavelengths, 405 nm and 635 nm. The 405 nm peak is a natural by-product of diesel (marked or unmarked), while the 635 nm peak is a by-product of the custom marker. Measuring and dividing the intensity of the two peaks provides a self-referenced measurement of the marker concentration strength.

1 Garvey, Jane F. Statement to the U.S. House, Committee on Public Works and Transportation. *Shortfall in Highway Trust Fund Collection*. Hearing, August 10, 1994. Available at: testimony.ost.dot.gov/test/pasttest/94test/garvey3.pdf.

The prototype system includes

- a stable, ORNL-developed fuel marker, compatible with legacy fuels and engines, that can be detected in the parts-per-billion range;
- a suite of prototype fuel transport vehicle sensors to monitor, among other things, whether any of the access points to the trailer are opened;
- a communications system designed to collect sensor signals from the trailer (for example, fuel level, weight), convey the sensor signals wirelessly from the trailer to the tractor, receive sensor data from the trailer, condition and format the sensor signals for acceptance by the onboard computer, and be capable of sending data packets to a back office system for processing;
- an ORNL-developed intelligent geographical information system to facilitate near real time notification of suspicious variation in standard delivery processes, tracking the tanker as it travels to its destinations on the delivery route; and
- a control center designed to communicate with law enforcement personnel in a timely manner, enabling interdiction and investigation of potential fuel diversion activities on a real time basis.



Visible fluorescence during the excitation of the fuel marker.

Publications

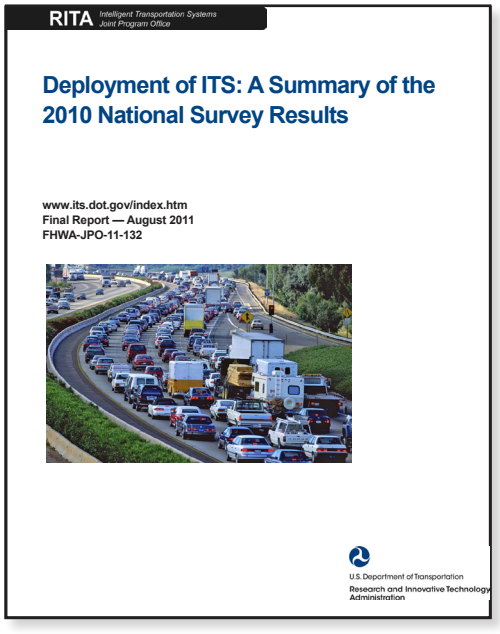
- Capps, G., et al. 2011. *Supply Chain–Based Solution to Prevent Fuel Tax Evasion: Proof of Concept Final Report.* ORNL/TM-2011/132, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

National Intelligent Transportation Systems Deployment Survey

For nearly 20 years, the U.S. Department of Transportation (DOT) has had an ambitious program to create a national infrastructure of intelligent transportation systems (ITS) technologies consisting of sensors to gather data on traffic conditions, media to disseminate traffic advisories to travelers, and systems to manage transit, incident management, and public safety. ORNL has been on board since the beginning, supporting management of the national ITS program by gathering, collating, and analyzing data; and helping disseminate the information. Starting in 1996, the DOT ITS Joint Program Office tasked ORNL to gather data on the status of ITS deployment in major cities and to analyze the data to track progress toward national goals.

Data are gathered through a series of surveys covering a variety of information on the extent and character of ITS deployment. The surveys cover nearly 2000 state and local agencies in 108 of the nation's largest cities. The data collected are used by DOT to manage the ITS program, to respond to Congressional inquiries, and to allocate federal grants to support ITS deployment. The Deployment Tracking Website (www.itsdeployment.its.dot.gov), created and maintained by ORNL, provides access to survey results as well as a national summary report of the latest results. The website is the only publicly available source for this type of information, serving as a resource for researchers, private vendors, other agencies, the general public, and decision makers.

The data from the most recent survey in 2010 reveal that the ITS program has moved from being experimental to mainstream, and interest in continuing investments in ITS technologies is very strong. When asked about near term deployment plans, most of the different agency types reported they will expand current deployments, and about half are planning to invest in new technologies. Other trends highlighted in the 2010 national summary report include:



- the almost total automation of toll collection, which has improved safety, mobility, and accuracy while reducing costs;
- the growth of real-time data collection through traffic sensors and cameras, allowing agencies to provide real-time traffic advisories and take a more active role in traffic management;
- technical advances that support proactive control of traffic through mechanisms like managed lanes, ramp metering, and adaptive traffic signals;
- migration of traveler information from infrastructure systems such as radio and dynamic message signs to personalized messaging through mobile devices and social media.

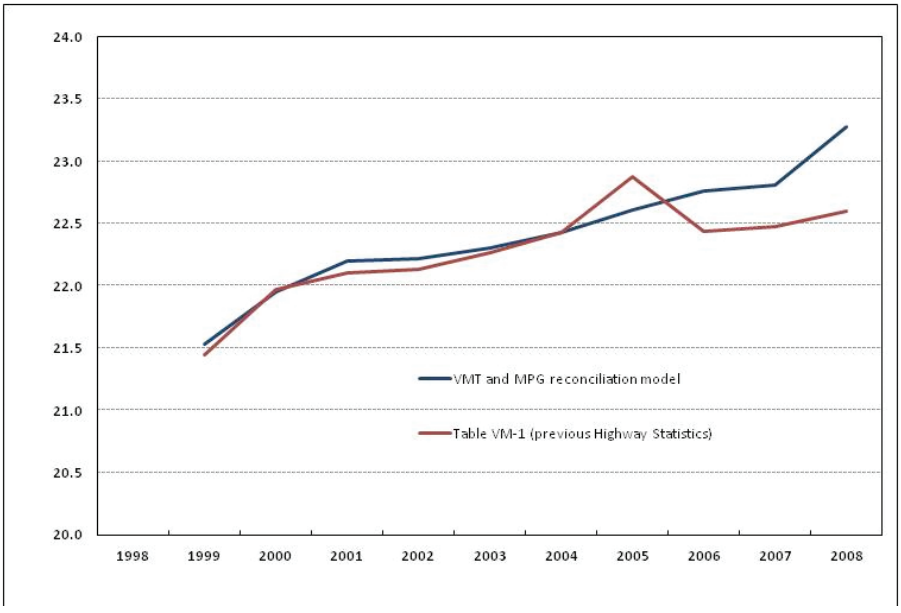
Publications

- Gordon, Steve, and Jeff Trombly. 2011. *Deployment of ITS: A Summary of the 2010 National Survey Results*. FHWA-JPO-11-132, ITS Joint Program Office, Research and Innovative Technology Administration, U.S. Department of Transportation, Washington, D. C.

New Method for Estimating Fuel Economy by Vehicle Class

ORNL was tasked by the Federal Highway Administration (FHWA) Office of Highway Policy Information to develop a new method to generate annual, national estimates of average fuel economy (in terms of mpg) and number of vehicles registered by vehicle class for the annual publication *Highway Statistics*. The data published in *Highway Statistics* is used by all levels of government to assess the performance of the U.S. highway transportation system, and to identify future highway system options. The data are extensively used by federal, state, and local agencies; academia; industry; consultants; professional organizations; and the public for a host of purposes.

The goal of the new methodology is to ensure that the statistics on total vehicle miles traveled, number of vehicles, and total fuel consumption are consistent and reasonable. It takes a two-step approach. First, fleet fuel economy by vehicle class is estimated based on vehicle stock models[1]. Then a reconciliation model is used to adjust the initial estimates from the vehicle stock models and match vehicle miles traveled information and total fuel consumption. This reconciliation model uses a systematic approach that produces documentable and reproducible results. The basic framework is based on a mathematical programming formula to minimize the deviations between the



For 1998–2003, passenger vehicle fuel economy results from the reconciliation model are similar to those published in Table VM-1 of ***Highway Statistics****. Since 2004, passenger vehicle fuel economy results from the reconciliation model show less variation than those published in Table VM-1.*

1 Vehicle stock models, also known as vehicle fleet models, are econometric models used by transportation analysts and traffic engineers to estimate and forecast policy impacts related to overall fleet performance.

fuel economy estimates published in the previous year's *Highway Statistics* and the results from the vehicle stock models, subject to the constraint that fuel consumption for different vehicle classes must sum to the total fuel consumption estimate in the current year's *Highway Statistics.*

For ease of use, the new method was implemented in a Microsoft Office 2007 Excel-based computer program with a simple user interface designed using macros. A "solver" was built into the program to allow "one click" model runs.

The results generated by this new methodology compare favorably with previous numbers generated manually and with industry trends; however, the method provides a smoother time series for the fuel economies by vehicle class. It also has the advantage that it uses the most up-to-date and best available data with sound econometric models. Further, the formula used in the reconciliation model will enable a relatively smooth transition from FHWA's current procedure to the new method, avoiding a "kink" in the statistics in the year the transition is made.

Publications

• Chin, S.-M., K. Dabbs and H.-L. Hwang. 2011. "New Methodology for Estimating Fuel Economy by Vehicle Class." Presented at the Transportation Research Board 90th Annual Meeting, Washington, D.C., January 23–27.

Hydrogen and Fuel Cell Technologies

R&D

Reducing the Production Cost of High Strength Carbon Fibers for Storage

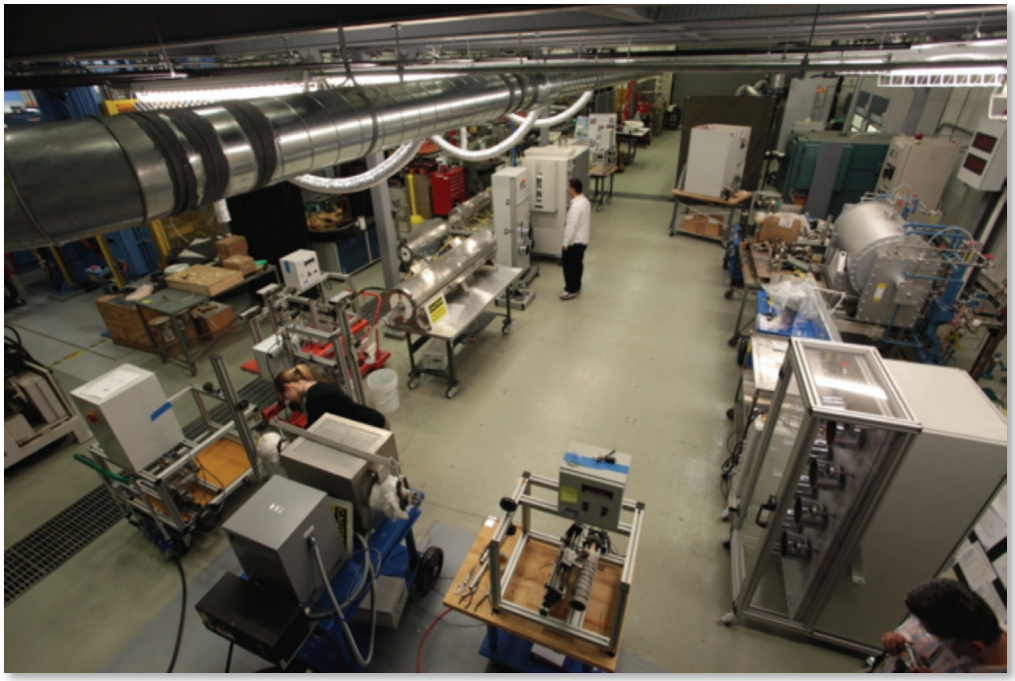
Investigating Aging and Associated Degradation of Membrane Electrode Assemblies

Vessel Design and Fabrication Technology for Stationary Hydrogen Storage

Reducing the Production Cost of High Strength Carbon Fibers for Hydrogen Storage

ORNL is investigating new precursor materials and production processes to yield lower cost high-strength fibers. Because of its remarkable strength-to-weight ratio and damage tolerance, high strength carbon fiber is the material of choice for durable, lightweight storage vessels for high pressure gas in both vehicular and stationary storage applications. However, these storage vessels are expensive, and carbon fiber is the reason. Between 40% and 70% of the storage vessel cost is for the carbon fiber (the precursor material accounts for about 40-60%). The conventional precursor for high strength carbon fibers is solution spun polyacrylonitrile (PAN). Melt spun PAN, if successful, will be much cheaper because it has fewer process steps and there is no cost for solvent or solvent operations; however, it is technically far more challenging.

Until specific cost and property targets for compressed hydrogen storage are established, the goal is a 24K tow with700 Ksi ultimate tensile strength, and 33 Msi tensile modulus fiber with a 25% reduction in cost. To date, the ORNL team has successfully prepared and characterized acrylonitrile copolymers, including those with methyl acrylate, in controlled molecular weights. The team has also demonstrated the generation of melt spun PAN using only modified water as a plasticizer



ORNL's highly versatile, modular precursor and fiber evaluation system capable of processing fibers in tow counts from 20 to more than 50,000 filaments.

(no solvents) and produced melt spun PAN precursor fibers with the desired denier (10 to 20 µm in diameter) using a one-step spinning/drawing process.

Converting precursor fibers into carbon fibers is normally accomplished by time- and energy-intensive thermal treatment. The project team is investigating revolutionary new processing methods that could potentially deliver higher line speeds with lower energy use and costs. The team is also establishing a modular carbon fiber research pilot line to evaluate these processes against conventional industrial processes using a conventional pilot line for benchmarking advanced technologies. In the near future, an advanced technology pilot line will be assembled to demonstrate that the advanced process modules work together as a functional system and to perform system optimization. Advanced carbon fiber conversion processes would not only increase production but also significantly reduce the required capital investment and energy demand per unit of output, potentially reducing cost by half, and expanding U.S. competitiveness into the manufacturing of higher strength carbon fibers.

Publications

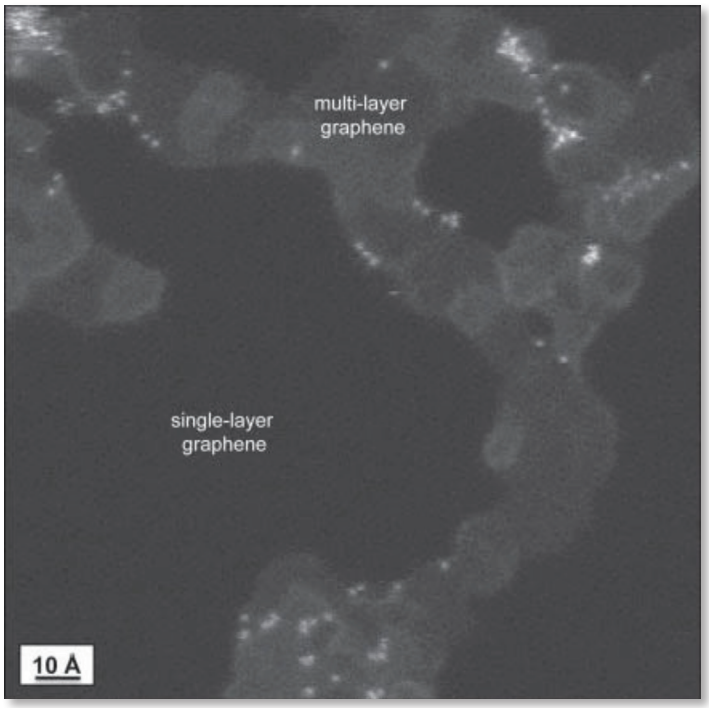
- Paulauskas, F. L. 2011. "Melt Processable PAN Precursor for High Strength, Low-Cost Carbon Fibers." Presented at the Hydrogen and Fuel Cells Program 2011 Annual Merit Review and Peer Evaluation, Arlington, Virginia, May 9–13. Available at www.hydrogen.energy.gov/pdfs/review11/st093_paulauskas_2011_o.pdf.

- Paulauskas, F. L. 2011. "Development of Low- Cost, High Strength Commercial Textile Precursor (PAN-MA)." Presented at the Hydrogen and Fuel Cells Program 2011 Annual Merit Review and Peer Evaluation, Arlington, Virginia, May 9–13. Available at www.hydrogen.energy.gov/pdfs/review11/st099_warren_2011_p.pdf.

Investigating Aging and Associated Degradation of Membrane Electrode Assemblies for Proton Exchange Membrane Fuel Cells

To reach DOE's technical targets for membrane electrode assemblies (MEAs), ORNL is leading a multiorganization effort to characterize the microstructures of MEA materials. ORNL's approach involves using advanced microscopy techniques and establishing collaborations with leading researchers in the field. Researchers are able to apply knowledge gained on this project to optimize the design and manufacture of fuel cell materials and assemblies.

Proton exchange membrane fuel cells (PEMFCs) are of interest as efficient, zero-emission power sources for vehicles. The performance of PEMFCs degrades during use, and this degradation can be directly correlated with the durability of the individual material components that make up the PEMFC MEAs. However, many of the microstructural and compositional attributes that contribute to decreased stability of the MEA during long-term use are not fully understood



Z-contrast scanning transmission electron microscopy image showing graphene sheet (single- and multi-layered) with individual Pt atoms (brightly imaging) deposited on surface. Note that all the Pt atoms deposit preferentially at the edge sites (or steps where graphene layers overlap) and not on sites associated with the sp^2-bonded flat (002) surfaces.

and must be directly correlated with performance as a function of aging protocols in order to identify mitigating strategies and improve fuel cell lifetimes.

ORNL is using advanced microstructural and microchemical analysis techniques to characterize as-processed and electrochemically aged MEAs. These techniques, which include high-resolution scanning, transmission, and analytical electron microscopy, are being used to evaluate structural changes and degradation phenomena under load. Large areas of extremely thin (less than 50 nm), fully intact MEAs, prepared for transmission electron microscopy, have allowed team scientists to quantitatively characterize the atomic-scale structural and chemical changes within the proton exchange membrane and electrodes. Furthermore, individual constituents and their assemblages within the electrodes (carbon-based support, ionomer, electrocatalyst particles, and interfaces between the electrode and membrane) are continually being evaluated, pre- and post-aging. This microstructural evaluation of MEAs is enabling significant stability and performance improvements, and is invaluable for identifying the mechanisms contributing to MEA degradation and/or failure.

To more fully elucidate the role of catalyst-support interactions on long-term stability during aging, a collaboration has recently been established with Nissan Technical Center to evaluate platinum (Pt) catalysts (in terms of dispersion, size, and morphology) deposited on a series of carbon supports exhibiting varying degrees of graphitization. In addition, ORNL has initiated a fundamental study of Pt deposition on model carbon substrates (single-layer graphene) to understand Pt nucleation and growth mechanisms on extended graphitic surfaces. These studies are focused on identifying critical bonding, chemical, and structural factors that contribute to catalyst degradation/stability during aging.

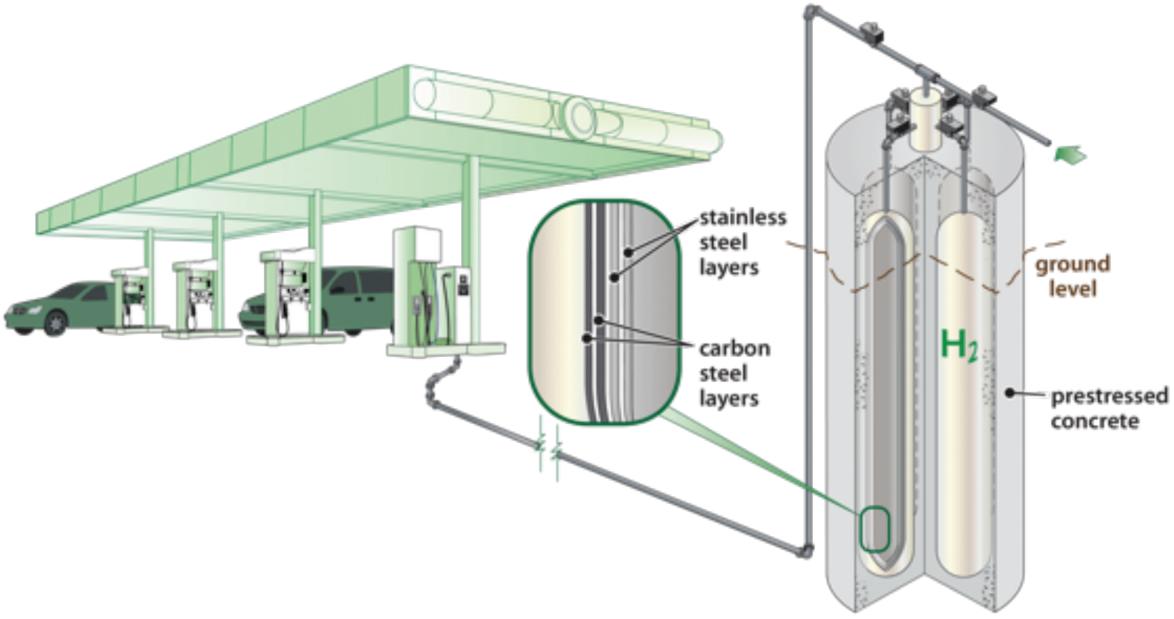
Publications

- Wang, C., et al. 2011. "Correlation Between Surface Chemistry and Electrocatalytic Properties of Monodisperse Pt_xNi_{1-x} Nanoparticles." *Advanced Functional Materials* 21(1):147–152.
- Wu, G., K. L. More, and P. Zelenay. 2011. "High-Performance Electrocatalysts for Oxygen Reduction Derived from Polyaniline, Iron, and Cobalt." *Science* 332:443–447.

Vessel Design and Fabrication Technology for Stationary High-Pressure Hydrogen Storage

ORNL has successfully completed the first year of a multiyear project to develop a stationary hydrogen storage system, and is on target to meet the DOE cost goal for off-board bulk storage. Stationary hydrogen storage is a critical element in the overall hydrogen production and delivery infrastructure. In this project, ORNL leads a multidisciplinary team consisting of government, industry, and academia to develop and demonstrate design and fabrication technologies for an integrated steel and concrete high-pressure hydrogen storage vessel that is cost effective and scalable. The integrated approach will enable

- a systematic, integrated design to mitigate hydrogen embrittlement associated with the use of high-strength steel for high-pressure hydrogen storage,
- cost-effective structural materials,
- high-productivity, low-cost fabrication technologies, and
- embedded sensors to ensure the safe and reliable operation of the storage system.



Schematic drawing of ORNL's innovative composite vessel for safe and cost-effective storage of high-pressure hydrogen.

The size and volume of stationary hydrogen storage vessels are expected to vary considerably depending on intended use, location, and other economic and logistic considerations. For instance, a storage vessel at a renewable energy generation site may have a lower pressure but much larger volume compared to one at a refueling station. Therefore, it is important that vessel design is scalable for different sizes and pressures.

This project demonstrated that the preliminary engineering design of an inner-layered steel vessel can sustain 5,000 psi pressure based on the relevant American Society of Mechanical Engineers Boiler and Pressure Vessel code. The preliminary designs for an outer prestressed concrete vessel and the steel-concrete interface were also completed. Detailed design and engineering analyses (including system cost), mockup vessel construction, and testing and demonstration are ongoing or planned. In addition to meeting the technical challenges, all aspects of the project will be optimized to meet or exceed the DOE capital cost goal of $300/kg hydrogen by the year 2015 (note: this goal is under revision at the time of publication).

Publications

- Feng, Z., J. Wang, and W. Zhang. 2011. "Vessel Design and Fabrication Technology for Stationary High-Pressure Hydrogen Storage." Presented at the Hydrogen and Fuel Cells Program 2011 Annual Merit Review and Peer Evaluation, Arlington, Virginia, May 9–13. Available at www.hydrogen.energy.gov/pdfs/review11/pd088_zhang_2011_o.pdf

Vehicle Technologies

R&D

Policy Analysis

Combustion Engines

Energy Storage

Fuels

High Temperature Materials Laboratory

Lightweight Materials

Propulsion System Materials

Power Electronics & Electric Machines

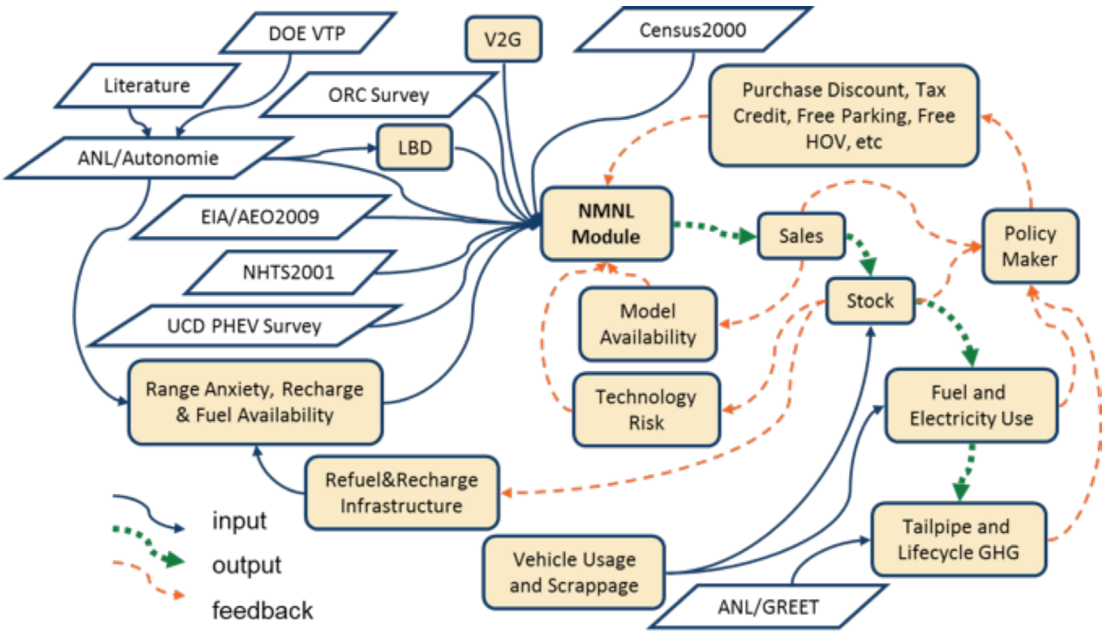
Vehicle & Systems Simulation & Integration

Policy Analysis

Modeling the Market Acceptance of Advanced Automotive Technologies

Understanding the diverse purchasing behaviors among individuals is crucial for designing effective policies to promote advanced vehicle technologies. To address this need, ORNL developed a market simulation model called Market Acceptance of Advanced Automotive Technologies (MA^{3}T). Implemented using Microsoft Excel for Windows, MA^{3}T simulates market demand for advanced vehicle technologies by representing attributes such as technological learning by doing, range anxiety, access to recharging points, daily driving patterns, and willingness to accept technological innovation. Much remains to be learned about how consumers will evaluate novel vehicle technologies and how these vehicles are likely to be operated. Because of this, the approach taken in developing MA^{3}T was to create a framework for integrating data and behavioral models at an appropriate level of detail, whether or not the data are fully available or the behaviors fully understood. As more is learned about advanced vehicle technologies and consumer preferences toward them, the model will be updated and improved.

Characteristics distinguishing MA^{3}T from other vehicle market models are technology richness, detailed consumer segmentation, market dynamics, daily distance distribution, and range-infrastructure characterization. MA^{3}T includes



MA3T model framework.

40 choices consisting of 20 powertrain technologies for each of 2 vehicle size classes: passenger cars and light duty trucks. MA^{3}T considers U.S. household users of these vehicles as the consumer market, which is disaggregated into 1,458 segments based on 6 dimensions: census divisions, residential areas, attitudes toward novel technologies, driving patterns, home recharging situations, and work recharging situations. MA^{3}T projections cover the period from 2005 to 2050 and capture the temporal interaction between market penetrations and product diversity and risk. MA^{3}T characterizes daily driving distance variation with the Gamma distribution, validated with real-world high-resolution travel data. MA^{3}T explicitly quantifies range anxiety for electric vehicles and reflects the effect of charging and refueling infrastructure on the appeal of plug-in electric vehicles and alternative fuel vehicles.

The core of the model is a nested multinomial logit method that predicts purchase probabilities among the 40 choices by each of the consumer segments based on value components associated with vehicle attributes, user behavior, infrastructure, energy prices, and policies. The purchase probabilities are translated into market penetrations, sales, populations, petroleum use, and greenhouse gas emissions. Some of the outputs serve as feedback signals and, together with exogenous inputs from various sources, affect the purchase probabilities.

Publications

- Lin, Zhenhong, Jing Dong, Changzheng Liu, and David Greene. 2011. "PHEV Energy Use Estimation: Validating the Gamma Distribution for Representing the Random Daily Driving Distance." *Transportation Research Record: Journal of the Transportation Research Board* (forthcoming).

- Lin, Zhenhong, and David L. Greene. 2011. "Assessing Energy Impact of Plug-In Hybrid Electric Vehicles: Significance of Daily Distance Variation over Time and among Drivers." *Transportation Research Record: Journal of the Transportation Research Board* 2252:99–106.

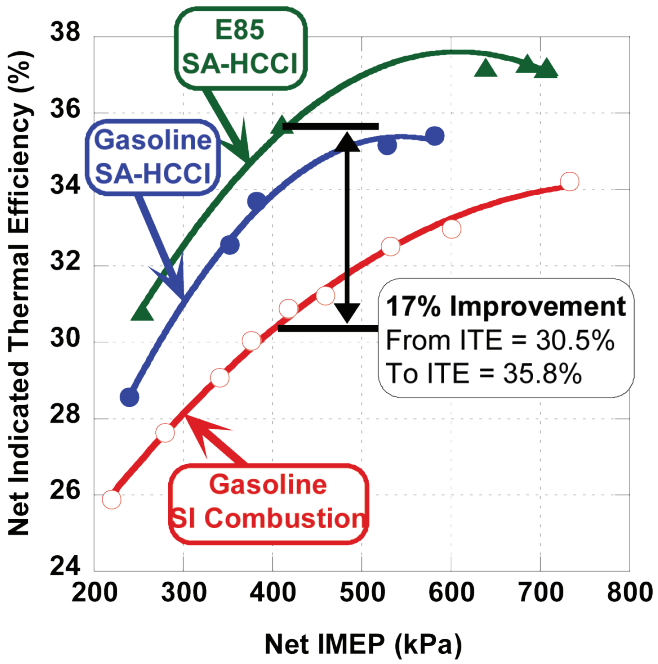
- Lin, Zhenhong, and David Greene. 2010. "Who Will More Likely Buy PHEV: A Detailed Market Segmentation Analysis." Presented at the 25th World Battery, Hybrid and Fuel Cell Electric Vehicle Symposium & Exhibition, Shenzhen, China, November 5–9.

Combustion Engines

Spark Assisted Stoichiometric HCCI with E85, a Potential Path to Higher Efficiency Engines

ORNL researchers have developed an engine combustion strategy that demonstrates a 17% increase in engine indicated thermal efficiency, relative to conventional spark ignited (SI) combustion with gasoline, by using E85 (a blend of 85% ethanol, 15% gasoline) under advanced mixed-mode combustion conditions. Efficiency improvements were achieved over a wide range in load, making them applicable over a large portion of the engine map.
The advanced combustion strategy uses mixed-mode combustion to take advantage of the desirable characteristics of conventional SI combustion and homogeneous charge compression ignition (HCCI). Combustion of a dilute fuel-air mixture is initiated with a spark, consuming up to 40% of the fuel, and the remaining fuel is consumed rapidly in a manner similar to HCCI. As a result, the combustion strategy has been named spark assisted HCCI (SA-HCCI).

HCCI achieves greater fuel efficiency than conventional SI combustion because of unthrottled operation and rapid combustion; however, the process is difficult to control. The spark assist provides enhanced



Net indicated thermal efficiency at 2,000 rpm as a function of net IMEP for conventional SI combustion with gasoline and SA-HCCI combustion with gasoline and E85.

control of combustion and an expanded operational load range. HCCI studies typically report a maximum load of about 4.0 bar net indicated mean effective pressure (IMEP), whereas SA-HCCI can be operated at up to 7.0 bar net IMEP with E85. As a result, the efficiency benefits of SA-HCCI can be realized over a larger portion of the engine map. Greater control over the HCCI combustion process enables stoichiometric operation and thus greater compatibility with emissions control devices.

This advanced combustion strategy was tested with E85, gasoline, and a blend of iso-butanol and gasoline. It was found that E85 produces higher indicated thermal efficiency and higher maximum net IMEP. Thus, this ORNL-developed SA-HCCI process holds the promise not only of improved performance, but also of greater use of alternative fuels.

Publications

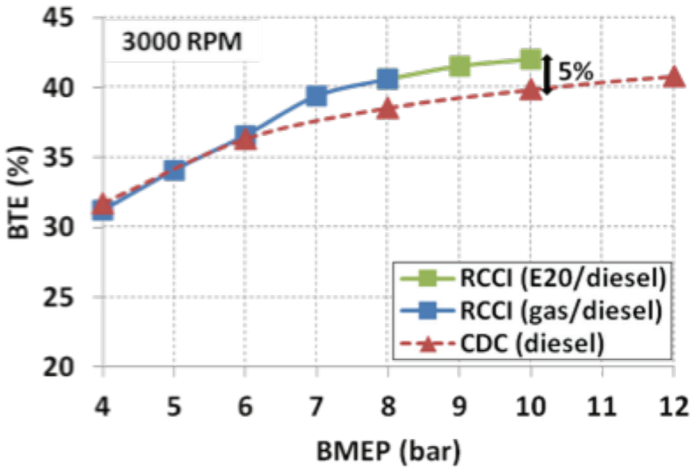
- Weall, Adam J., and James P Szybist. 2011. "The Effects of Fuel Characteristics on Stoichiometric Spark-assisted HCCI." Technical Paper ICEF2011.60122. *ASME Conf. Proc. 2011*, pp. 243–259.

Dual-Fuel RCCI Combustion Enables Efficiency Improvements with Lower NO_x Emissions

ORNL researchers are teaming with universities and major automotive parts manufacturers to evaluate real-world challenges and opportunities of reactivity controlled compression ignition (RCCI). RCCI combustion, a variant of homogeneous charge compression ignition, makes use of in-cylinder blending of two fuels with different reactivities for improved control of the combustion process. The less reactive fuel (for example, gasoline or ethanol with diesel) slows the reaction and lessens the chance for autoignition. While this approach has been shown in simulations and single-cylinder engine experiments to have the potential for high efficiencies and very low nitrogen oxide (NO_x) and particulate matter (PM) emissions, this project is among the first to study the potential of this approach under near-real-world conditions.

The project employed a light duty multi-cylinder engine in experiments designed to bridge simulation and single-cylinder research engine progress to production-viable hardware. Results show that RCCI can reduce NO_x and PM emissions while achieving diesel-like or higher brake thermal efficiency—as much as 5% higher at higher loads. This potential was demonstrated across a wide range of steady-state operating points consistent with the light duty federal drive cycle.

The experiments explored fuel injection strategy, dilution levels, piston geometry including compression ratio, fuel properties, and emissions. NO_x emissions were up to 90% lower than in conventional diesel combustion; howev-



RCCI (blue) using gasoline and diesel compared with conventional diesel (red), showing up to 5% increase in brake thermal efficiency as engine load is increased at 3,000 rpm. The load expansion of RCCI with E20 (20% ethanol, 80% gasoline) is shown in green.

er, carbon monoxide and hydrocarbon emissions were much higher than in conventional diesel combustion and were more similar to levels seen in gasoline engines. The combination of high carbon monoxide and hydrocarbon emissions with low exhaust gas temperatures will be a significant challenge due to the limited effectiveness of current oxidation catalysts at low temperatures.

Other challenges for the multi-cylinder engine implementation included matching turbomachinery with high exhaust gas recirculation (EGR) and providing sufficient EGR cooling with production viable hardware. EGR, which can be challenging to implement, is important for additional control of in-cylinder pressure rise rates, combustion noise, and reactivity stratification at higher engine loads.

Various fuel blends were investigated, including ethanol-gasoline blends. The high octane and charge cooling effects of ethanol were found to have the benefit of expanding RCCI operation with reduced or no EGR. This effectively allows for operation at higher loads with better matching of turbomachinery and reduced heat rejection requirements, which are more consistent with production viable hardware.

The data are being used in combination with a vehicle model to estimate the drive-cycle fuel economy/emissions potential of RCCI operation.

Publications

- Curran, S., R. Hanson, and R. Wagner. *Effect of E85 on RCCI Performance and Emissions on a Multi-Cylinder Light-Duty Diesel Engine.* SAE Paper 2012-01-0376 (forthcoming).
- Wagner, R., et al. 2011. "Addressing the Challenges of RCCI Operation on a Light-Duty Multi-Cylinder Engine." Presented at the 2011 Directions in Engine-Efficiency and Emissions Research (DEER) Conference, Detroit, Michigan, October 3–6.

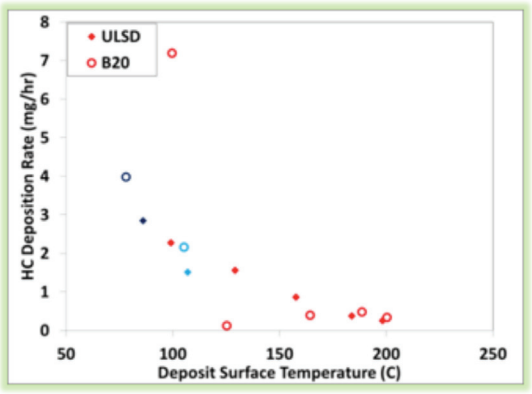
New Understanding of EGR Cooler Fouling Mechanisms Provides Information for Improving Designs

Scientists at ORNL and the University of Michigan are teaming with engineers from some of the leading diesel engine manufacturers to gain greater understanding of the processes involved in fouling of exhaust gas recirculation (EGR) coolers. EGR is a key aspect of many advanced combustion technologies and has become a mainstay for controlling emissions of nitrogen oxides (NO_x) from diesel engines. Typically this is at the expense of engine efficiency/fuel economy and increased levels of hydrocarbon (HC) and carbon monoxide emissions. This in turn can lead to fouling or failure of the EGR system.

Fouling of the EGR cooler by HCs and particulate matter (PM) from the exhaust gas stream can reduce the performance of the cooler in a matter of hours, causing the temperature of the EGR stream to rise, potentially producing higher NO_x emissions and changing the dynamics of the combustion process. Research has shown that under moderate engine loads and speeds the fouling process tends toward development of a frangible porous layer that is highly insulative. However, extended operation at low loads and speeds can result in a deposit layer that is less insulative because the void volume is substantially filled with condensed HCs. The increased thermal conductivity of the layer enables continued fouling at relatively high rates. High HC concentrations relative to the PM concentration in the gas stream, as is typical of advanced combustion processes, can increase the likelihood of this situation. Experience has shown that incidences of plugging in the field are most often associated with deposit layers high in HCs, which result in a less frangible deposit that can become cohesive enough to inhibit the EGR flow through the cooler.

Fouled EGR cooler after 200 h fouling test.

A key aspect of high rates of deposition of HCs relative to PM is the gas flow velocity through the cooler during low-temperature conditions. If the velocity is low compared to the maximum design velocity, deposition tends towards HC-dominated layers. Thus, applications that operate frequently at cold start, low-load, or idle conditions are much more likely to experience EGR cooler plugging, particularly if the EGR cooler design process focuses primarily on high-temperature conditions. Project team members are currently exploring design solutions to reduce the risk of plugging in these circumstances, including the use of an oxidation catalyst upstream of the cooler or multiple EGR coolers with one cooler sized and used for low-load conditions, and another sized for moderate- and high-demand conditions.



HC deposition rate versus temperature for 0.05 kg/min/tube EGR stream containing 100 ppm HCs.

Publications

- Sluder, C. Scott, John M. E. Storey, and Michael J. Lance. 2011. "Hydrocarbon and Deposit Morphology Effects on EGR Cooler Deposit Stability and Removal." Presented at the 2011 Directions in Engine Efficiency and Emissions Research (DEER) Conference, Detroit, Michigan, October 3–6.

- Storey, John M. E., et al. 2011 "Exhaust Gas Recirculation Cooler Fouling in Diesel Applications: Fundamental Studies, Deposit Properties, and Microstructure." *Proceedings of International Conference on Heat Exchanger Jouling and Cleaning - 2011,* edited by M.R. Malayeri, H. Müller-Steinhagen and A.P. Watkinson, 65-73.

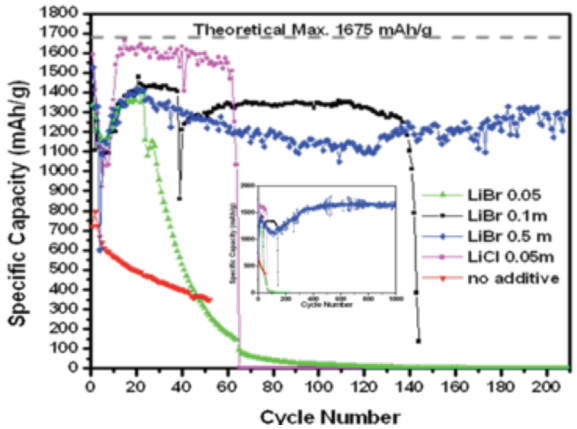
Energy Storage

Improving Lithium-Sulfur Battery Technology for Electric Vehicles

Significant market barriers for both plug-in hybrid electric vehicles (PHEVs) and electric vehicles (EVs) are technology cost and vehicle range. ORNL is conducting research and development on new battery technologies to address those barriers, enabling meaningful reductions in U.S. petroleum consumption.

Lithium-sulfur (Li-S) battery technology has significantly lower raw material costs and offers a much higher energy density (that is, provides longer vehicle range) than lithium ion batteries. The challenges for Li-S batteries are short cycle-life and poor efficiency.

Three key phenomena cause the short cycle-life of the Li-S batteries: the irreversible deposition of lithium sulfide (Li_2S) on the lithium anode through the intrinsic polysulfide shuttle, and Li_2S and sulfur on the cathode; and the formation of lithium dendrites. Earlier research revealed that these three obstacles could be overcome by using nanostructured sulfur-carbon composite cathodes with electrolyte additives. ORNL scientists devised a cell that achieved a cycle-life of 1,000 cycles with no indication of capacity decay. In spite of this dramatic improvement, the lithium bromide (LiBr) additive discovered at ORNL had significant drawbacks: the electrochemical intermediates of LiBr are highly corrosive and cause severe problems with the current collectors and other metal parts in the battery.



Cycle performance of Li-S batteries with and without electrolyte additives.

The incompatibility of LiBr with battery components is driving the search for alternative additives that do not corrode. There is an additional challenge in that the coulombic efficiency and the round-trip energy efficiency are very low for Li-S batteries unless the polysulfide shuttle is suppressed or eliminated and the electrochemical reversibility of Li_2S formation is improved. The ORNL team is investigating new materials that could improve both the energy efficiency and the cycle life of Li-S batteries by optimizing the structure of the sulfur-carbon composite to suppress the polysulfide shuttle, thereby improving the coulombic efficiency; exploring electrolyte additives that can reverse the formation of Li_2S; and protecting the lithium metal anode by solid electrolyte coating.

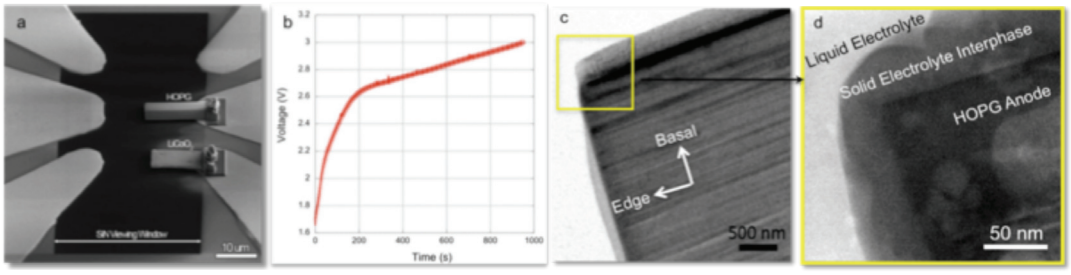
Publications

- Zengcai, L., W. Fu, and C. Liang. 2011. "Lithium Sulfur Batteries." In *Handbook of Battery Materials, Second Edition*, edited by Claus Daniel and Jürgen O. Besenhard, 811–840. Weinheim, Germany: Wiley-VCH Verlag GmbH & Co. KGaA.
- Liang, C. 2011. "Carbon/Sulfur Nanocomposites and Additives for High-Energy Lithium Sulfur Batteries." Presented at the 2011 Hydrogen Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting, Arlington, Virginia, May 9–13.
- Liang, C. 2011. "Advanced Materials for Li-S Batteries." Presented at the 4th Symposium on Energy Storage: Beyond Lithium Ion, Richland, Washington, June 7–9.

In Situ Electron Microscopy of Electrical Energy Storage Materials

ORNL has developed an electrochemical cell capable of performing in situ microscopy experiments. Before now, there were no high resolution electrochemical characterization techniques that can be used to directly observe dynamically evolving electrochemical reactions during charge/discharge cycling in volatile battery electrolytes. This technique has allowed ORNL to study the formation and growth of the solid electrolyte interphase on graphite electrodes in real time and at high spatial resolution.

Understanding how interfaces—particularly electrode-electrolyte solid-liquid interfaces—control the physical and electrochemical energy conversion processes is a critical challenge in the accelerated development of materials used in electrical energy storage systems. For example, in lithium ion–based systems, when the liquid electrolyte decomposes, a passive multiphase layer grows at the electrode-electrolyte interface. Once formed, this solid electrolyte interphase (SEI) protects the active electrode materials from degrading and regulates the transport and intercalation of lithium ions during charge/discharge cycling. Due to the dynamically evolving nature of this nanometer-scale interface, it is difficult to design experiments that will not only elucidate the fundamental mechanisms controlling SEI nucleation and growth, but will also track the microstructural and chemical evolution of the SEI as a function of charge/discharge cycling to be monitored in real time.



(a) Scanning electron microscopy micrograph of battery electrodes [highly oriented pyrolytic graphite (HOPG) anode and lithium cobalt oxide cathode] attached to the biasing microchips and across the silicone nitride membrane, (b) charging curve, (c) bright-field TEM image of HOPG anode before experiment, and (d) snapshot acquired during in situ electrochemistry experiment depicting the formation of the SEI on the surface of the graphite anode.

The in situ electron microscopy technique, which uses an electrochemical cell holder built specifically for in situ transmission electron microscopy (TEM) characterization, will enable scientists to evaluate critical nanometer-scale microstructural and microchemical changes as a function of test conditions, electrode materials, electrolytes, and electrolyte additives. Preventing the evaporation of high vapor pressure and volatile organic liquid electrolytes has been a major challenge that has been overcome by sealing fluid between thin electron transparent viewing membranes. To create the electrochemical cell, two silicon microchips are stacked upon one another and placed within the tip of a precision-machined TEM holder. Biasing contacts are deposited onto the lower chip or "window" of the cell, which also serves as a platform for attaching battery electrodes and for interfacing with an external potentiostat for electrochemical testing. A 500 nm spacer material patterned on the upper chip controls the thickness of the liquid electrolyte layer in the cell. The cell incorporates a liquid delivery system (microfluidic syringe pump and microfluidic tubing) to allow liquid electrolyte to flow between the silicon nitride membranes that make up the cell. The TEM holder was built specifically for the Hitachi HF3300 S/TEM at the ORNL ShaRE User Facility, which is equipped with imaging detectors and a Gatan GIF Quantum for electron energy loss spectroscopy and energy-filtered TEM.

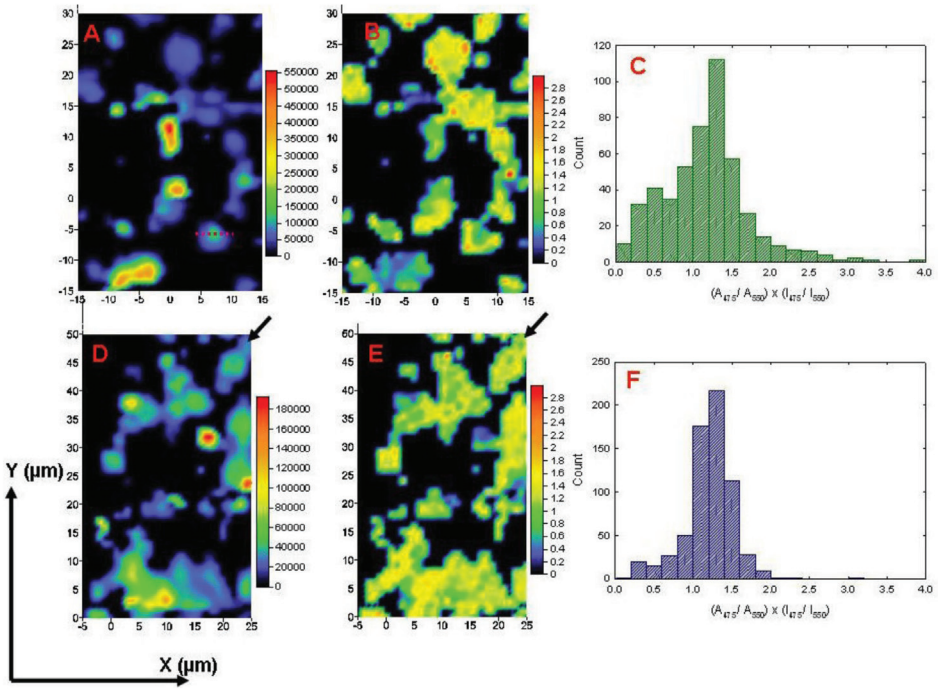
Publications

- Unocic, R. R., et al. 2011. "The Versatility of In-Situ Environmental Fluid Cells for Materials Science Research." Presented at Materials Science & Technology 2011, Columbus, Ohio, October 16–20.
- Unocic, R. R., et al. 2011. "Use of In-situ TEM Characterization to Probe Electrochemical Processes in Li-ion Batteries." Presented at 2011 Materials Research Society Spring Meeting and Exhibit, San Francisco, California, April 25–29.
- Unocic, R. R., et al. 2010. "In Situ TEM Characterization of the SEI in Li-ion Batteries." Presented at the 218th Electrochemical Society Meeting, Las Vegas, Nevada, October 10–15.

Study of Local State of Charge and Underlying Structures in Lithium Battery Electrodes

An ORNL-led research team consisting of scientists from ORNL and Ford Motor Company are using combined confocal micro-Raman imaging and electron microscopy for studying lithium ion electrodes subjected to various state of charge (SOC) and stress cycles. This study will provide important insights into cycle-life and voltage depression issues in lithium-rich manganese nickel cobalt (MNC) compositions, and correlate electrochemical performance with microstructural phase changes.

Key challenges with lithium-rich compositions are that they have a very high first cycle irreversible capacity loss upon high voltage cycling, and undergo structural transition upon repeated high voltage cycling (more than 4.6 V). They also have very limited rate capability because of the lower intrinsic electronic and ionic conductivity. Accomplishments include doubling the rate performance for lithium-rich MNC obtained from Toda America Inc. and successful elec-



Raman maps showing local SOC variation across NCA electrodes cycled at 4.1 V under constant current condition at 3-C rate with 1 hour potentiostatic step. SOC plots show the local inhomogeneity across the electrode surface and could vary under electrochemical conditions.

trochemical benchmarking of lithium-rich composition to address the issue of voltage suppression.

The project team monitored SOC variations on the surface of commercial lithium nickel cobalt aluminum oxide (NCA) electrodes subjected to various charge-discharge protocols. A battery's SOC is a macroscopic indicator of the amount of its stored energy and is often used as a diagnostic tool for observing battery performance. The microscopic origin of the SOC in connection to lithium ion electrodes is related to the local lithium content (or lack of it) in the individual electrode particles. Commercial electrodes for lithium ion batteries are composite materials composed of active electrode material, polymeric binders, and carbon diluents. At an electrode level, the local SOC could be nonuniform with variations becoming more apparent as the cell degrades, resulting in either power fade, capacity fade, or both. Understanding the spatial variation of SOC on the electrode surface could provide a microscopic picture of the degradation occurring at a local scale.

As mentioned above, the team carried out ex situ Raman mapping of electrodes that have been electrochemically cycled under different conditions. Using a particle-level SOC, the team obtained an SOC Raman map showing electron distribution at a micron-length scale. The ex situ SOC map is expected to change as the electrodes are cycled at different rates and under extreme duty cycle conditions. This provides a statistical means for studying the micron-scale SOC variation of commercially fabricated electrodes to identify key failure modes at the electrode (or materials) level that affect the cycle life of the lithium ion cell.

Publications

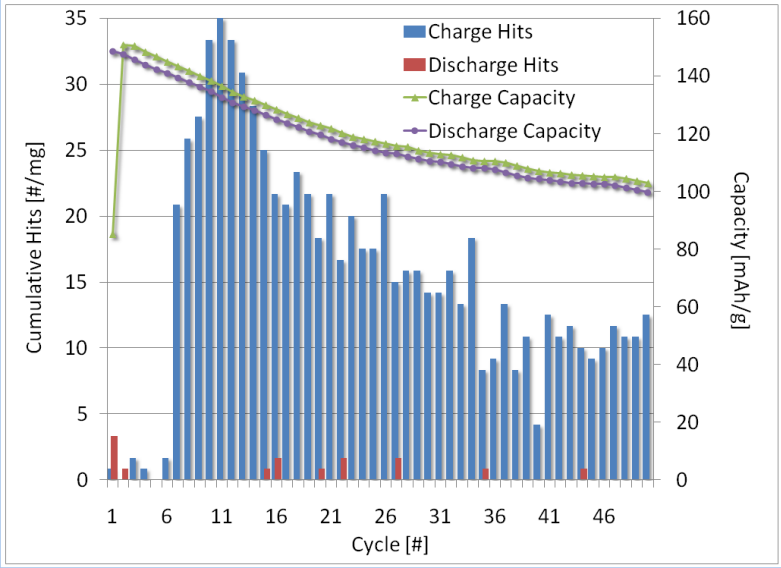
- Nanda, J., et al. 2011. "Observation of Local State of Charge Distributions in Lithium-ion Battery Electrodes." *Adv. Funct. Mater*. 21:3282–3290.
- Varadaraajan, Vikram, et al. 2011. "Direct Synthesis of Nanostructured V2O5 Films using Solution Plasma Spray Approach for Lithium Battery Applications." *J. Power Sources* 196(24):10704–10711.

Mechanical Degradation of Electrodes

The role of mechanical degradation in lithium ion battery lifetime and capacity fade is not thoroughly understood. Research has been limited by the parameters of available characterization techniques. A better understanding is important to the development of next-generation lithium ion (Li-ion) batteries. ORNL has developed a laboratory-scale method for using acoustic emission (AE) and x-ray diffraction (XRD) to monitor degradation in Li-ion batteries that will enable the development of cost effective in situ characterization tools. In situ AE-XRD is safe, uses inexpensive components, and is adaptable for either anode or cathode materials, making it a useful method for a wide variety of situations.

AE is used to detect, sort, and classify mechanical events such as particle fracture inside cycling Li-ion batteries. Special in situ methods of XRD are used to directly correlate the observed fracture events with strain in the active materials. Changes in electrode materials—lattice strain and phase transformation in cathodes (nickel-manganese-cobalt, manganese oxide, and $Li_{1.2}Ni_{0.15}Mn_{0.55}Co_{0.1}O_2$) and tin anodes—were measured and correlated well with the observed AE activity.

ORNL's novel beryllium-free in situ AE-XRD cell uses a metalized Mylar or Kapton window to allow x-ray penetration during cycling in standard coin cell hardware. This technique provides a safe, in-



Bar graph of AE activity for each charge and discharge step. A clear majority of events were observed during charging, and a fatigue-type AE activity onset was seen.

expensive alternative to current in situ XRD methods. It also provides data for a depth of understanding that before was possible only with special miniature cells and very short synchrotron beam time. The new cell allows for extended beam time in inexpensive laboratory-scale diffractometers. Mylar or Kapton disks sputtered with compatible metals can be used in direct contact with active materials. AE-XRD will enable further fundamental understanding of material degradation mechanisms and their correlation with capacity fade and cell failure.

Publications

- Rhodes, Kevin, et al. 2011. "Evolution of Phase Transformation Behavior in $Li(Mn_{1.5}Ni_{0.5})O_4$ Cathodes Studied by In Situ XRD." *J. Electrochem. Soc.* 158(8):A890–A897.

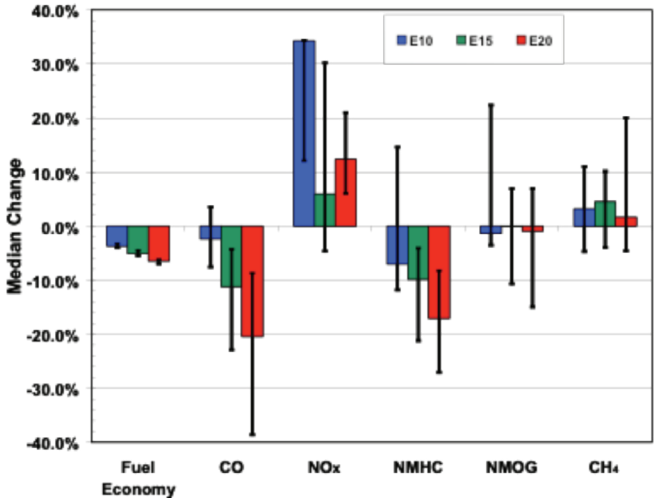
- Rhodes, Kevin, et al. 2011. "Novel Cell Design for Combined In Situ Acoustic Emission and X-Ray Diffraction Study During Electrochemical Cycling of Batteries." *Rev. Sci. Instr.* 82:075107.

Fuels

Study Charts the Impacts of Intermediate Ethanol Blends on Vehicle Emissions

ORNL has been working with the National Renewable Energy Laboratory and others to assess the viability of using intermediate ethanol blends—blends of gasoline with up to 20 vol % ethanol—in conventional vehicles to meet energy needs, decrease U.S. reliance on petroleum products, and meet U.S. goals for using renewable fuels. In 2011 the research team completed a groundbreaking study on the effects of intermediate blends on vehicle emissions and emissions systems.

The study, which was unprecedented in size and scope, included 82 vehicles (both cars and light trucks) from the 6 largest vehicle manufacturers, and new and pre-owned vehicle models from 2000 through 2009. Vehicles were acquired to establish matched sets of two, three, or four vehicles of each model being tested, and each vehicle of a set was dedicated to a specific gasoline-ethanol blend for aging. Vehicles were aged using the U.S. Environmental Protection Agency's Standard Road Cycle, the official driving cycle for aging studies to assess exhaust system durability, and emissions were tested periodically throughout the program. Emissions tests on all vehicles were conducted using emissions certification gasoline (E0—i.e., no ethanol) and splash blends of this same fuel with denatured ASTM D4806 ethanol to produce "certification



Median change in fuel economy and carbon monoxide (CO), nitrogen oxides (NO_x), non-methane hydrocarbon (NMHC), non-methane organic gas (NMOG), and methane (CH_4) emissions relative to ethanol-free gasoline. Range bars show interquartile range (25^{th} to 75^{th} percentile). Results for Federal Test Procedure at start-of-test.

grade" E10, E15, and E20. In addition to emissions testing, powertrain component inspections were also performed on six of the vehicle sets at the end of the program.

Data analysis on the full suite of vehicle data was completed in 2011, and the entire project has been detailed in a comprehensive report, *Intermediate Ethanol Blends Catalyst Durability Program.* In general, emissions increased with increasing mileage accumulation for all vehicles, whether aged on ethanol blends or ethanol-free gasoline, and aging with ethanol blends did not affect emissions changes over time differently than aging with ethanol-free gasoline. The examination of the powertrain components showed no signs of increased corrosion or wear from the use of ethanol blends compared to gasoline. Vehicles aged with ethanol blends did have higher intake valve deposit mass, however, detergent additive concentrations were not adjusted in consideration of adding ethanol to the fuel.

The information from this study has already been used by the Environmental Protection Agency to grant a partial Clean Air Act waiver[1,2] allowing increased ethanol in gasoline, and it is anticipated that the study and its accompanying report will have even more far reaching effects in the future.

Publications

- Shoffner, Brent A., et al. 2012. *Powertrain Component Inspection from Mid-Level Blends Vehicle Aging Study.* Prepared by Southwest Research Institute for Oak Ridge National Laboratory, November 2010. ORNL/TM-2011/65, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

- West, B. H., et al. 2012. *Intermediate Ethanol Blends Catalyst Durability Program.* ORNL/TM-2011/234, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

1 "Partial Grant and Partial Denial of Clean Air Act Waiver Application Submitted by Growth Energy To Increase the Allowable Ethanol Content of Gasoline to 15 Percent; Decision of the Administrator." *Federal Register* 75(213), November 4, 2010, pp. 68094–68150.

2 "Partial Grant of Clean Air Act Waiver Application Submitted by Growth Energy To Increase the Allowable Ethanol Content of Gasoline to 15 Percent; Decision of the Administrator." *Federal Register* 76(17), January 26, 2011, pp. 4662-4683.

Effects of Alternative Fuels on EGR System Performance

Greater use of alternative, non-petroleum-based fuels is heavily dependent on increased understanding of their effects on conventional automotive systems. ORNL researchers are working to quantify the effects of non-petroleum-based fuels on exhaust gas recirculation (EGR) system performance and to identify fuels or fuel properties that may reduce the effectiveness of EGR systems through fouling, or problematic deposits on EGR coolers.

As has been mentioned elsewhere in this report, EGR is a key aspect of many advanced combustion technologies and has become a mainstay for controlling nitrogen oxide (NO_x) emissions in diesel engines. Fouling of the EGR cooler by hydrocarbons and particulate matter from the exhaust gas stream can reduce the performance of the cooler in a matter of hours, causing the temperature of the EGR stream to rise and potentially producing higher NO_x emissions.

Some non-petroleum-based fuels (for example, biodiesel) have unique fuel chemistries and/or combustion behavior that may cause changes in the fouling tendencies of EGR coolers. If this is found to be the case, it represents a very significant technical hurdle that must be overcome if these fuels are to achieve significant market penetration. The first step toward overcoming this potential hurdle is to gain a better understanding of the scope of the problem, which ORNL is doing through experiments using an engine and sampling system with surrogate EGR cooler tubes to examine the nature of the deposits caused by operation with non-petroleum-based fuels.

In 2011 a series of experiments was conducted to determine the effect of various surface treatments on EGR deposits under both transient and steady state flow conditions. The results showed that surface

treatments do not have a significant impact on fouling and thus do not represent a means of avoiding the cooler fouling issue. Furthermore, the transient flow experiments demonstrated that deposit removal requires high gas flow rates that may be a challenge in practical EGR systems.

Experiments aimed at further understanding the impact of non-petroleum-based fuels on the EGR fouling process are planned in the coming year. These studies will focus on separating the conditions that may generate plugged coolers from those that produce more frangible layers, and further investigation of the potential role of fuel-related hydrocarbons on the stability of the deposit layer.

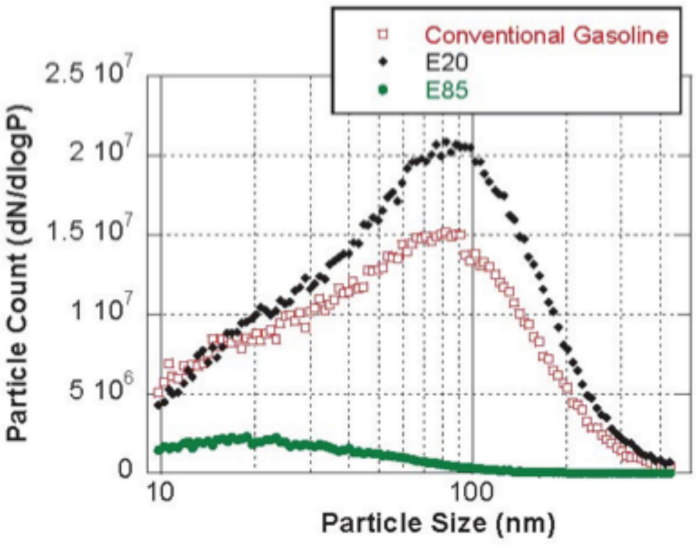
Publications

- Storey, J. M. E., et al. 2011. "Exhaust Gas Recirculation Cooler Fouling in Diesel Applications: Fundamental Studies, Deposit Properties, and Microstructure." Presented at the 2011 Eurotherm Heat Exchanger Fouling and Cleaning Conference, Crete Island, Greece, June 5–10.
- Styles, D., et al. 2010. "Factors Impacting EGR Cooler Fouling—Main Effects and Interactions." Presented at the 2010 Directions in Engine Efficiency and Emissions Research (DEER) Conference, Detroit, Michigan, September 27–30.
- Lance, M., S. Sluder, S. Lewis, and J. Storey. 2010. "Characterization of Field-Aged EGR Cooler Deposits." *SAE Int. J. Engines* 3(2):126–136.

Enabling High-Efficiency Ethanol Engines

As part of a multiyear Cooperative Research and Development Agreement, researchers at ORNL and Delphi Automotive Systems have been investigating methods to remove barriers to more widespread use of ethanol and ethanol blends in the United States. Prior years' efforts focused on identifying and demonstrating potential efficiency gains for ethanol fuels. The effort in 2011 was focused on determining the effect of ethanol content on particulate emissions in a gasoline direct injection (GDI) engine relative to gasoline and port fuel injection (PFI) fueling. PFI has been the standard in spark ignition engines for the last 20 years but is being eclipsed by GDI because it promises increased fuel efficiency and power while controlling emissions levels. However, expected changes in regulations for particulate emissions make it essential to understand the impact of fuel compositions on particulate emissions under different fueling regimes.

The research platform used for this research was a multicylinder production engine modified by Delphi to make it capable of optimization for E85. The engine was also modified for PFI, allowing direct comparison of particle emissions at the same engine load on a common engine with two different fueling strategies. Engine operation focused on a single operating point at 1,500 rpm and 8 bar brake mean effective pressure—a



Particle emissions for conventional gasoline, E20, and E85 under throttled operation at 1,500 rpm, 8 bar indicated mean effective pressure, and a fuel injection timing of 320 crank angle degrees before top dead center. Under these conditions E20 produced the highest concentration of particle emissions, followed by conventional gasoline and E85. The differences between conventional gasoline and E20 were dependent on the fueling and breathing strategies, with E20 producing highest particle emissions under some conditions and conventional gasoline producing the highest emissions at other conditions. In all cases, however, E85 produced by far the lowest concentration of particle emissions.

condition known to produce high smoke (particulate) emissions. The engine was operated with gasoline, E20, and E85.

The main finding of the 2011 campaign was that use of E85 results in a reduction in particulate emissions of up to 2 orders of magnitude relative to GDI fueling with gasoline and E20. Furthermore, GDI particulate emissions with E85 are similar to those for PFI fueling with gasoline. Thus, an increase in particulate emissions beyond that of PFI engines can be prevented while gaining the efficiency of GDI engines using E85.

Four-cylinder research engine modified from a production engine by Delphi.

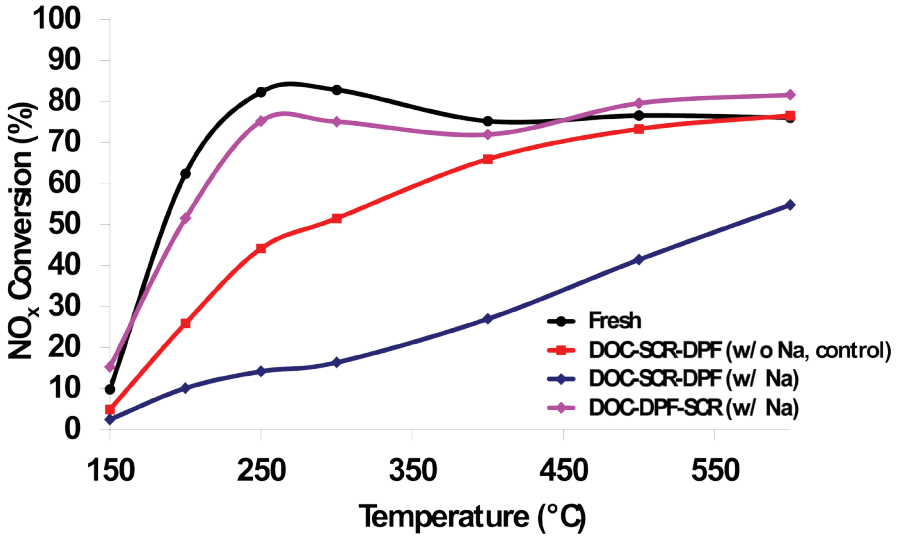
Publications

- Szybist, J. P., et al. 2011. "Ethanol Blends and Engine Operating Strategy Effects on Light-Duty Spark- Ignition Engine Particle Emissions." *Energy & Fuels* 25(11):4977–4985.

Investigation of Impacts of Emerging Fuels and Lubricants on Emissions Control Devices

To enable use of alternative fuels and advanced lubricants, it is critical to evaluate their compatibility with emissions control devices. ORNL researchers are working with industry partners to investigate the impact of emerging fuels and lubricants on emissions control devices using accelerated aging techniques. A key element of this research is the development of (1) protocols for accelerated aging and poisoning of emissions control devices and (2) laboratory experiments that accurately mimic field use. Such protocols do not exist for current emissions control devices, and their development will enable more rapid implementation of new fuel and lubricant formulations and improvements in the emissions control devices being developed.

Biodiesel fuel, a domestic renewable energy source synthesized from vegetable oil or animal fat, combusts similarly to diesel fuel; however, greater use has been hampered by unknowns such as the impact on emissions control devices. One particular concern is the potential effect of the trace elements of sodium and/or potassium in biodiesel. (The American Society for Testing and Materials specifies a maximum of 5 ppm combined sodium and potassium in biodiesel.) To address this concern, efforts in 2011 focused on a comparison of selective catalytic reduction catalysts [SCR, used for nitrogen oxides (NO_x) control in conjunction with ammonia/urea] and diesel particulate filters (DPF, used for



SCR NO_x reduction performance illustrating the impact of Na in the DOC-SCR-DPF arrangement compared to the minimal effects when the DPF is in front of the SCR (DOC-DPF-SCR).

particulate emissions control) exposed to sodium in the emissions control device configurations used in light duty vehicles [diesel oxidation catalyst (DOC)-SCR-DPF] and heavy duty vehicles (DOC-DPF-SCR).

The results showed that while sodium can significantly impact SCR catalysis, placing the DPF in front of the SCR protects the catalyst from sodium and its effects. Some protection from thermal stresses is also gained by this placement. Placement of the DPF in front of the SCR, however, led to significant sodium penetration of the cordierite wall of the DPF, which other studies have shown to affect the strength of the DPF. The location of the sodium contamination in the accelerated aged samples mimicked that seen in long-term engine aged catalysts, suggesting the accelerated aging protocol is valid.

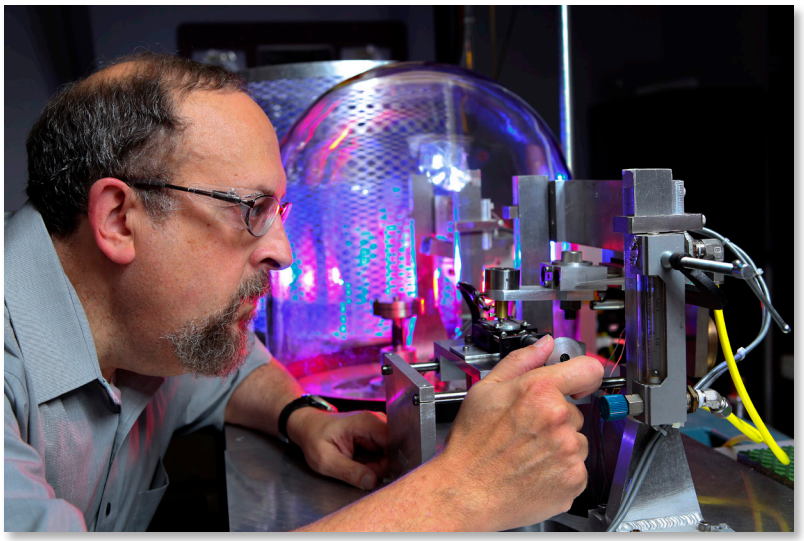
Based on these results, a large collaboration was formed between ORNL, the National Renewable Energy Laboratory, National Biodiesel Board, the Manufacturers of Emission Controls Association, and Ford Motor Company to determine appropriate limits for trace amounts of sodium in biodiesel.

Publications

- Brookshear, D. W., et al. 2011. "Investigation of the Effects of Biodiesel-Based Na on Emissions Control Components." *Catalysis Today* (forthcoming). Available online January 24, 2012. doi:10.1016/j.cattod.2011.12.001.
- Ottinger, N. A., et al. 2011. "Effect of Lean/Rich High Temperature Aging on NO Oxidation and NO_x Storage/Release of a Fully-Formulated Lean NO_x Trap." *Applied Catalysis B: Environmental* 101(3–4):486–494.

High Temperature Materials Laboratory

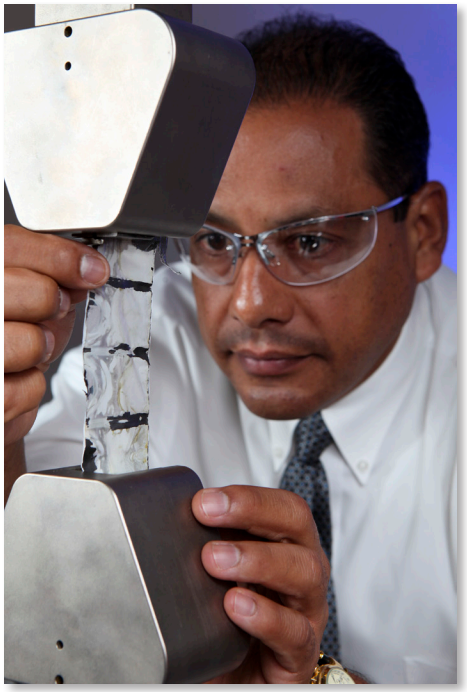
The ORNL High Temperature Materials Laboratory (HTML), a DOE User Facility dedicated to solving materials problems, presents scientists and students with unique opportunities for collaborative world-class research. The HTML is dedicated to solving materials problems that limit the efficiency and reliability of systems for power generation and energy conversion, distribution, and use. A particular focus is the development of materials based, energy efficient, and environmentally friendly transportation technologies that will enable the United States to use less petroleum. HTML's six user centers—Diffraction, Materials Analysis, Mechanical Characterization and Analysis, Residual Stress, Thermography and Thermophysical Properties, and Tribology Research—are clusters of specialized equipment designed for specific types of property measurements. They provide users with extensive capabilities for characterizing the microstructure, microchemistry, and physical and mechanical properties of materials over a wide range of temperatures. HTML also manages a neutron beam line facility at the ORNL High Flux Isotope Reactor, and a synchrotron beam line at the National Synchrotron Light Source at Brookhaven National Laboratory.



A reciprocating tribometer is used to measure the friction forces between battery materials during repeated charging and discharging.

In addition to the physical facilities, HTML User Program participants also have access to HTML's professional staff who:

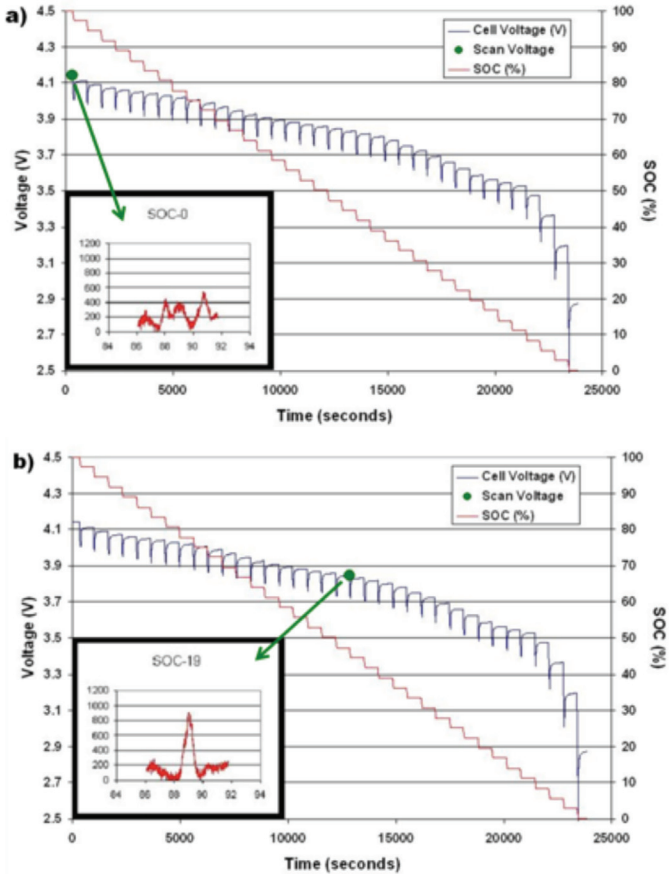
- participate in the planning, performance, and interpretation of research, including co-preparation of technical papers and presentations from nonproprietary research;
- assist users in the safe and efficient operation of user center research equipment; and
- maintain instruments to maximize their availability for research.



A mechanical testing machine used to characterize the stress-strain response of various battery materials.

General Motors Analyzes Lithium Ion Battery Performance with Customized Neutron Scattering Technique

Researchers from the GM R&D Center in Warren, Michigan, and the HTML User Program have developed a customized nondestructive monitoring technique for analyzing the large format lithium ion batteries used in GM's electric vehicles. Using neutron scattering and high resolution infrared imaging, they conducted in situ analysis of cathode and anode materials inside fully functioning lithium ion cells. Baseline data were collected on internal volume changes, surface temperature changes, and distribution of active materials during charging and discharging. One of the technical barriers to overcome in the neutron scattering study was extracting small electrode-related signals from the large background signals from polymer-based pouch and separator materials. Using ORNL's High Flux Isotope Reactor and special features in scanning selected 2θ angles (6 degrees) at the HB-2 beam line, characteristic diffraction changes associated with electrode materials were monitored successfully.



Plots of a GM 15-Ah cell from this project showing the fully charged state (open circuit voltage, V_{OC} = 4.15 V) in dark blue and state of charge at the midpoint of discharge (V_{OC} = 3.85 V) in red, as a function of time: a) before discharging and b) during discharging. Insets at lower left are neutron intensity vs 2θ scans.

The infrared in situ imaging captured small changes in temperature at critical stages and locations, while the neutron scattering experiments confirmed charge/discharge cycle models. The techniques used in this project are a significant advance over conventional tools and techniques and will be applicable in other research projects. The information obtained during the project will help GM ensure that the performance of production batteries is consistent with that predicted from laboratory studies.

Dr. Yang prepares to load a large format lithium ion cell for testing.

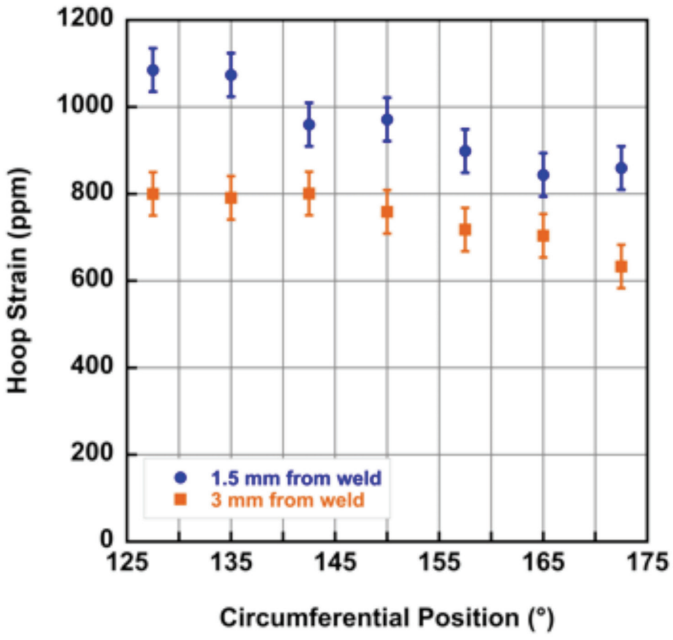
Residual Stresses in Turbocharger Shaft-Wheel Assembly Welds

Honeywell Turbo Technologies visited the HTML as part of a two-pronged study to better understand residual stresses in the weld joints of turbocharger shaft wheel assemblies (SWAs). Honeywell researchers conducted neutron and x-ray scattering characterization studies of stress relief methods applied during the manufacturing process. One element of the experimental plan was to create a map of the residual strains in the region near the electron beam (EB) weld joining the shaft to the turbine wheel in both through-thickness and circumferential directions using the HTML second generation neutron residual stress facility (NRSF2). NRSF2's combination of small gauge volumes (1.5 × 1.5 × 0.5 mm) and good intensity made these through-thickness measurements feasible. The deep penetration that only neutrons provide was critical for the study of stresses near the EB weld. The team observed significant changes in hoop and radial strains around the circumference, localized within a 30° angular range of the as-welded sample and the standard "stress relieved" SWAs. These changes show that the industry's standard manufacturing method is not fully effective in relieving residual stresses from the EB weld operation. Measurements on an SWA subjected to 1100°C furnace stress relief showed that effectively all residual stresses were relieved and no localized stresses remained.

Honeywell SWA mounted on the NRSF2 beam line sample stage.

The second element of the study was to quantify defect density by mapping the near-surface residual stresses and peak breadth along the shaft in the two bearing regions. X-ray diffraction (XRD) measurements of surface stresses were made at the bearing regions along the shaft. Mapping data were collected using the new PROTO I XRD instrument on SWAs in three conditions: as-welded, standard stress relieved, and furnace treated at 1100°C. Analysis of the XRD data confirmed the neutron scattering results that showed furnace heat treatment removed stresses caused by welding.

Turbochargers are key elements in advanced fuel-efficient engines, so ensuring their reliability is important to manufacturers of these engine boosters. Quantifying the role that residual stresses play in the lifetime of the SWA and turbocharger housings will aid Honeywell in designing the highest quality SWAs and monitoring manufacturing processes. Planned future collaborations with Honeywell include the evaluation of cost-effective ways to mitigate residual stress and thereby extend component life and ensure reliability of both the SWA and turbine housing in the company's turbochargers.

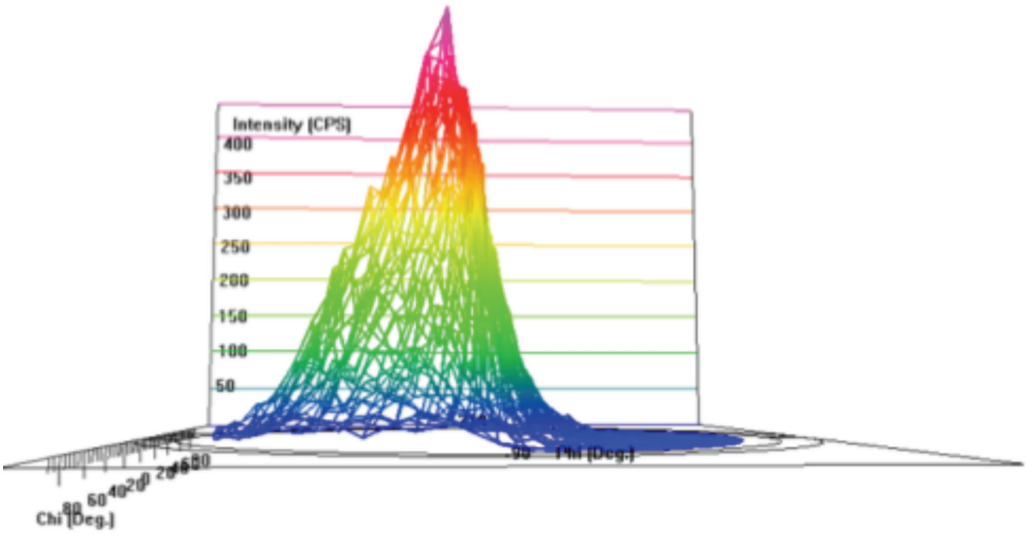


Neutron circumferential strain mapping of SWA showing variation of hoop strain at two distances from weld.

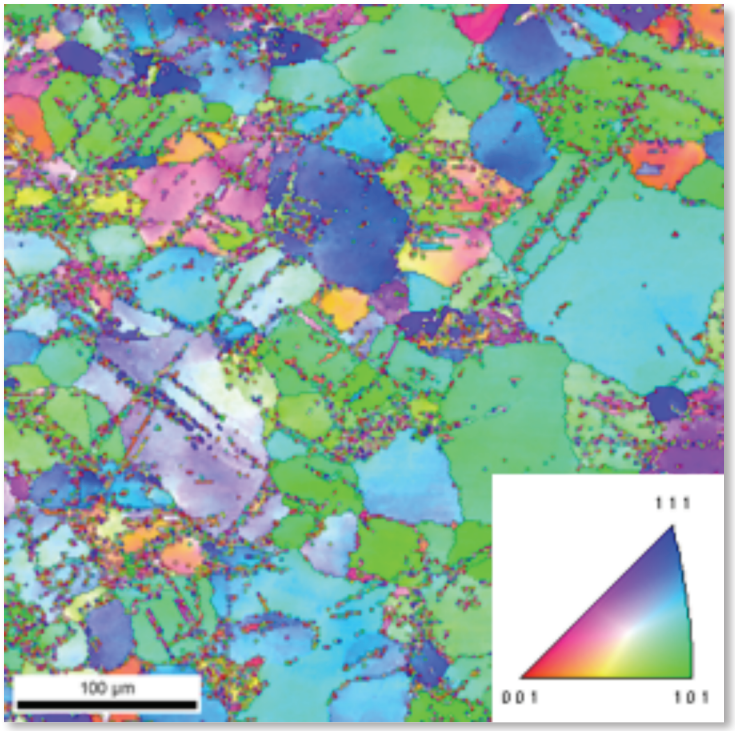
Magnesium Elektron Characterizes Magnesium Sheet Alloy Materials to Produce Improved Automotive Structures

Magnesium Elektron North America researchers came to HTML to work on a user project focused on two goals: enhancing formability of sheet alloys and producing lighter weight automotive components. Experimental data were collected to help determine the manufacturing process adjustments needed to improve magnesium sheet formability. X-ray diffraction of crystallographic texture data from heated, asymmetrically rolled AZ31B and ZEK100 sheet show the orientation of the (002) pole is out of plane after asymmetric rolling (see figure below). That is, after asymmetric rolling the majority of basal planes are no longer parallel to the plane of the sheet, which is important for formability purposes. The microstructure and microtexture of the two magnesium alloys as a function of hot working were also investigated with electron backscatter diffraction (EBSD) microscopy. Different grain orientations by color, as well as the presence of shear bands (linear features cutting across grains) are shown in the figure on the right. With higher levels of deformation, the density of shear bands increased and more deformation twinning was observed.

Characterization results from both electron backscatter and x-ray diffraction will enable Magnesium Elektron to design manufacturing processes for large-scale production of magnesium alloys for automotive structures.



Three-dimensional x-ray pole figures plotting intensity of the (002) or basal planes as a function of azimuthal and tilt angle for the asymmetrically rolled AZ31B.



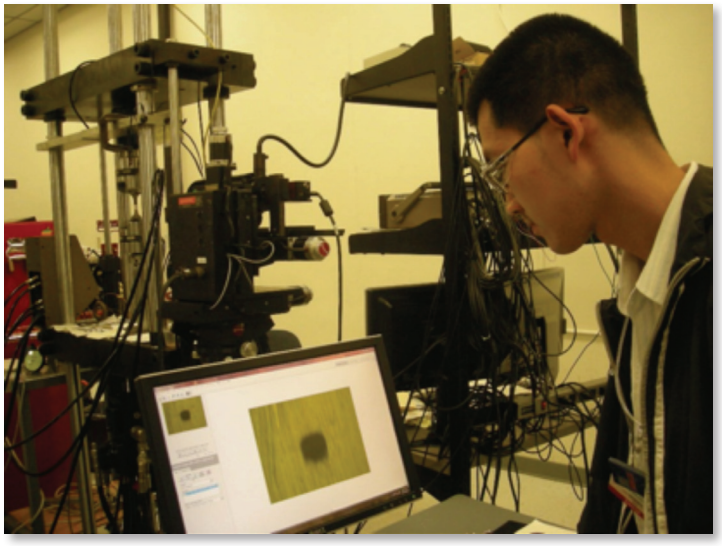
EBSD image showing the microstructure and microtexture of ZEK100 asymmetrically rolled at 150°C after a 5% reduction. The inverse pole figure map (inset) provides a key to the color-crystallographic orientation relationship.

Publications

- Randman, D., et al. 2011. "The Effect of Rare Earth Elements on the Texture and Formability of Shear Rolled Magnesium Sheet." *Magnesium Technology 2011*, edited by W. H. Sillekens, S. R. Agnew, N. R. Neelameggham and S. N. Mathaudhu. Hoboken, New Jersey: John Wiley & Sons.

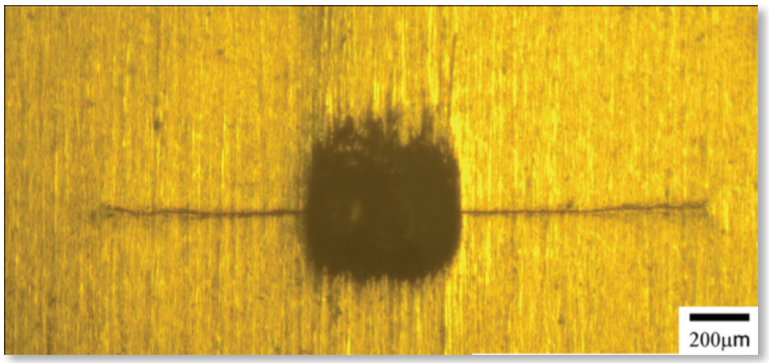
Investigating Fatigue Crack Growth in High-Strength Magnesium Alloy

The first comprehensive study of small fatigue crack propagation behavior in a magnesium alloy subjected to various thermomechanical heat treatments was undertaken by Michigan State University in an HTML user project. Magnesium alloys are lightweight alternatives to structural alloys used in engine and other automotive components, but their low fatigue strength and high cost has inhibited widespread use. Michigan State has been studying the small fatigue crack growth behavior of a high-strength nanoMAG AM60 magnesium alloy subjected to various thermomechanical processing treatments. They partnered with the HTML User Program to characterize the effects of thermomechanical processing and subsequent heat treating on the fatigue crack growth behavior of a Thixomolded® AM60 magnesium alloy. Notches a few hundred microns in size were machined on test specimens, and the growth behavior of small fatigue cracks emanating from the notches was directly measured using a telescopic system recently installed at HTML. The effect of mechanical loading parameters such as maximum stress and load ratio on the small fatigue crack growth behavior was also determined. The interactions of the small fatigue cracks with porosity and other material defects were found to determine the overall fatigue lifetime, while the role of grain size was found to be secondary across the various thermomechanical treatments investigated.



Michigan State's Zhe Chen examines a microscope image of a fatigue crack in an AM60 magnesium alloy sample subjected to the Thixomolded® thermomechanical processing heat treatment.

The results of this project can be used directly to estimate fatigue life for the different heat treatments under various mechanical loading conditions. In addition, Michigan State will use the results of its investigation to support development efforts at Thixomat, Inc., owner of the Thixomolding® manufacturing process, for a new product line aimed at replacing existing aluminum alloys with magnesium alloys for automotive light-weighting applications.



Close up look at the microscope image of a fatigue crack in an AM60 magnesium alloy sample subjected to the Thixomolded® thermomechanical processing heat treatment.

Publications

- Chen, Z., et al. 2011. "The Effect of Thermomechanical Processing on the Creep Behavior and Fracture Toughness of Thixomolded® AM60 Alloy." *Magnesium Technology 2011*, edited by W. H. Sillekens, S. R. Agnew, N. R. Neelameggham, and S. N. Mathaudhu. Hoboken, New Jersey: John Wiley & Sons.

- Chen, Z., et al. 2011. "The Small Fatigue Crack Growth Behavior of an AM60 Magnesium Alloy." Presented at the Materials Science & Technology 2011 Conference & Exhibition, Columbus, Ohio, October 16–20.

Influence of Molding Processes on Properties of Glass Fiber–Reinforced Polymers

In the first Toyota Research Institute of North America user project at the HTML, Toyota is undertaking a project to characterize the microstructure and mechanical properties of glass fiber–reinforced thermoplastics. These materials can reduce vehicle weight and improve fuel efficiency without sacrificing safety. In particular, Toyota wants to understand the influence of different molding processes on the structural properties of glass fiber–reinforced polymers. These materials may be produced using injection molding, injection compression, compression, or direct injection techniques. Each process results in different material microstructures and properties and carries a different production cost. Optical and x-ray tomography methods were used to measure length distribution, orientation, and dispersion of fibers. This work resulted in the first successful correlation of optical and computed tomography fiber orientation measurement results on these materials. Tensile properties of these materials at various strain rates were also evaluated to assess the effect of microstructure on mechanical properties.

Discontinuous fiber thermoplastic composites are low cost, recyclable, lightweight materials with increasing use in automotive applications. Understanding microstructure and its influence on material properties is critical for proper design and application of these materials to achieve the goals of the DOE Vehicle Technologies Program. Increased use of lightweight thermoplastic composite materials will contribute to reaching the target of a 50% reduction in vehicle weight.

Cross section of material showing discontinuous glass fibers in quasi-random orientation (diameter 15 μm).

Umesh Ghandi, Toyota Research Institute, prepares a tensile sample for high strain rate tensile testing with digital image correlation.

Publications

- Gandhi, U., S. DeBoodt, and V. Kunc. 2011. "Investigation of Fiber Orientation in Fiber Reinforced Polymers." Presented at Digimat Users' Meeting 2011, Munich, Germany, October 10–12.

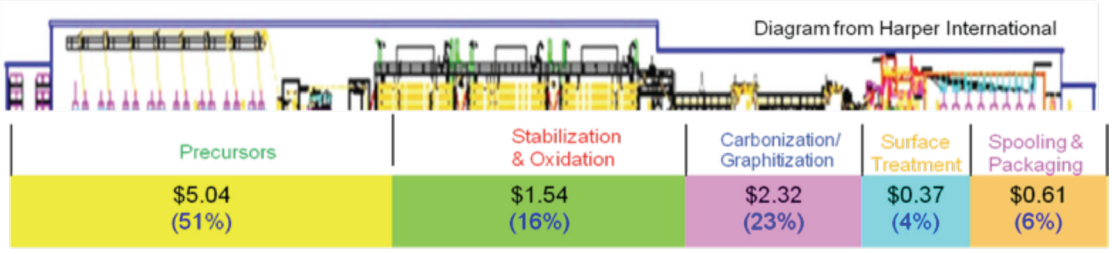
Lightweight Materials

Low Cost Carbon Fiber Development

In efforts to produce lighter weight vehicles and achieve corresponding gains in fuel economy, ORNL and DOE are taking a multipronged approach aimed at making carbon fiber (CF) more attractive to manufacturers. The major barrier to greater use of CF is its cost. Fifty-one percent of the cost of producing CF is attributable to the precursor, and 39% to conversion of the precursor into CF. A significant amount of the ORNL effort has been devoted to developing lower cost precursors and lower cost, higher rate production technologies.

- ORNL's successful collaboration with fiber manufacturer Fibras Sineticas de Portugal S.A. (FISIPE) to render textile-based polyacrylonitrile (PAN) suitable for conversion to CF is nearing completion. Textile PAN sells for about half the cost of conventional CF precursors. ORNL and FISIPE developed an alternative pretreatment for the textile PAN, which was installed in a FISIPE production facility. It was verified that the CF produced met or exceeded strength and modulus requirements. Commercialization plans are in development.

- Melt spun polyolefins are the lowest cost potential precursors due to low raw material cost, simpler spinning process, and inherently high carbon content. During 2011, greater understanding of the mechanical properties of polyolefin precursors and their relation to processing parameters was achieved, and previously identified issues of incomplete functionalization of the fiber core and interfilament bonding during thermal treatment were successfully resolved. A polyolefin based CF with a tensile strength of 237 Ksi was produced, while a different sample yielded a modulus of 17.2 Msi. In FY 2012 work will continue on enhancing the



Breakdown of CF production costs (Base diagram courtesy of Harper International.)

properties to meet the program targets of tensile strength of at least 250 Ksi and modulus of at least 25 Msi.

- To decrease conversion costs, ORNL has developed a new plasma based process resulting in oxidation times of as little as 20 minutes for aerospace grade PAN (compared to 90–120 minutes for conventional processing) and 45 minutes for the first samples of textile grade PAN. All mechanical property requirements were met except for modulus (5% under minimum). The research team is optimizing the new process for textile grade fibers. In addition, the team completed exhaustive fiber damage analyses in conjunction with mechanical properties analyses of aerospace grade PAN processed with the advanced oxidation process. The project team is currently completing the work necessary to design a larger oxidation reactor for installation in the ORNL Small Pilot Line.

Textile tow precursor as produced by FISIPE and supplied to ORNL on spools for evaluation. Note the golden color of this precursor fiber, which is indicative of the specialized pretreatment that was developed and implemented by ORNL and FISIPE.

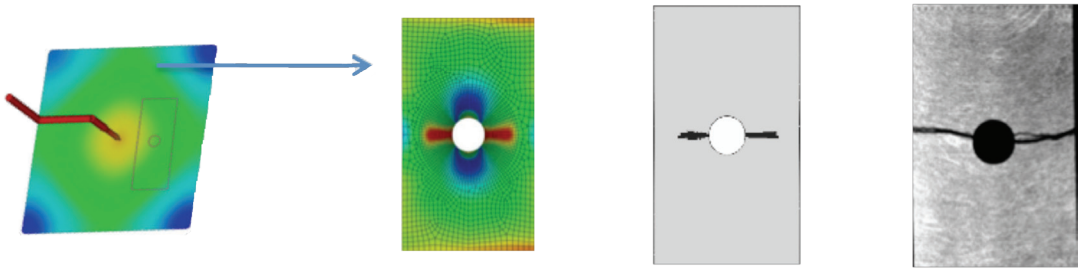
Publications

- Hunt, Marcus A., et al. 2012. "Patterned Functional Carbon Fibers from Polyethylene." *Advanced Materials.* First published online: March 21, 2012. dol: 10.1002/adma.20110455/1.
- Warren, C. David. 2012. "Low Cost Carbon Fiber Development—Oak Ridge National Laboratory." *Lightweight Materials FY 2011 Annual Report.* DOE/EE-0674. U.S. Department of Energy, Washington, D.C..

Predictive Models for Long Fiber Thermoplastic Injection Molding

Long-fiber reinforced thermoplastics have generated interest in the automotive industry due to their low cost, rapid production, and good mechanical properties. However, use of these materials has been limited by an inability to accurately predict their stiffness, strength, long-term durability, and service life. A collaborative program between ORNL and Pacific Northwest National Laboratory (PNNL) has been conducting research to address this by developing, implementing, and validating models for injection molding and property prediction, allowing complete prediction from process to property in as-formed components.

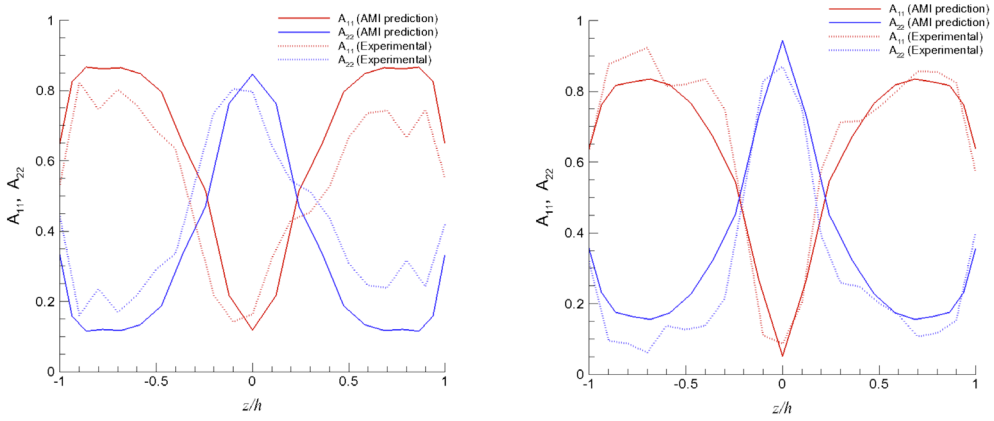
Validation of the predictive models was completed for two dimensional geometries in fiscal year 2011. Large plaques were molded using materials representative of the automotive industry—polypropylene/40% and PA6,6/40% glass. Radial and linear flow was achieved by center gating and edge gating of samples. To change the microstructure of the resulting material and exercise the predictive models, fill speed and back pressure were varied. Experimental data measured for the plaques point to consistent material properties, including appropriate dispersion, lack of weld lines in sample regions, and an entangled fiber network with a relatively wide core. Therefore, the test data obtained are well suited for model validation.



ORNL and PNNL models support prediction from process to property. Left to right: global injection molding flow prediction, global stress prediction, progressive failure prediction, and x-ray of failed sample.

Accurate prediction of fiber orientation is crucial for prediction of material properties. Three locations in each plaque type were evaluated experimentally and compared to predictions, which were performed with a single set of parameters for a given material. Predicted and experimental results for the 24 cases evaluated matched within 8% on average, exceeding the project target of 15%. The nature of flow, including the variation in core and shell thickness, was captured for all cases. Subsequent predictions of mechanical properties based on these orientation results further confirmed the high fidelity of the predictive models. Platforms prevalent in the automotive industry were selected to commercialize the tools developed in this project. The injection molding models are implemented by Autodesk Inc. in their commercial code, Moldflow. Licensing by PNNL for the property prediction tool developed under the Abaqus FEA software environment of Dassault Systemes is in progress. Both tools are being tested by industry professionals.

To complete development of the tools, a complex three-dimensional automotive part was selected in collaboration with industry experts. Test articles will be molded with materials identical to those used for validation on plaque geometry, under similar processing conditions, and measured values will be used to validate the models.



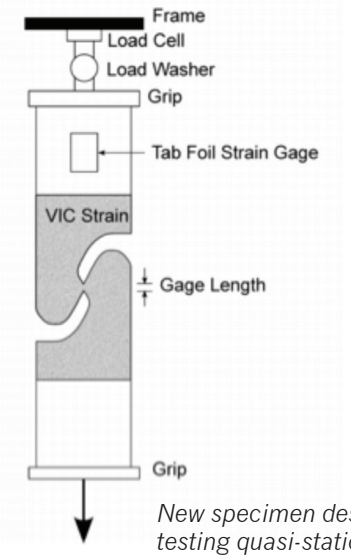
Comparisons of the experimental and predicted fiber orientation results for (left) the 40% slow-fill glass/PP center-gated plaque, worst case; and (right) the 40% fast-fill glass/PA6,6 center-gated plaque, best case. Series designated A11 represent flow direction orientation, and series designated A22 represent cross-flow direction orientation.

High Strain Rate Characterization of Magnesium Alloys

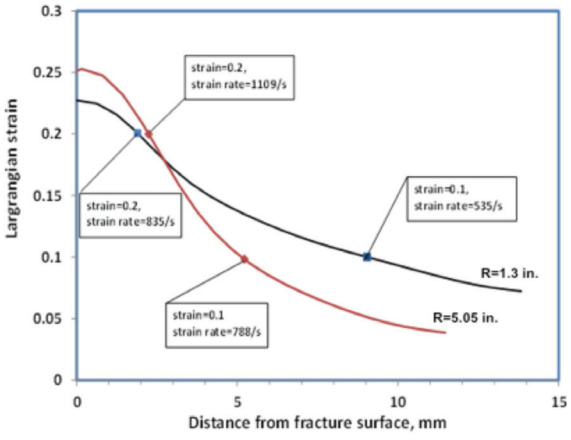
Low-density magnesium (Mg) alloys are good candidates for lightweight automotive components to achieve significant vehicle weight reductions, which in turn enable increased fuel economy. Because these materials are not well characterized with regard to mechanical properties under impact, Mg alloy components are overdesigned in order to compensate for uncertainties in deformation and failure mechanisms. ORNL is addressing this problem by developing new methods for characterizing material behavior at high strain rates and for determining underlying mechanisms of load-induced property degradation. The information and models that result from this research will reduce uncertainties in component design thereby reducing overdesign and vehicle weight. Test methods, test data, and material data gathered during the project are available on the World Wide Web at thyme.ornl.gov/Mg_new.

The ORNL team has developed several new test procedures and methods that can be standardized for widespread use. These include:

- New techniques to generate reliable tensile stress-strain data in the intermediate strain rate regime (quasi-static up to 1,000/s) corresponding to strain rates experienced in high speed forming and vehicle crashes. The tests are conducted on a custom-designed high speed servohydraulic machine combined with a three-dimensional digital image correlation method. For both Mg alloys tested, the yield strength and ultimate tensile strength increased slightly when the strain rate was increased from 1 s^{-1} to 1,000 s^{-1}.



New specimen design for testing quasi-static shear strength of Mg alloy sheet.



Strain distribution of AM60B specimens with two different radii. Tests were conducted at nominal speed of 500 in./s.

- A new specimen design for use in determining quasi-static shear strength of sheet materials, which achieves constraint shear strain within the shear ligament. Both tested Mg alloys showed very small strain rate sensitivity in shear.
- A technique that enables measurement of material behavior with continuous strain levels and under multiple strain rates using a single specimen design. This new specimen design and testing procedure can produce continuously varying levels of plastic strain achieved at various locations in the specimen and at different strain rates. The specimen design also reduces the size of conventional test matrices and overall testing time and permits more focus on test analysis and modeling.
- Procedures for quantifying the evolving stages of damage based on image processing, void growth, and mechanical tests with the controlled strain application. Results show that void growth is dependent not only on the applied strain rate but also on the strain rate.

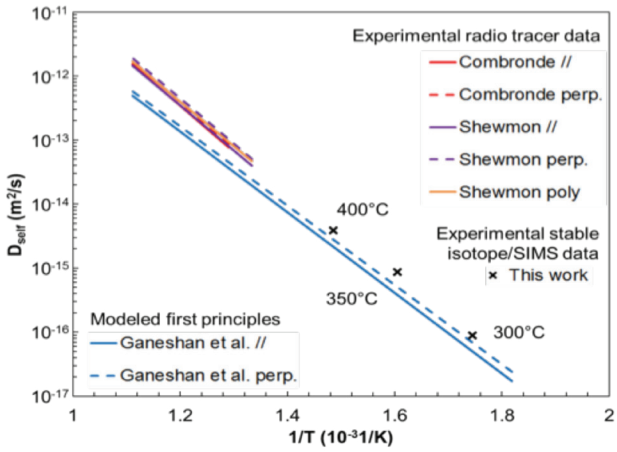
Publications

- Wang, Y., et al. 2011. "Characterization of High Strain Rate Mechanical Behavior of AZ31 Magnesium Alloy Using 3D Digital Image Correlation." *Advanced Engineering Materials* 13(10):943–948.
- Wang, Y., D. L. Erdman, V. Kunc, and S. Simunovic. "Material Mechanical Characterization Method for Multiple Strains and Strain Rates." U. S. Patent Application 61/485,163 filed May 12, 2011.

Understanding the Diffusion of Elements in Magnesium Alloys for use in Lightweight Components for Vehicles

ORNL scientists and engineers are working with an international team to develop a comprehensive understanding of the diffusion of elements in magnesium (Mg) alloys. The low density of Mg alloys makes them good candidates for lightweight components for use in automobiles; replacing steel chassis components with Mg alloys could reduce their weight by 50%, enabling higher fuel economy in vehicles. Typical Mg alloys are brittle during vehicle crash events and are difficult to form without elevated temperature processing. More ductile Mg alloys could address these barriers. Greater understanding of the diffusion of alloy elements will facilitate development of new Mg alloys with improved formability and ductility, and enable increased use of Mg in vehicles. Additionally, modeling precipitation and dissolution phenomena during heat treatment of super-vacuum die casting of Mg alloys requires knowledge of the diffusivities of the alloy constituents in the cast alloys. The Mg Integrated Computational Materials Engineering activity is an international effort that will result in an integrated suite of validated computational materials modeling tools for Mg alloy development.

The team's approach involves obtaining Mg tracer diffusion data using secondary ion mass spectrometry (SIMS) for diffusion depth profile measurements of stable isotopes (for example, ^{25}Mg) in Mg-rich alloys. This approach is based on the thin film method using stable isotopes rather than radioactive isotopes as tracers, reducing the cost associated with handling and processing the radioisotopes and extending historic



Arrhenius plot of the self-diffusion coefficients in pure Mg using the SIMS-based stable isotope thin-film technique. Comparison with an extrapolation of the published self-diffusion radioactive tracer data at high temperatures (more than 400°C) shows excellent agreement.

radiotracer measurements to lower temperatures. The data for pure Mg self-diffusion showed very good agreement with available radioisotope tracer data. An ultrahigh vacuum system was designed and developed to minimize isotopic losses and provide high-purity isotopic thin films. New SIMS techniques were developed such as measurements on angled (less than 2 degrees taper) polish sections for deep diffusion depths, and parameters were optimized to minimize sputter roughness in polycrystalline samples. Interdiffusion/intrinsic diffusion experiments (involving traditional diffusion couples) were used along with thermodynamics to extract tracer diffusivities of monoisotopic elements such as aluminum (Al). The project has undertaken three-dimensional molecular dynamics modeling of volume and grain boundary diffusion in polycrystalline Mg alloys to incorporate microstructure effects.

Work will continue in 2012 with tracer diffusion experiments and interdiffusion analysis in Mg-Al-Zn and Mg-Al-Zn-Mn alloys. Tracer diffusion studies are also planned in select rare earth and rare earth replacement alloys, and grain boundary and effective diffusion modeling will be extended to polycrystalline Mg-Zn and Mg-Al-Zn.

Publications

- Brennan, S., K. Bermudez, N. Kulkarni, and Y. H. Sohn. 2011. "Growth Kinetics of γ-$Al_{12}Mg_{17}$ and β-Al_3Mg_2 Intermetallic Phases in Mg vs. Al Diffusion Couple." In *Magnesium Technology 2011*, edited by W. H. Sillekens, S. R. Agnew, N. R. Neelameggham, and S. N. Mathaudhu, 549-552. Warrendale, Pennsylvania: The Minerals, Metals & Materials Society.

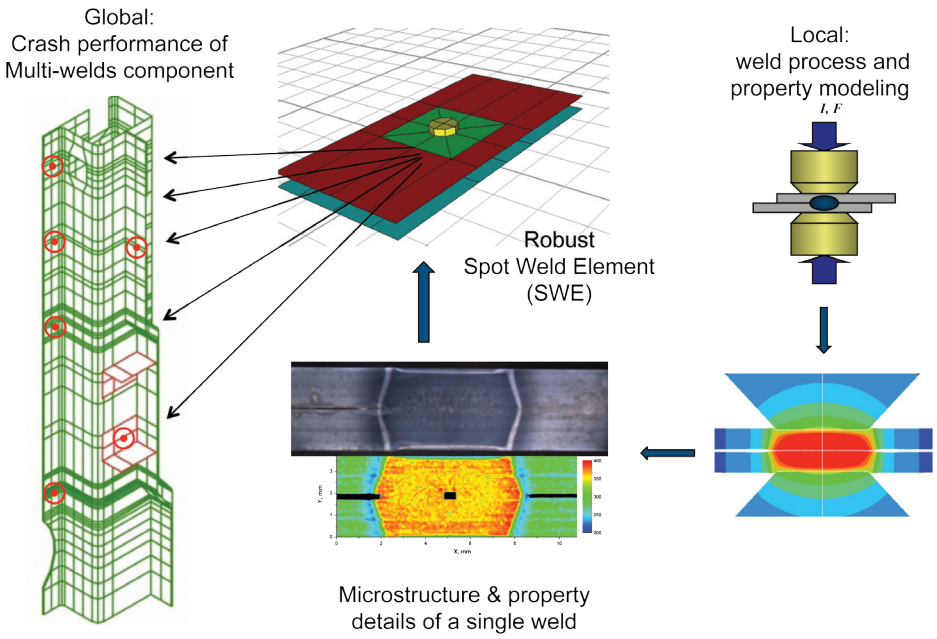
- Brennan, S., K. Bermudez, N. Kulkarni, and Y. H. Sohn. "Diffusion Couple Investigation of the Mg-Zn System." In *Magnesium Technology 2012*, edited by S.N. Mathaudhu, N. Hort, W.H. Sillekens N.R. Neelameggham. Warrendale, Pennsylvania: The Minerals, Metals & Materials Society. Forthcoming.

- Brennan, S., et al. "Aluminum Impurity Diffusion in Polycrystalline Magnesium." *Journal of Phase Equilibria and Diffusion.* Forthcoming.

- Belova, I. V., T. Fiedler, N. Kulkarni and G. E. Murch. "The Harrison Diffusion Kinetics Regimes in Solute Grain Boundary Diffusion." *Philosophical Magazine A.* Forthcoming.

Dynamic Characterization of Spot Welds in Advanced High Strength Steels

An ORNL team is developing a fundamental understanding of the behavior of spot welds in advanced high-strength steels (AHSSs). This project will enable more widespread use of AHSSs in vehicles, resulting in drastic improvements in performance while reducing vehicle weight. Resistance spot welding is the most common joining process used in automotive manufacturing, however, spot weld failure behavior in a dynamic crash event is not well understood for AHSSs. Typically there are several thousand spot welds in a vehicle, and spot weld failure can affect the crash response of welded structural components. ORNL is developing a spot weld modeling tool that is easy for engineers to use in advanced auto-body crashworthiness computer aided engineering. The end product will be an optimized model that can be implemented in crash simulation finite element analysis codes. The development employs a three-pronged approach:



Local-global approach for developing robust spot weld crash simulation framework.

- a spot weld element formulation and associated constitutive models for robustness in computer aided engineering simulation, with the complexity to incorporate weld geometry and microstructure effects;
- a physics based integrated electrical-thermal-mechanical-metallurgical spot weld process model to generate the weld geometry, microstructure, and residual stress results needed by the spot weld element; and
- a companion weld characterization and impact test database for development and validation of the new spot weld modeling approach.

In 2011 the team completed comprehensive testing and characterization of resistance spot welds, generating a data set of static strength and failure modes under 4 loading conditions covering 17 groups of AHSS grades, coatings, and thicknesses. For each group, welds were produced with three different weld nugget sizes. The welded samples were tested under lap-shear, cross-tension, and coach-peel conditions and a specially designed in-plane torsion condition. The testing matrix covered more than 220 unique combinations of materials, welding, and mechanical testing conditions. Multiple duplicates of welds were produced for each combination for microstructure characterization, microhardness mapping, and miniature mechanical property testing to be carried out in 2012. A project web page has been created to distribute FEM models, formulations, and results at thyme.ornl.gov/SPW.

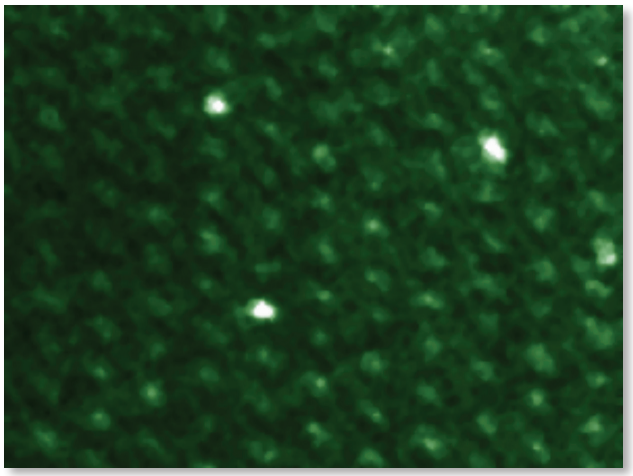
The integrated spot welding process and performance model has been successfully developed with all essential features to handle various materials, joint geometries, and welding process conditions typically encountered in resistance spot welding of AHSS auto body components and has been shown to be stable and robust. The model will be further validated in 2012 using the experimental data set generated in 2011.

Propulsion System Materials

Ultrahigh-Resolution Electron Microscopy for Catalyst Characterization

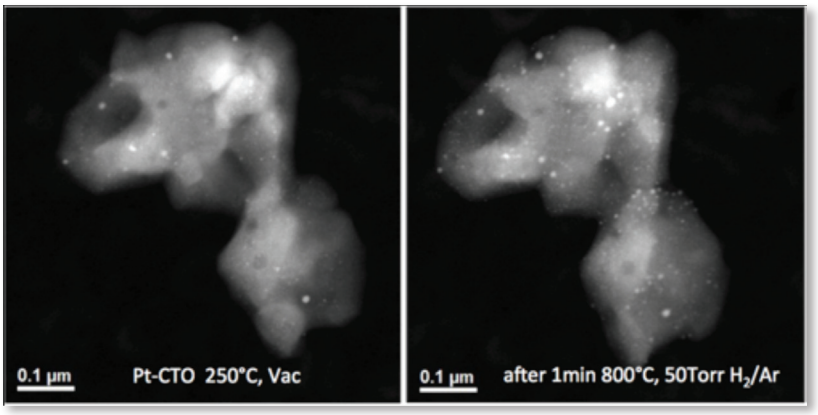
Oak Ridge National Laboratory (ORNL) is using the ultrahigh-resolution aberration-corrected electron microscope at the High Temperature Materials Laboratory to advance fundamental understanding of how catalysts behave at the atomic level. This research has shown, through sub-Ångström resolution imaging coupled with surface analytical techniques, that single atoms can catalyze reactions and be stable for long periods. The first demonstration of the efficacy of single-atom catalysis offers the promise of after-treatment systems that lower vehicle emissions at a reduced cost (due to lower catalyst loading) with a higher performance level than conventional catalysis. ORNL is partnering with universities, industry, and another national laboratory to use these capabilities for studies of catalytic materials and reactions leading to improved automotive catalysts.

ORNL contributions to this project are furthering catalyst studies through the development of innovative capabilities for imaging catalytic materials in situ at elevated temperatures and pressures up to a full atmosphere, and under reactive gas conditions. This allows atomic-level imaging in ORNL's aberration-corrected electron microscope that elucidates mechanisms of catalyst behavior. The team is employing a third-generation design environmental cell, or "Gen 3 E-cell," holder that incorporates a unique heater manufactured by an industry partner. The Gen 3 E-cell is used to study new nitrogen oxide reduction materials called "intelligent catalysts," which are composed of



The first example of a "single-atom" catalyst; the three bright spots are platinum atoms on the surface of an iron oxide support material.

precious metal species such as platinum and rhodium in perovskite. Through in situ oxidation and reduction cycling experiments, researchers are obtaining a fundamental understanding of the mechanisms and kinetics of the cyclic dissolution and subsequent reformation of catalytic nanoparticles on support surfaces during the redox cycles. Remarkably, studies of a rhodium-perovskite catalyst in the Gen 3 E-cell showed atomic structure at the Ångström level can be imaged at elevated temperatures in gas pressures up to a full atmosphere in the cell with essentially no loss of signal. ORNL's in situ heating technology is the only method in the field that presently allows such precision control of a reaction process, in time, temperature, and pressure.



Results of a reduction experiment on a platinum-perovskite material using ORNL's specialized in situ heating technology. Bright spots are platinum nanoparticles. Image on the left was taken before the reduction treatment; image on the right is after a reduction treatment for 1 minute in a 50 Torr reducing atmosphere at a nominal temperature of 800°C.

Publications

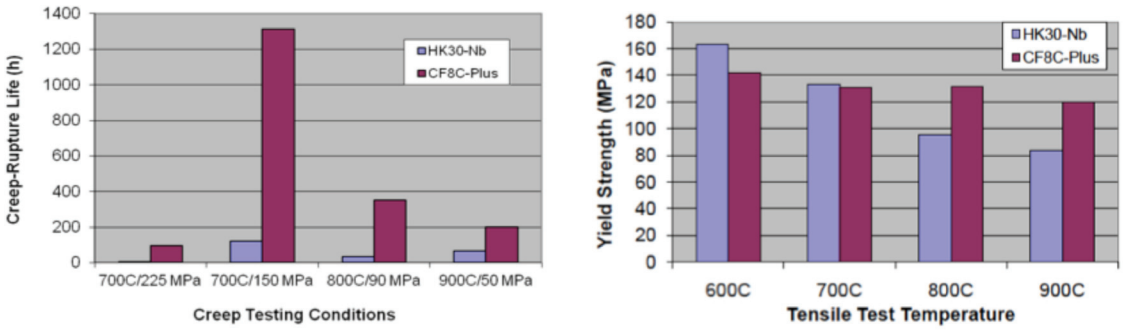
• Qiao, B., et al. August 2011. "Single-atom Catalysis of CO Oxidation using Pt_1/FeO_x." *Nature Chemistry* 3(8):634–641.

ORNL's CF8C-Plus Stainless Steel Targeted for High Temperature Turbocharger Applications

ORNL is partnering with Honeywell, a major international turbocharger manufacturer, to develop new materials for advanced turbocharger components.

Turbochargers are key components in advanced fuel-efficient engines. They are used to increase power output and efficiency by increasing the ratio of mass to air to the cylinders, thereby enabling higher fueling rates, more power, and reductions in engine size without increasing regulated emissions. Recent advances in turbocharging have yielded higher intake pressures resulting in efficiency improvements up to 20% in gasoline engines and up to 40% in diesel engines. Additional efficiency gains are expected with further increases in pressure; however, these increases in pressure and the accompanying increases in temperature are stressing traditional turbocharger materials and driving the search for newer, more robust materials and designs to withstand these more extreme conditions.

Honeywell and ORNL initially assessed the effects of higher exhaust temperatures on turbocharger materials and components and identified turbocharger housings as priority components for consideration under this project. Several years ago ORNL developed a special cast austenitic stainless steel, CF8C-Plus, with higher temperature capabilities and greater durability. CF8C-Plus is in commercial use in advanced diesel engine exhaust component applications. Alloying additions of manganese and nitrogen give this alloy excellent castability and improved high-temperature strength based on nanoscale dispersions of carbide and nitride precipitates. The CF8C-Plus steel also has good fatigue



Comparison of creep rupture (top) and yield strength (bottom) for CF8C-Plus and HK30Nb cast austenitic stainless steels.

resistance and aging resistance. Honeywell and ORNL have targeted this material for more in-depth study as a potential upgrade material for the turbocharger housing application.

Turbocharger housings for diesel and gasoline engines are typically made of cast irons, which have limitations in terms of temperature capability. To date, comparisons of CF8C-Plus steel to various cast irons have established CF8C-Plus' superiority. The CF8C-Plus steel alloy has also demonstrated much better creep rupture resistance and greater tensile strength in the temperature range from 700°C to 900°C compared to other more expensive commercial stainless alloys such as HK30Nb. In addition, use of CF8C-Plus in turbocharger housings would reduce turbocharger weight relative to cast iron further contributing to fuel efficiency and life cycle energy savings.

CF8C-Plus has not yet been commercialized for Honeywell turbochargers, but the material is showing promise as a turbo housing material. Honeywell and ORNL are continuing to partner on turbocharger housing materials under this project and are expanding the search to alternate high-temperature materials for other turbocharger components.

Publications

- Maziasz, Philip J., and Pat Pattabiraman. 2011. "CRADA NFE-08-01671—Materials for Advanced Turbocharger Design." Presented at the 2011 DOE Hydrogen Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting, Washington, D.C., May 9–13.

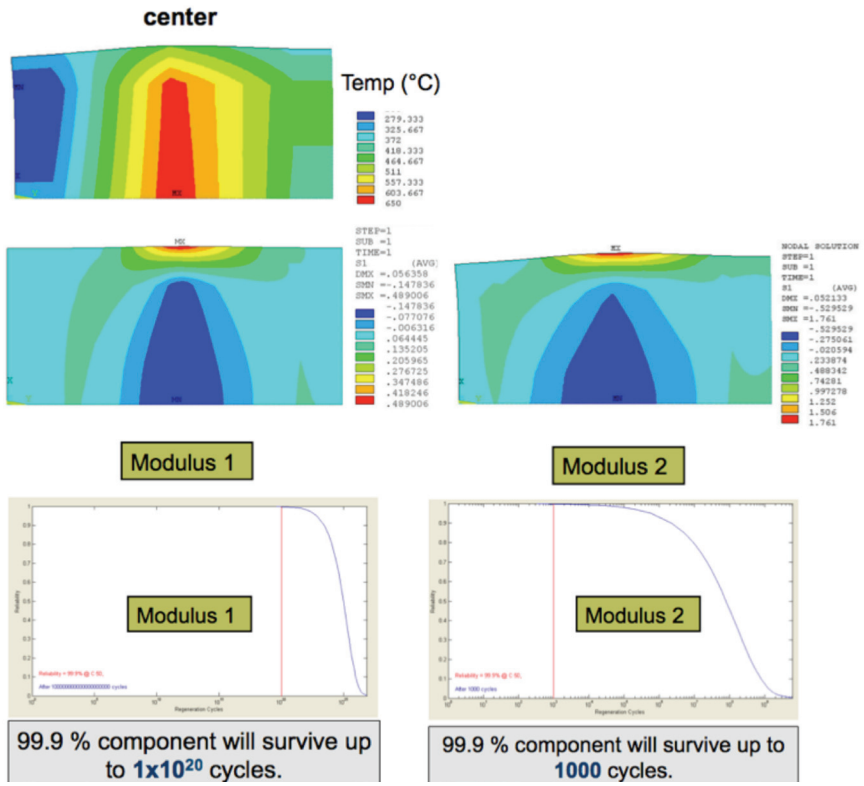
- Maziasz, P. J., A. Shyam, and N. D. Evans. 2010. *Cast CF8C-Plus Stainless Steel for Turbocharger Applications*. ORNL/TM-2010/86, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Durability of Diesel Particulate Filters

ORNL's modeling capabilities, which have proven successful in elucidating materials science phenomena that impact industry, were recently put to use in modeling diesel particulate filter (DPF) service life.

DPFs reduce emissions of particulate matter (PM), or soot; hydrocarbons; and carbon monoxide by 60–90% thus enabling advanced diesel engines to meet the stringent regulation of PM that went into effect in 2007. DPF service life predictions are therefore of great importance to the automotive and truck industries.

Ceramic honeycomb devices are typically used as DPFs. They collect PM in the exhaust stream of the engine. Because ceramics are highly heat resistant, they can withstand the high temperature of the exhaust (approximately 500°C) needed to break down or oxidize PM inside the filter. This process is called filter regeneration and is triggered when a specified level of PM accumulates in the DPF.

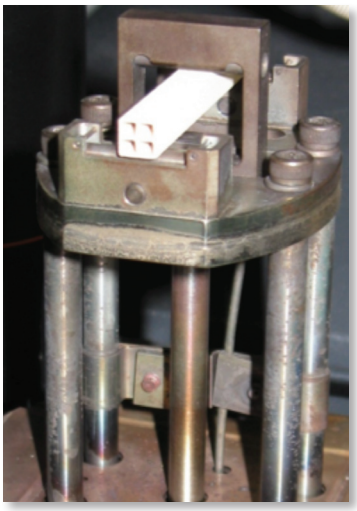


The top image shows an axisymmetric DPF with a predefined thermal profile. As the exhaust flows left to right, the profile is hottest in the center. The middle images show the corresponding thermal strain for two DPFs, one (modulus 2, on the right) with an elastic modulus twice that of the other (modulus 1, on the left). The bottom graphs show a lower elastic modulus results in a significantly higher predicted number of regeneration cycles before DPF failure.

DPF service life predictions are based on a combination of experimentally determined strength data, stress analyses (for example, that produced using finite-element analysis), and selection of appropriate failure criteria. Typically, experimental material data are collected and then used in predictive models to estimate filter lifetimes in terms of regeneration cycles.

Recent end-user observations of DPF performance indicate service lifetime expectations longer than ever before—positive news for manufacturers and industry. To explore the cause of the low failure rate, General Motors and ORNL researchers found the apparent elastic modulus of the filter ceramics to be almost an order of magnitude lower than industry-accepted values when using more appropriate means for its measurement. According to ORNL's Andrew Wereszczak, "The measurements indicate that while the filter is under thermally induced strain, such as that during regeneration, the actual internal stresses are much lower and mechanical reliability is much higher than manufacturer models have predicted in the past because of that lower actual elastic modulus."

Further understanding of the relationships between microstructural material properties and their performance in DPFs will lead to improved materials and designs that will enhance the effectiveness and efficiency of diesel engines in general. Cleaner diesel operation will help increase public acceptance of the more fuel-efficient diesel with a resulting concomitant reduction in petroleum use.



Experimental set up for measuring elastic modulus. The 2 × 2 cell specimen is loaded in 3-point-bending apparatus, and its deflection response is measured as a function of frequency while oscillation amplitude is held constant.

Publications

- Lance, M. J., et al. January 2012. "Agreement 20091 - Electrically-Assisted Diesel Particulate Filter Regeneration." In *2011 Progress Report for Propulsion Materials,* 253–271. ORNL/TM-2011/34212, U.S. Department of Energy, Washington, D.C.

Power Electronics & Electric Machines

Inverter Using Current Source Topology

ORNL researchers have designed, fabricated, and tested a 10 kW Z-source current source inverter (ZCSI) prototype that promises to overcome the drawbacks of traditional voltage source inverters (VSIs) and significantly advance electric vehicle technology toward DOE and U.S. DRIVE goals for size, weight, and cost.

VSIs using film capacitors are universally employed in hybrid, plug-in, and battery electric vehicles. The technology, although mature and well established, has many drawbacks. For example, it requires an expensive and bulky direct current (dc) bus capacitor, and it produces high electromagnetic interference, detrimental voltage stresses on the motor insulation, high frequency losses, and harmful bearing leakage currents. Long-term reliability issues also exist due to possible dc bus shoot-through conditions. Additionally, to increase the output voltage of a VSI a larger battery pack must be used or a dc-dc converter must be incorporated into the system. Both of these options result in unwanted cost, weight, and volume.

To overcome the limitations of VSIs, ORNL researchers are using new reverse-blocking semiconductor devices in a new topology called ZCSI, which integrates the boost converter, inverter, and battery charger functions; improves fault tolerance; and substantially reduces capacitor requirements. The new design is capable of functioning as a universal charger for plug-in hybrid electric vehicles, allowing charging of low-voltage and high-voltage batteries from single- (120 V/240 V) or three-phase supplies. In testing, the prototype has demonstrated the following advances over the conventional VSI technology.

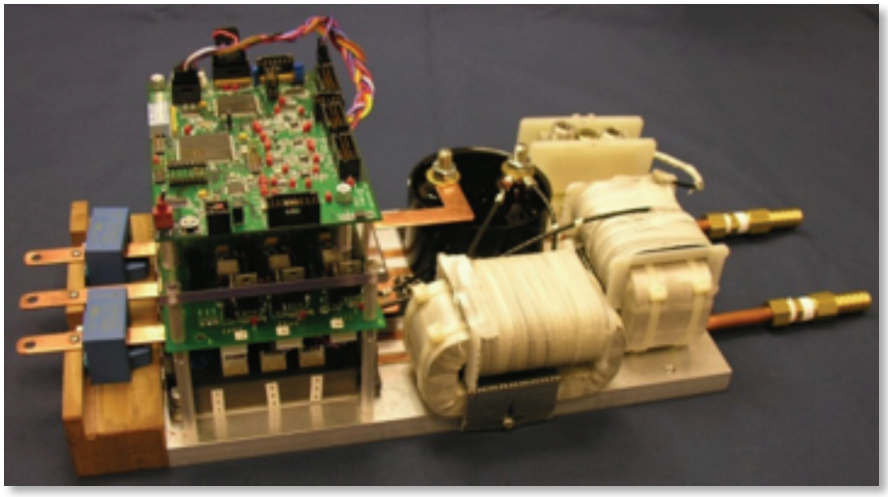
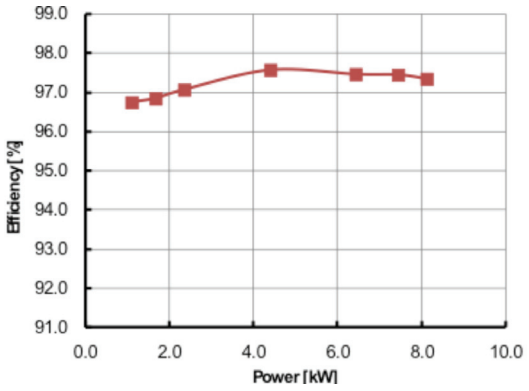


Photo of the 10 kW ZCSI prototype.

- Capacitance reduction to 200 µF (2,000 µF for VSI)
- Output voltage boost capability ranging from 0 to 3 times the battery voltage (0–0.99 for VSI)
- Output voltage total harmonic distortion factors of 6%–12% (70%–200% for VSI)
- Power density and specific power of 4.9 kW/kg, 16.6 kW/L (4.3 kW/kg, 7.1 kW/L for Camry VSI)
- More than 97% efficient even with a relatively low source voltage of 250 V

The prototype 10 kW ZCSI was designed using first generation reverse blocking semiconductor device technology. The project team plans to design, fabricate, and test a 55 kW ZCSI prototype when new reverse blocking switching devices become available.



Efficiency chart for the ZCSI prototype, indicating a maximum efficiency of 97.6%.

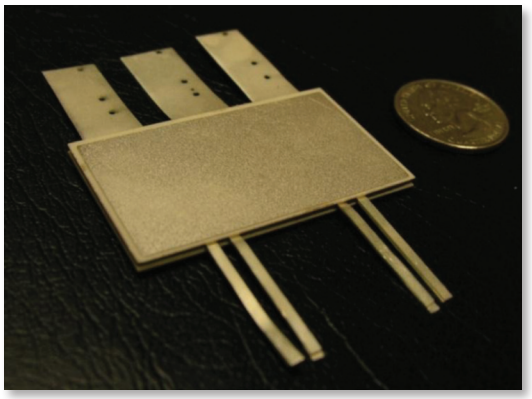
Publications

- Tang, L., and G. J. Su. 2011. "A Novel Current Angle Control Scheme in a Current Source Inverter Fed Surface-Mounted Permanent Magnet Synchronous Motor Drive." *Energy Conversion Congress and Exposition (ECCE), 2011 IEEE,* 2358–2364.
- Su, G. J. "Power Conversion Apparatus and Method." U.S. Patent 8,110,948, filed March 6, 2009, and issued February 7, 2012.

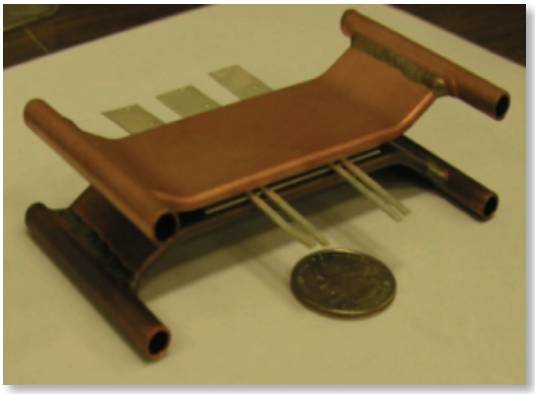
Planar Bond Power Electronics Module

ORNL is developing advanced automotive power electronics packaging technologies to help achieve DOE and U.S. DRIVE targets for power density and cost. This involves multidisciplinary capabilities including material development and characterization; thermal, electrical, and thermomechanical expertise; and reliability, process, and manufacturing considerations.

A prototype 200 A/1,200 V phase leg power module, called "Planar_Bond_All," has been fabricated in-house at the ORNL Power Electronics Packaging Laboratory. The module features double-sided planar electrical interconnections and integrated mini-coolers. The versatility of the module allows it to be air cooled on pin fins or cooled with liquid mini-coolers on one or both sides for increased heat rejection. The module's planar interconnections allow large bonding contact areas. The package is constructed so that the switch die are oriented in face up/face down insulated gate bipolar transistor/diode die pairs. This packaging arrangement leads to significantly reduced parasitic parameters—80% less than the state-of-the-art module in the 2010 Toyota Prius; and the double-sided cooling capability reduces the thermal resistivity of the whole module assembly to 0.33°C·cm^2/W—30% less than the 2010 Prius module.



Planar_Bond_All photo showing double-sided planar interconnections.



Planar_Bond_All photo showing double-sided planar interconnections and integrated mini-coolers.

But what makes Planar_Bond_All truly a paradigm shift in power module packaging is the processing technology used to create the module. It reduces the conventional multiple hybrid packaging processes to just two steps. In the first step all the components are assembled into a fixture for processing. The second step involves heating of the assembly to form the bonds and create the final package. The simplicity of the process will reduce costs and improve the manufacturability of the module.

Publications

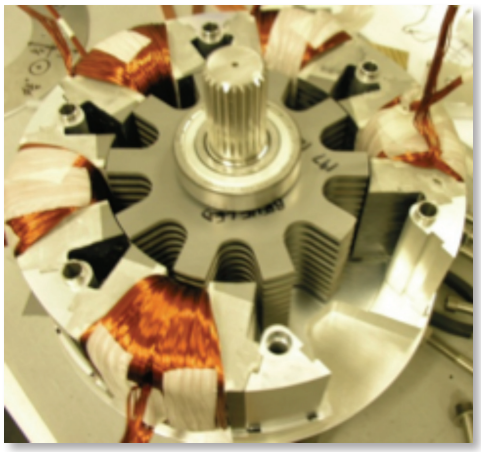
- Liang, Zhenxian, Fred Wang, Puqi Ning, and Laura Marlino. Power Module Packaging with Double Sided Planar Interconnection and Heat Exchangers. U.S. Patent application serial number 61/509,312.
- Liang, Zhenxian, Puqi Ning, Fred Wang, and Laura Marlino. 2011. "Power Module Packaging with Double Sided Planar Interconnection and Heat Exchanger." Presented at ORNL Power Electronics Symposium, Oak Ridge, Tennessee, July 22.

Novel Switched Reluctance Motor Design

Switched reluctance (SR) motors are of interest to automotive manufacturers because they do not use rare earth permanent magnets, which are subject to unpredictable availability and cost; and because their simplicity offers many cost and manufacturing benefits. Two primary drawbacks of the SR motor are the level of torque ripple and the acoustic noise inherently associated with its stator and rotor geometry. ORNL has developed a novel SR motor with isolated multiple flux paths (IMFPs) to facilitate better control over torque ripple and acoustic noise with a secondary goal of improving power density and specific power. An SR motor stator and/or rotor with IMFP segments has the potential to locate teeth within closer proximity of each other while maintaining magnetic saliency, which is the fundamental manner in which torque is produced in SR motors.

The final SR motor design consists of 6 segmented stator pieces forming 12 stator teeth and a conventional SR rotor with 10 teeth. The use of segmented stator pieces opens up design opportunities that can lead to increased power density and/or reduced torque ripple and acoustic noise. One primary advantage is the capability to have yoke-wound stator coils, as shown in the figure. While using this winding technique at first seems insignificant, a closer look reveals the following benefits.

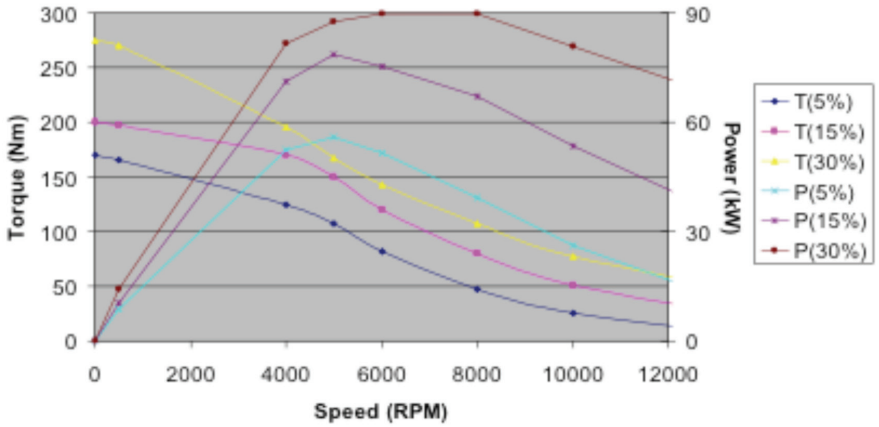
- Copper windings are located on the outer perimeter of the motor and are well positioned for interfacing with a heat exchanger for improved heat transfer. This will increase continuous operation capability.



Partially assembled prototype showing yoke-wound stator coils.

- Broader teeth allow the torque production from each phase to overlap the torque production between phases. Increased overlap of torque production between phases can reduce torque ripple, and because the broader teeth are more substantial, they are less likely to vibrate and create acoustic noise.
- Slots contain one coil instead of two, thereby eliminating issues with interference between coils.
- Stator pieces can be wound before installation, facilitating manufacturability.
- Voids between stator pieces can be filled with noise damping material.

Because of the unconventional nature of the IMFP SR motor, ORNL developed custom design and simulation tools that were used in optimization studies and in formulating control algorithms. In simulations the novel SR motor achieved 52.4 kW (125 Nm at 4,000 rpm) with 5% torque ripple and 93% efficiency. A prototype has been fabricated and is being testing in the dynamometer facility at ORNL's Power Electronics and Electric Machinery Research Center.



Simulated peak torque and power versus speed for various torque ripple levels.

Publications

- Burress, T., and C. Ayers. Isolated Multiple Flux Path Reluctance Motors with Yoke-Wound Coils and Wedge Supports. U.S. Patent application serial number 61/509,213.

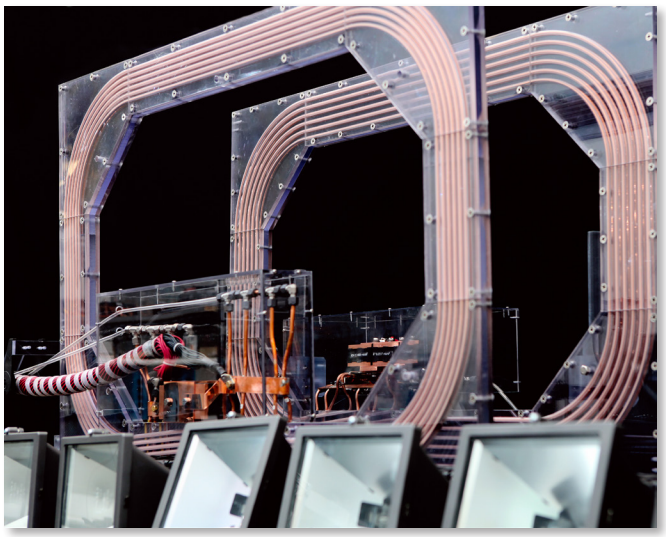
Vehicle & Systems Simulation & Integration

Wireless Plug-In Electric Vehicle Charging Development and Demonstration

Wireless power transfer (WPT) permits a plug-in electric vehicle (PEV) to recharge its battery without plugging in. It is seen as a key enabling technology supporting widespread acceptance of PEVs. ORNL has developed and demonstrated, in laboratory-scale experiments, a new WPT concept that has achieved efficiencies in the low 90% range. Current WPT systems operating at high power typically have efficiencies in the high 70% to high 80% range. ORNL's objectives were twofold: (1) to develop full analytical, computational, and experimental understanding of the physics of wireless power charging so that implementation designs will meet industry requirements for efficiency, safety, cost, and vehicle packaging criteria; and (2) to develop WPT stationary charging sufficiently for integration into a demonstration vehicle.

ORNL leveraged its "evanescent wave" experimental hardware, a Laboratory Directed Research and Development technology, to show the flexibility of WPT in accommodating arbitrary receiver-side voltage levels (120 Vdc, 240 Vdc, and moving to 270 Vdc). This will be required for WPT in future vehicle applications because there is not a standardized PEV battery pack voltage level.

Work to date has established a firm foundation in the fundamentals of WPT opera-



WPT Laboratory apparatus in copper tube coil configuration.

tion from both analytical and experimental investigations. Primary activity has focused on coupling coil electromagnetic performance, magnetic field strength, emissions levels, and closest approach boundary for compliance with international standards. Coupling coils constructed of copper tube and flat designs were compared in experimental tests; both exhibited comparable efficiency with the ac resistance of each being within 2%. A more fundamental finding, based on analytical work, was that the insulated gate bipolar transistors (current technology) are limiting the operation to suboptimal conditions. Recent announcements indicate that new insulated gate bipolar transistors capable of high current switching up to 200 kHz may be available in the near future; if not, the team will work with ORNL's Power Electronics Packaging Laboratory to fabricate high-frequency power modules.

Future work includes optimizing the coupling coil designs and fabricating and testing suitably packaged transmit (primary) and receiver (secondary) pads based on those optimized designs. The effects of concrete, asphalt, plastic and plywood on coupling coil transfer efficiency and system tuning have been evaluated. The full WPT system will be bench validated and then integrated into a vehicle for demonstration on the ORNL Hardin Valley campus.

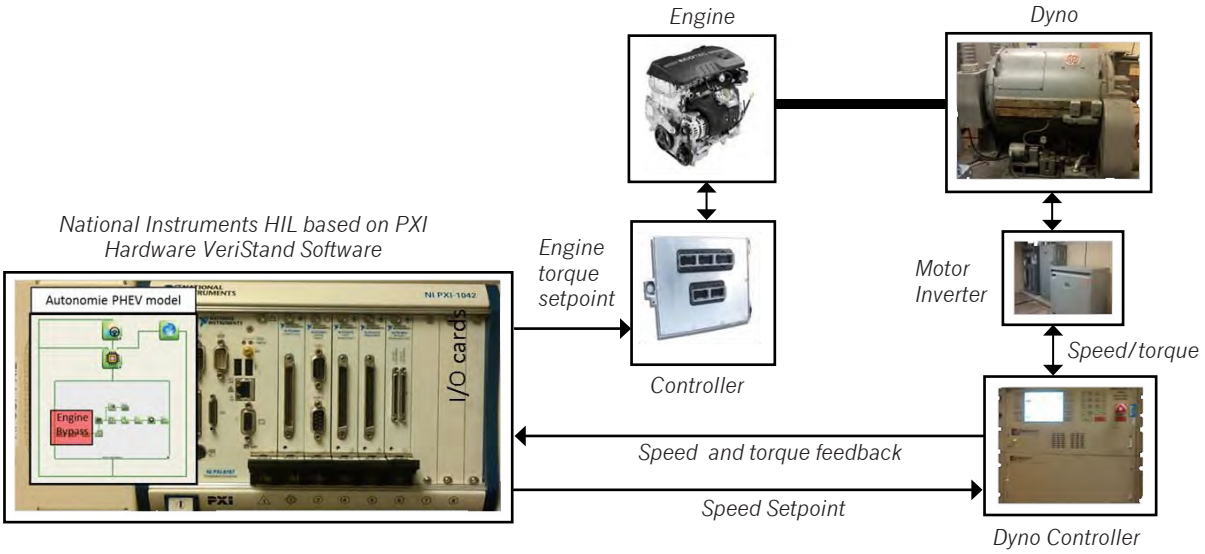
Publications

- Scudiere, M., J. McKeever, and J. M. Miller. 2011. "Wireless Power Transfer for Electric Vehicles." Presented at SAE World Congress, Detroit, Michigan, April 12–14. Paper number 2011-01-0354. doi:10.4271/2011-01-0354
- Miller, J. M. "Coupling Coil ac Resistance Minimization Using Graphene Coatings." U.S. Patent Application 61/510,206, filed July 21, 2011.
- Miller, J. M. "Regulation Control and Energy Management Strategy for Wireless Power Transfer." U.S. Patent Application 61/510,210, filed July 21, 2011.
- Miller, J. M., and P. T. Jones. "WPT EVSE Installation and Validation Tool." U.S. Patent Application 61/510,231, filed July 21, 2011.

Plug-In Hybrid Electric Vehicle Engine Control and Energy Management Strategy

Plug-in hybrid electric vehicles (PHEVs) have the potential to reduce petroleum consumption considerably; however, this is at the expense of increased tailpipe emissions due to multiple cold start events for the gasoline engine. PHEVs operate predominantly as electric vehicles (EVs) with intermittent assist from the engine during high power demands (for example, accelerating from urban traffic to highway driving). As a consequence, the engine experiences multiple cold start events that have a significant impact on tailpipe emissions due to degraded catalyst performance and starting the engine under less than ideal conditions. ORNL is working with industry partners, universities, and other national laboratories to address the cold start challenge in PHEVs through novel engine control strategies targeted at rapid engine and catalyst warming to mitigate tailpipe emissions. The project team also aims to validate and optimize hybrid supervisory control techniques developed during other research projects by integrating them into the vehicle level control system and complementing them with modified engine control strategies to further reduce emissions during both cold start and engine restarts.

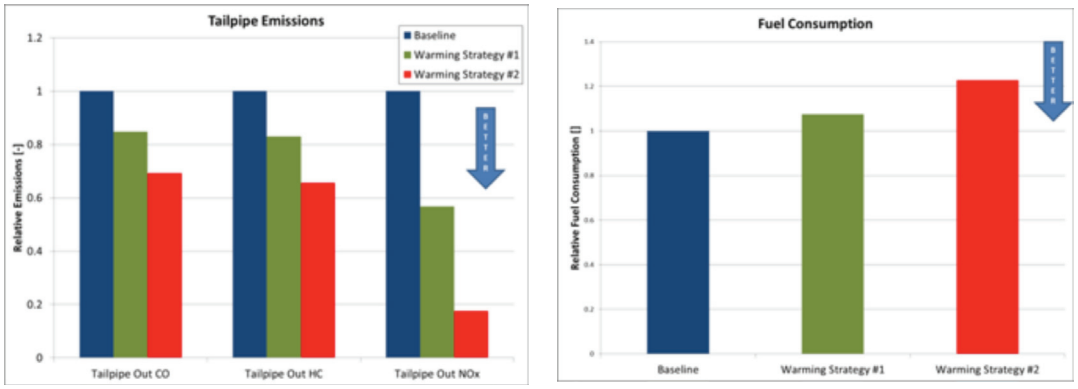
A modified production engine controller from Robert Bosch LLC is being used on a GM Ecotec LNF engine; the engine and controller were commissioned on an engine test cell in the ORNL Fuels, Engines and Emissions Research Center. The open-calibration controller allows modification of cold start strategies to assess the effects of different operat-



Engine-in-the-loop test platform.

ing modes on the engine and emissions mitigation systems. The project team is using the Autonomie simulation program (developed by Argonne National Laboratory) in a unique "engine-in-the-loop" test system that allows interfacing the Autonomie PHEV model with the real engine on a dynamometer test stand.

The control system has been tested to demonstrate the impact of various engine control parameters on cold start emissions, and the test setup was used to demonstrate the potential for further emissions reduction and faster catalyst warm-up by modifying engine cold start calibration. During 2012, the project team will proceed with combined optimization of both engine- and vehicle-level strategies to achieve lower cold start emissions in the hybrid powertrain configuration.



Emissions improvements and fuel penalty associated with vehicle supervisory strategies that prewarm the engine and filter out transient conditions while the engine is cold.

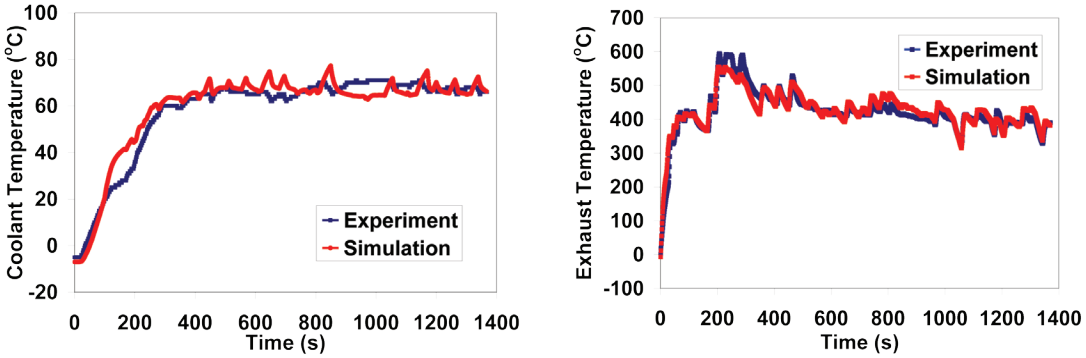
Publications

- Chambon, Paul H. 2011. "PHEV Engine Control and Energy Management Strategy." Presented at the 2011 U.S. DOE Hydrogen Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting, Washington, D.C., May 9–23.

Advanced Modeling and Analysis for Hybrid Vehicle Systems

Accurate predictions of the fuel efficiency and environmental impact of advanced vehicle propulsion and emissions control technologies are vital for informed decision making about DOE programmatic priorities and optimal use of DOE resources. To this end, DOE tasked ORNL with providing component data and models that enable simulations of hybrid vehicle systems with advanced engines and emissions controls. ORNL's progress includes numerous experimental measurements of emissions and fuel efficiency for advanced diesel and lean-burn gasoline engines and their associated emissions control components. These data have been transformed into maps and low-order transient models that support vehicle performance simulations. In 2011, the ORNL team collaborated with Argonne and Pacific Northwest National Laboratories to develop integrated transient engine and aftertreatment component models suitable for implementation in PSAT and Autonomie. These models were then used to generate improved simulations of emissions and fuel economy for hybrid electric vehicles (HEVs) and plug-in hybrid electric vehicles (PHEVs) powered by both stoichiometric and lean-burn engines. Major accomplishments included the following.

- Constructed and made preliminary parameter estimates for a computational model of a passive adsorber for exhaust hydrocarbons and nitrogen oxides (NO_x), and applied the adsorber model to simulations of HEVs and PHEVs with stoichiometric gasoline engines and three-way catalyst (TWC) emissions controls.
- Enhanced a previously developed transient engine model to explicitly include thermal interactions among the engine block, coolant, and radiator.
- Evaluated the potential benefits of advanced combustion and aftertreatment technologies on fuel efficiency and emissions control of diesel-powered hybrid vehicles equipped with appropriate aftertreatment trains.



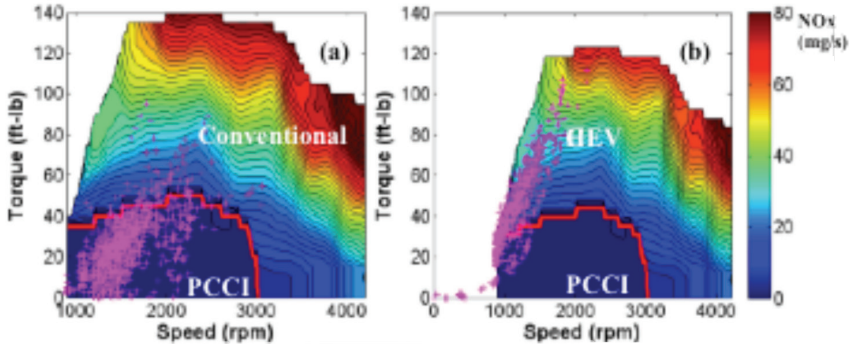
Comparison between predicted and measured coolant temperature and exhaust temperature for the PHEV Prius with a cold start at -7°C.

- Successfully translated ORNL's low-order TWC, diesel oxidation catalyst, lean NO_x trap, catalyzed diesel particulate filter, and transient engine models from PSAT into Autonomie.

- Developed an independent graphical input simulation tool for TWC for research use.

Modeling and research results were made available to the public in a series of articles including one comparing the simulated emissions and fuel efficiencies of diesel and gasoline hybrid electric vehicles and another on a phenomenological computer model for rapidly estimating NO_x and particulate emissions from advanced diesel engines operating in the premixed-charge compression ignition mode.

The tools developed to date will be transferred to system simulation tasks associated with a Cooperative Research and Development Agreement between ORNL and Meritor, and simulations of cold-start effects and control system optimization in collaboration with other national laboratories.



Engine speed-load map illustrating opportunities for premixed-charge compression ignition use during an urban driving duty cycle for (a) a conventional (nonhybrid) passenger vehicle and (b) an equivalent size HEV. Pink crosses correspond to engine operating points. Solid colors correspond to engine-out NO_X levels.

Publications

- Gao, Z., V. K. Chakravarthy, and C. S. Daw. 2011. "Comparisons of Simulated Emissions and Fuel Efficiency of Diesel and Gasoline Hybrid Electric Vehicles." *Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering* 225(7):944–959.

- Gao, Z., R. M. Wagner, C. S. Sluder, C. S. Daw, and J. B. Green Jr. 2011. "Using a Phenomenological Computer Model to Investigate Advanced Combustion Trajectories in a CIDI Engine." *Fuel* 90(5):1907–1918.

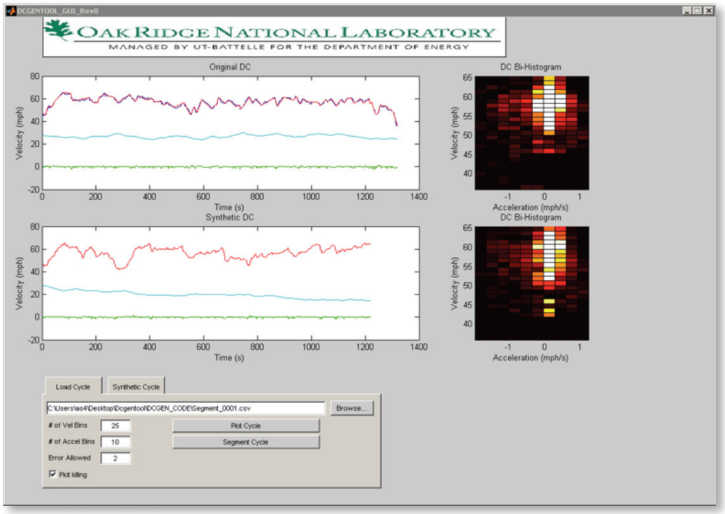
Medium Truck Duty Cycle Project

ORNL's Medium Truck Duty Cycle (MTDC) project—involving data collection, analysis, and reporting for Class 6 and 7 trucks—is producing a database of duty cycle and vehicle performance data available nowhere else in the world. The MTDC project complements a prior, similar effort that focused on Class 8 trucks. Together, the data represent an unprecedented 800 million records of heavy- and medium-size vehicle information in one database. The information is supporting DOE's modeling efforts and technology investment decision-making, as well as specialized energy efficiency studies. The MTDC project collected 73 channels of data related to fuel use, engine parameters, speed, direction of travel, time of day, geographic position, road grade, weather conditions, and road conditions. Transit buses, Class 7 combination tractor-trailers, utility trucks, and towing and recovery trucks were included in the study. Data collection has been completed and analysis is ongoing. Overall, the MTDC project has produced about 245 GB of data. In the future, a public website will be developed where researchers can access analyzed and summarized data.

The project team has developed a set of software tools to quickly interrogate the data available on a candidate vehicle, wirelessly transfer data from the vehicles, validate the data, and select data segments for analysis. In addition, a Duty Cycle Generation Tool is being developed that will allow the research community to generate customized, real world–based duty cycles; for example, a duty cycle for a metropolitan area during peak travel times, or one for a rural area with steep grades. The Duty Cycle Generation Tool can also be used to generate synthetic duty cycles statistically representative of original duty cycles, but much smaller, making analysis and modeling faster while giving the same or similar results.

Bucket truck (left) and flat-bed recovery vehicle (right) representative of vehicles used in the MTDC project.

The MTDC and heavy truck duty cycle projects are meeting diverse research needs. Argonne National Laboratory has used the database in support of its vehicle modeling using the Powertrain System Analysis Toolkit and Autonomie tools. The Department of Transportation's Federal Motor Carrier Safety Administration has joined with the project to collect brake and tire performance data. Heavy truck data were used in an ORNL study of the effects of weight and grade on fuel economy for the Department of Transportation's Federal Highway Administration. Additionally, methods for synthetically generating emissions data are being discussed and a potential partnership with the Environmental Protection Agency is being explored.



Duty Cycle Generation Tool showing comparison of original (top) and synthetic (bottom) duty cycles

Publications

- Franzese, O., M. B. Lascurain, and G. Capps. 2011. *Medium Truck Duty Cycle Data from Real-World Driving Environments: Project Interim Report.* ORNL/TM-2010/255, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

- Franzese, O., and D. Davidson. 2011. *Effect of Weight and Roadway Grade on the Fuel Economy of Class-8 Freight Trucks.* ORNL-TM-2011/471, Oak Ridge National Laboratory, Oak Ridge, Tennessee.