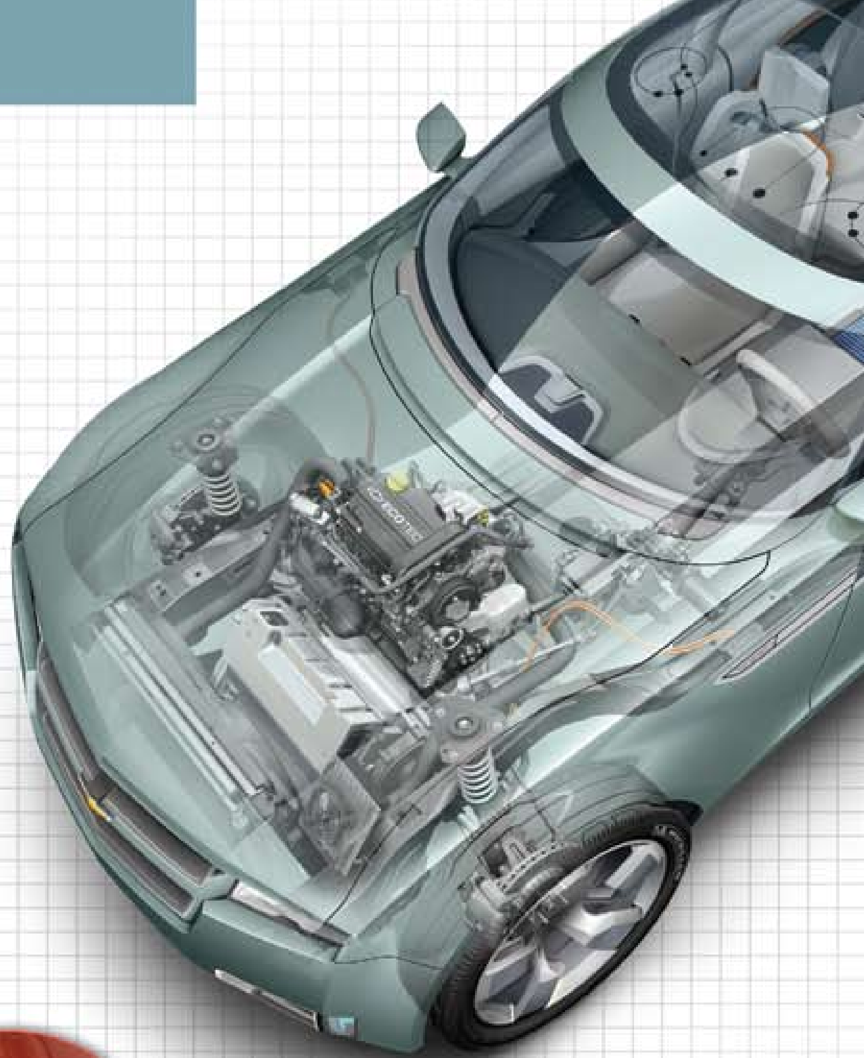


Transportation Technology Program

Annual Report Fiscal Year 2008

Compiled by
Kathy J. Graham, Oak Ridge National Laboratory
for Dr. Raymond G. Boeman, Director
Transportation Technology Program
Oak Ridge National Laboratory

Prepared for
Patrick B. Davis, Program Manager
Vehicle Technologies Program
Office of Energy Efficiency and Renewable Energy
U.S. Department of Energy

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
managed by
UT-BATTELLE, LLC
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

Contents

List of Acronyms Used

3D	three-dimensional
21CTP	21st Century Truck Partnership
ac	alternating current
ACC	Automotive Composites Consortium
ACEM	aberration-corrected electron microscope
ACERT	advanced combustion emissions reduction technology
AHSS	advanced high-strength steel
APEEM	Advanced Power Electronics and Electric Machines
ASE	Alliance to Save Energy
Au	gold
B20	fuel containing 20% biodiesel
BTE	brake thermal efficiency
CAE	computer-aided engineering
CLEERS	Cross-cut Lean Exhaust Emissions Reduction Simulation
CO	carbon monoxide
Co	cobalt
CSI	current source inverter
CRADA	Cooperative Research and Development Agreement
dc	direct current
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
DPF	diesel particulate filter
E85	85% ethanol : 15% gasoline blend
ECVT	electronic continuously variable transmission
EDS	energy-dispersive X-ray spectroscopy
EERE	Office of Energy Efficiency and Renewable Energy
EETT	Electrical and Electronics Technical Team
EGR	exhaust gas recirculation
EIA	Energy Information Administration
EISA	Energy Independence and Security Act
EPA	U.S. Environmental Protection Agency
EPFL	Ecole Polytechnique Federal de Lausanne
EV	electric vehicle
FACE	Fuels for Advanced Combustion Engines Group
FCV	fuel cell vehicle
FEA	finite element analysis
FEG	*Fuel Economy Guide*
FMCSA	Federal Motor Carrier Safety Administration
FSCW	fractional-slot concentrated winding
FY	fiscal year
GHG	greenhouse gas
HC	hydrocarbon
HCCI	homogeneous charge compression ignition
HECC	high efficiency clean combustion
HEV	hybrid electric vehicle

HTDC	heavy truck duty cycle
HTML	High Temperature Materials Laboratory
HTRI	high temperature, repetitive-impact
iBlends	intermediate ethanol blends
IC	integrated circuit
ICME	integrated computational materials engineering
IGBT	insulated gate bipolar transistor
IPM	interior permanent magnet
IR	infrared
LAST	lead-antimony-silver-tellurium
LDRD	Laboratory Directed R&D
LFT	long fiber thernoplastic
LM	lightweighting materials
LNT	lean NO_x trap
MEMS	microelectromechanical systems
MPG	miles per gallon
MSAT	mobile source air toxic
MSRP	manufacturer's suggested retail price
MSU	Mississippi State University
MTDC	medium truck duty cycle
MY	model year
NDE	nondestructive evaluation
NO_x	oxides of nitrogen/nitrogen oxide
NREL	National Renewable Energy Laboratory
NTRC	National Transportation Research Center
OEM	original equipment manufacturer
ORNL	Oak Ridge National Laboratory
P4	programmable powdered preform process
PAN	polyacrylonitrile
PbTe	lead telluride
PCCI	premixed charge compression ignition
PCU	power control unit
Pd	palladium
PDA	personal digital assistant
PED	power electronic device
PHEV	plug-in hybrid electric vehicle
PM	particulate matter
PNNL	Pacific Northwest National Laboratory
PSAT	Powertrain System Analysis Toolkit
Pt	platinum
PZT	lead zirconate titanate
R&D	research and development
RSW	resistance spot welding
SAcM	scanning acoustic microscopy

SCR	selective catalytic reduction
SI	spark ignition
Si_3N_4	silicon nitride
SiC	silicon carbide
SNL	Sandia National Laboratories
SOI	silicon-on-insulator
SpaciMS	spatially resolved capillary inlet mass spectrometer
SRIM	structural reaction injection molding
STEM	scanning transmission electron microscopy
SWE	spot weld element
TAGS-x	a family of thermoelectric materials comprising compounds made up of germanium, tellurium, silver, and antimony in various proportions
TBC	thermal barrier coating
TE	thermoelectric
TEG	thermoelectric generator
TER	thermal energy recovery
THC	total hydrocarbons
TiAl	titanium-aluminum
TWC	three-way catalyst
UDDS	Urban Dynamic Driving Schedule
UL	Underwriters' Laboratory
ULSD	ultralow sulfur diesel
USABC	United States Advanced Battery Consortium
VSATT	Vehicle Systems Analysis Technical Team
VSI	voltage source inverter
VTP	Vehicle Technologies Program
WFO	Work For Others
XRD	X-ray diffraction

Introduction

The Transportation Technology Program at Oak Ridge National Laboratory (ORNL) supports the mission of the Vehicle Technologies Program (VTP) within the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE). The VTP mission is "to develop more energy-efficient and environmentally friendly highway transportation technologies (for both cars and trucks) that will meet or exceed drivers' performance expectations and environmental requirements and that will enable America to use significantly less petroleum and reduce greenhouse gas (GHG) emissions."[1] The VTP mission supports national goals relating to energy security and GHG reductions. **Table 1** illustrates the flowdown of national goals to VTP performance measures.

ORNL provides VTP with expertise supporting each of the program's performance measures. ORNL performs research and development (R&D) and provides technical support in the areas of combustion, fuel utilization, systems analysis, materials science and technology, electrical engineering, data collection and analysis, and economic analysis of technology and policy options.

ORNL's FY 2008 R&D supporting the VTP performance goals is described in more detail beginning on page 7.

Much of the ORNL Transportation Technology Program R&D is performed in partnership with industry, primarily under two umbrella collaborative arrangements between DOE and industry: the FreedomCAR and Fuel Partnership and the 21st Century Truck Partnership. The FreedomCAR and Fuel Partnership comprises DOE, the U.S. Council for Automotive Research,[2] five energy companies, and two electric utility companies. The FreedomCAR and Fuel Partnership focuses on high-risk, precompetitive research "needed to develop the component and infrastructure technologies necessary to enable a full range of affordable cars and light trucks, and the fueling infrastructure for them that will reduce the dependence of the nation's personal transportation system on imported oil and minimize harmful vehicle emissions, without sacrificing freedom of mobility and freedom of vehicle choice."[3] The 21st Century Truck Partnership focuses on heavy-duty vehicles and includes engine manufacturers, truck and bus manufacturers, hybrid powertrain manufacturers, DOE,

Table 1. Cascade from National Goals to VTP Performance Measures[a]

Goals	**Energy Security and Greenhouse Gas Reductions**				
Strategies	More efficient use of petroleum fuels			Displacement by non-petroleum fuels	
Technical Strategies	More efficient engines	Lighter vehicles	Cost-competitive hybrid vehicles	Optimize combustion of alternative fuels/ blends	Enable cost-competitive plug-in hybrid vehicles
VTP Performance Measures	Improve engine efficiency for gasoline, diesel, and advanced combustion regimes	Reduce cost of advanced materials like carbon fiber	Reduce cost of high-power batteries	Improve gasoline and diesel engine efficiency when using alternative fuel blends	Reduce cost of high-power, high-energy batteries
	Capture and use waste heat		Reduce cost of power electronics and motors		Field demonstration of plug-in hybrid vehicles

[a]*Office of Chief Financial Officer. May 2009. FY 2010 Congressional Budget Request. DOE/CF-037 Vol. 3. U.S. Department of Energy, Washington, D.C.*

[1]Office of Chief Financial Officer. May 2009. *FY 2010 Congressional Budget Request.* DOE/CF-037 Vol. 3. U.S. Department of Energy, Washington, D.C.
[2]The U.S. Council for Automotive Research (USCAR) is a legal partnership among Chrysler Corporation, Ford Motor Company, and General Motors Corporation.
[3]FreedomCAR and Fuel Partnership. March 2006. *Partnership Plan.* Available at http://www1.eere.energy.gov/vehiclesandfuels .

U.S. Department of Defense (DOD), U.S. Department of Transportation (DOT), and U.S. Environmental Protection Agency (EPA). Its objective is "accelerate the introduction of advanced truck and bus technologies that use less fuel, have greater fuel diversity, operate more safely, are more reliable, meet future emissions standards and are cost-effective."[4]

Program Resources

The Transportation Technology Program received about $47M in new budget authority from VTP in FY 2008 **(Figure 1)**. ORNL received funding in every VTP activity except Advanced Vehicle Competitions, Graduate Automotive Technology Education, and Biennial Peer Reviews. The program costed out at about $45M during the fiscal year, with an additional $5M in outstanding commitments at year-end. The program supported about 160 direct full-time-equivalent staff members at ORNL, while sending approximately $12.5M to external subcontracts with industry, universities, and consultants.

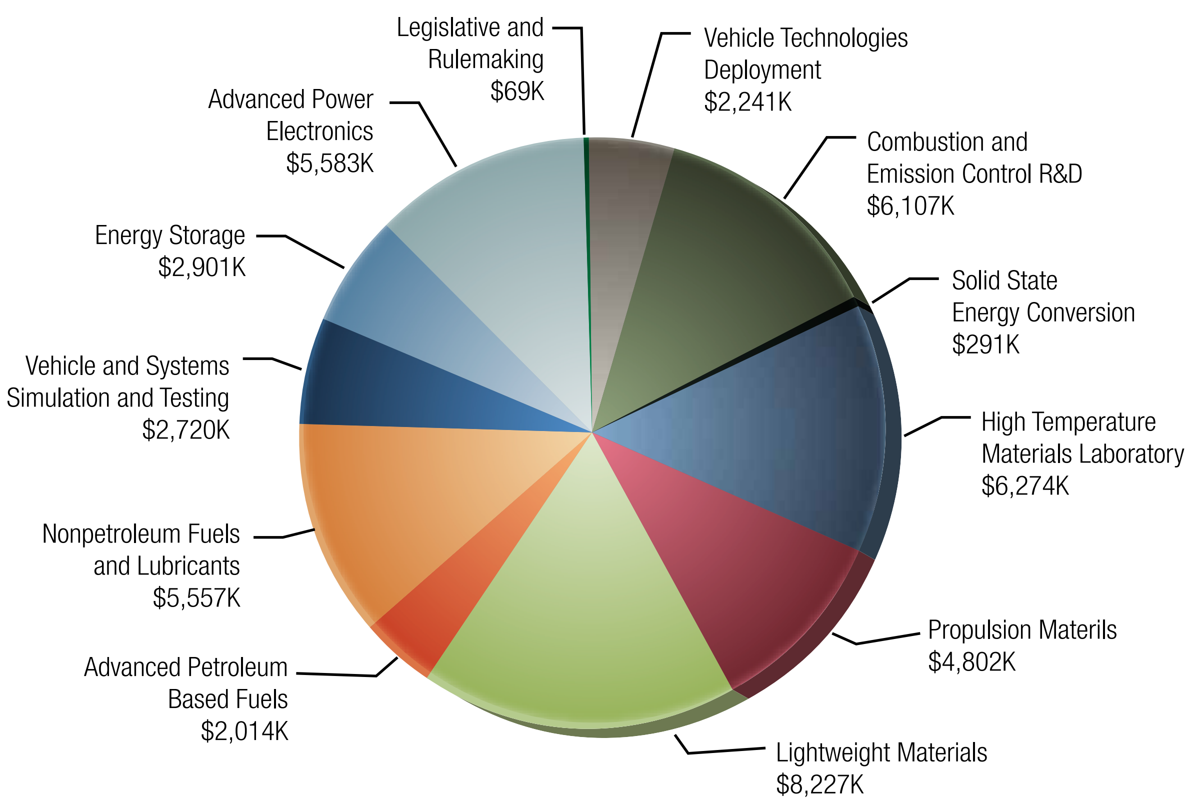


Figure 1. FY 2008 new budget authority by activity.

[4]21[st] Century Truck Partnership. December 2006. *Roadmap and Technical White Papers*. 21CTP-0003. Available at http://www1.eere.energy.gov/vehiclesandfuels.

Overhead Cost Savings

About half of the VTP-sponsored R&D at ORNL is conducted at the National Transportation Research Center (NTRC) in Knoxville, Tennessee.[5] R&D conducted at NTRC is subject to a reduced ORNL overhead rate, as many of the ORNL support services—for example, physical security and groundskeeping—are not applicable to NTRC because it is located away from the main ORNL campus. **Figure 2** shows the approximate annual and cumulative cost savings resulting from the NTRC's off-site location since FY 2002, the first year of full occupancy and beneficial facility operation. These overhead cost savings allow a larger percentage of VTP funds to directly support programmatic R&D in the activities conducted at NTRC.

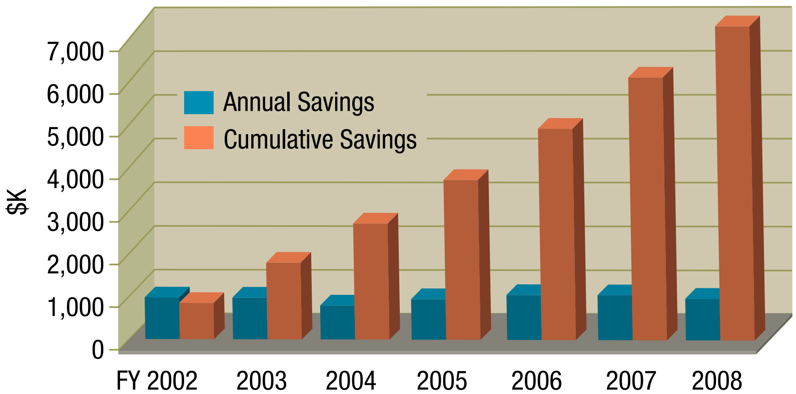


Figure 2. Cumulative overhead savings of nearly $7,000K have been applied to VTP-sponsored R&D at NTRC.

Sponsored Research — Work for Others

Transportation Program research staff often work with industry, other federal agencies, and universities under direct sponsorship and funding from those organizations. The R&D performed under these Work for Others (WFO) contracts complements the DOE VTP research program, contributes to the knowledge base that supports VTP R&D, and informs its analysis activities.

A statistical profile of FY 2008 WFO is shown in **Figure 3**. Information on the scope of these WFO R&D projects is presented in the relevant programmatic narratives beginning on page 7.

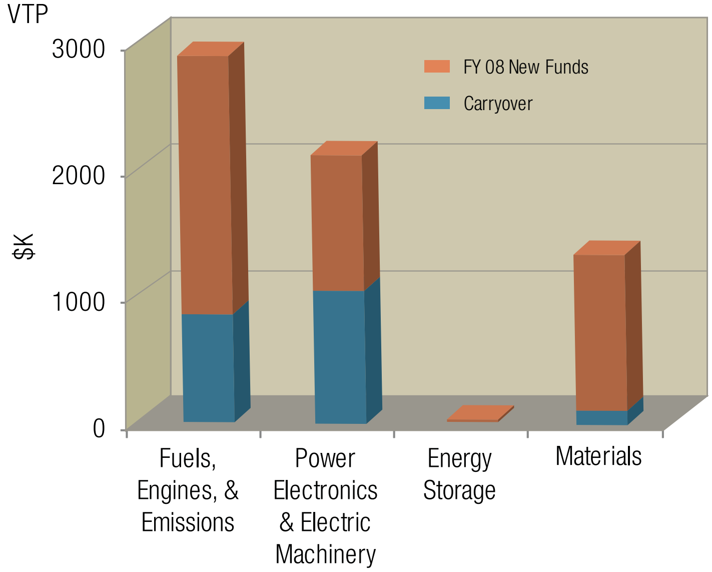


Figure 3. FY 2008 funding for research sponsored by industry, academia, and other federal agencies. Data include funds-in from industry partners working with ORNL on CRADAs.

[5] Activities primarily conducted at the National Transportation Research Center are advanced power electronics, legislative and rulemaking, vehicle technologies deployment, combustion and emission control research and development, advanced petroleum based fuels, nonpetroleum fuels and lubricants, and vehicle and systems simulation and testing.

Program Metrics

Patents

Transportation Program research staff members filed 8 invention disclosures and had 3 patent applications published in FY 2008. Five patents based on previous filings were awarded and issued during the period **(see Table 2)**.

Table 2. Patents Issued and Patent Applications Published in FY 2008

Inventors	Title
Z. Feng, S.A. David, and D.A. Frederick	Patent Application 12/051,972—Multiple Pass and Multiple Layer Friction Stir Welding and Material Enhancement Processes
A. Naskar, F. Paulauskas, C. Janke, and C. Eberle	Invention Disclosure 1924—Polyolefin based precursors and the processing of the materials for production of carbon fibers
A. Naskar, F. Paulauskas, and C. Eberle	Invention Disclosure 1926—Nano-reinforced high-strength carbon fibers
A. Naskar, F. Paulauskas, C. Janke, and C. Eberle	Invention Disclosure 1973—Novel compositions for PAN based carbon fiber precursors
F. Baker, P. Menchhofer, and D. Baker	Invention Disclosure 2051—In-situ Incorporation of Carbon Nanotubes into Lignin Fibers
P. Menchhofer, F. Baker, and F.C. Montgomery	Invention Disclosure 2060—Carbon Nanotubes Grown on Various Fibers
F. Paulauskas, and A. Naskar	Invention Disclosure 2069—Rapid stabilization/oxidation of lignin based precursors for carbon fibers
R. Ott, C. Blue, N. Dudney, and D. Harper	Patent 7220936—Pulsed Thermal Processing of Functional Materials Using Directed Plasma Arc
H.T. Lin , H. Wang, and A.A. Wereszczak	Invention Disclosure 2179—Dual-Rod Piezodilatometer and Method for Testing a Piezoceramic Plate
J.G. Sun	Patent Application 7,365,330—Method for Thermal Tomography of Thermal Effusivity from Pulsed Thermal Imaging
R. H. Wiles, A.A. Wereszczak, C.W. Ayers, and K.T. Lowe	Patent Application 61/037,129—Direct-Cooled Power Electronics Substrate
J.S. Hsu	Invention Disclosure 12/009,682; Reference No: 1859.1—Utilization of Rotor Kinetic Energy Storage for Hybrid Vehicles
G.J. Su	Patent 7,408,794—Triple Voltage dc-to-dc Converter and Method
Ronald L. Graves, Brian H. West, Shean P. Huff, and James E. Parks, III	Patent 7,469,693—Advanced engine management in individual cylinders for control of exhaust species
Robert M. Wagner, C. Stuart Daw, Johney B. Green Jr., and K. Dean Edwards	Patent 7,431,011—Techniques to diagnose and control combustion instabilities in HCCI and spark-assisted HCCI operation
Johney B. Green Jr., C. Stuart Daw, and Robert M. Wagner	Patent 7,277,790 B1—Combustion diagnostic for active engine feedback control

Awards and Professional Recognition

Program scientific and technical staff received numerous awards during the year **(Table 3)**. Several staff members were elected or appointed to positions in professional organizations, reflecting peer recognition.

Table 3. Significant Honors, Awards, and Professional Recognitions During 2008

Name	Award or Recognition
DOE and ACC Composites Team	2008 Outstanding Leadership Team Award for the advancement of plastics in automotive given by the Society of Plastics Engineers Automotive Division
Philip J. Maziasz	Chair of the ASM International Awards Policy Committee for 2008/09
A. Wereszczak	American Ceramic Society's Richard M. Fulrath Award
H.T. Lin	2008 ASM International-Indian Institute of Metals Visiting Lecturer
D.J. Singh	ORNL Distinguished Scientist Award
D.J. Singh	Fellow of the American Physical Society
D.J. Singh	ORNL Directors Award for Science and Technology in 2008
D.J. Singh	Publications Oversight Committee of the American Physical Society
D.J. Singh	Visiting Professor Appointment at the University of Paris (Orsay) in 2008
D.J. Singh	American Ceramic Society's Richard M. Fulrath Award
O. M. Jadaan; A. A. Wereszczak	2nd Place Best Paper, 32nd ICACC, Daytona Beach, Florida, January 2008, "Probabilistic Design Optimization and Reliability Assessment of High Temperature Thermoelectric Devices"
P. Blau	Chairman, ASTM Subcommittee G02.91 on Wear and Erosion Terminology
C. Ayers	ORNL Copyright and Patent Awards Ceremony
C. Coomer	ORNL Copyright and Patent Awards Ceremony
J. Hsu	ORNL Copyright and Patent Awards Ceremony
L. Marlino	ORNL Copyright and Patent Awards Ceremony
L. Seiber	ORNL Copyright and Patent Awards Ceremony
D. Adams	ORNL Copyright and Patent Awards Ceremony
GJ. Su	ORNL Copyright and Patent Awards Ceremony
C. Daniel	Session Chair "B1—Batteries General Session/Cells—Lithium and Lithium-Ion," 213th Electrochemical Society Meeting, Phoenix, Arizona, May 18–22, 2008
Edgar Lara-Curzio	Fellow, American Ceramic Society
Claudia J. Rawn	Outstanding Faculty Advisor, University of Tennessee College of Engineering
Peter J. Blau	Fellow, Society for Tribologists and Lubrication Engineers
Jun Qu	Outstanding Young Manufacturing Engineer Award, presented by the Society of Manufacturing Engineers
Harry Meyer	Recognized by Society of Automotive Engineers for authoring "one of the best" papers of 2007
Bill Partridge, Jae-Soon Choi, John Storey, Samuel Lewis	R&D 100 Award with Cummins for Spatially Resolved Capillary Inlet Mass Spectrometer (SpaciMS)
Brian West	SAE Lloyd Withrow Award for Outstanding Oral Presentations
Scott Sluder	SAE Forest R. McFarland Award for outstanding leadership
Bill Partridge	ORNL Distinguished Engineer Award for 2008

Publications and Presentations

ORNL R&D staff produced more than 190 papers and presentations on VTP-sponsored R&D during FY 2008. **Figure 4** provides a breakdown by type of publication or presentation for VTP subprograms.

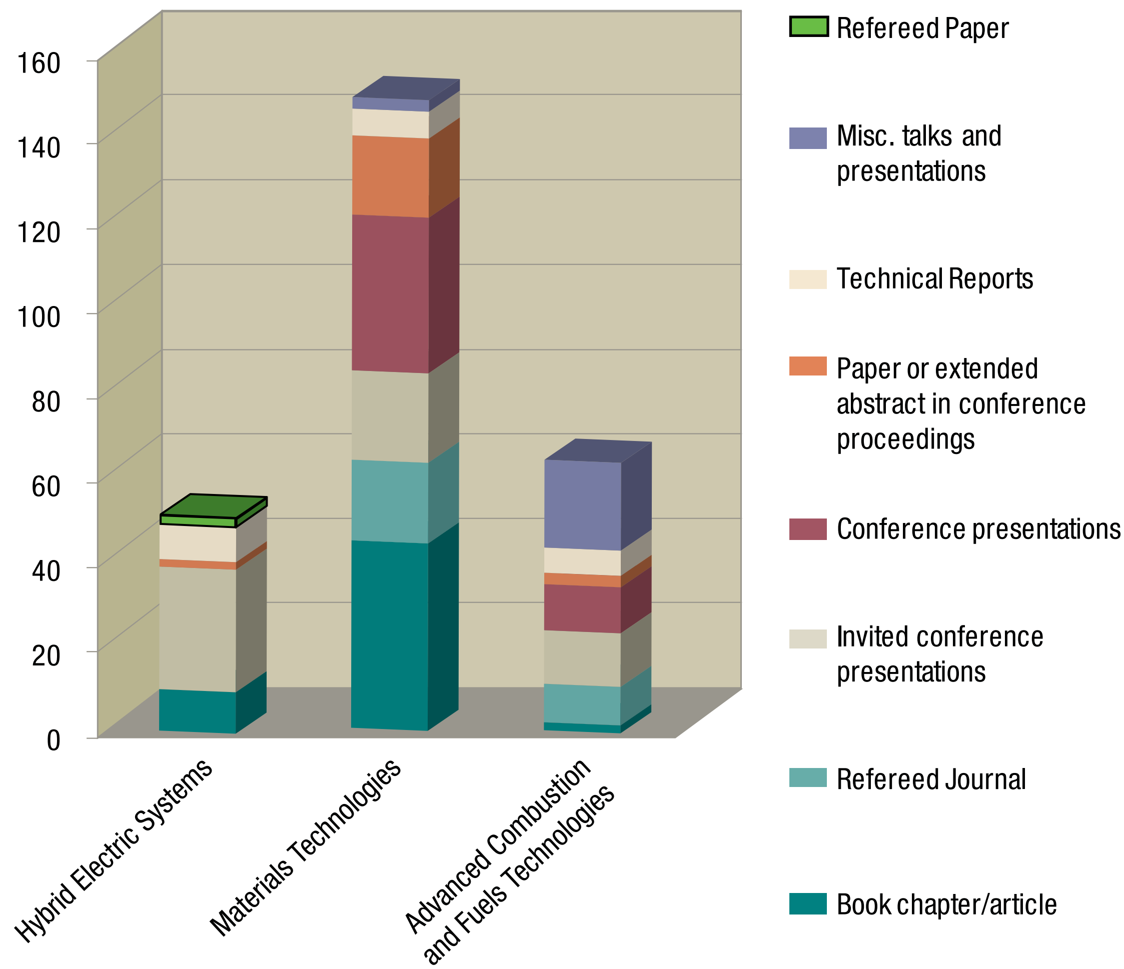


Figure 4. FY 2008 publications and presentations.

Program Summaries

Advanced Power Electronics and Electric Machines

The Power Electronics and Electric Machinery Research Center conducts high-risk, long-term research; evaluates hardware; and provides technical support to the DOE VTP Advanced Power Electronics and Electric Machines (APEEM) activity. In this role, ORNL serves on the FreedomCAR and Fuel Partnership Electrical and Electronics Technical Team, evaluates technical proposals for DOE, and lends its technological expertise to the evaluation of projects and developing technologies. ORNL also executes specific projects for DOE in the areas of power electronics, electric machines, thermal control, and integrated systems. These projects help remove technical and cost barriers so that technologies will be suitable for use in advanced vehicles that meet VTP goals and provide a portfolio of options that automakers can use when developing innovative solutions for hybrid electric vehicles (HEVs), plug-in HEVs (PHEVs), and fuel cell vehicles (FCVs).

In FY 2008, advances were made through efforts in several projects as highlighted below.

KEY TECHNICAL ACCOMPLISHMENTS

Direct water-cooled power electronics substrate

- Identified candidate materials and processing methods for a direct-cooled power electronics substrate.
- Determined the optimum ceramic materials for maximum heat transfer.
- Completed design analysis and thermal and structural finite element analyses (FEAs) on five designs.
- Continued an ongoing effort to analyze the compatibility of ceramic substrates with water/ethylene glycol.

Uncluttered rotor permanent magnet machine for continuously variable transmission design

- Developed a design conforming to the overall dimensions of the baseline machine (Toyota Prius).
- Performed simulations, which indicated that the radial-gap continuously variable transmission provided a significant torque increase of 30% with a weight gain of only 15%.
- Achieved significant advances in the simulation and design of highly complex machines using the uncluttered rotor principle with three-dimensional (3D) flux paths.

Application of concentrated windings to electric motors without surface-mounted permanent magnets

- Completed analysis of a 9-slot, 8-pole interior permanent magnet (IPM) with concentrated windings, and compared it with a 48-slot, 8-pole baseline IPM with distributed windings.
- Simulated both motor designs, and compared their performance running the US6 and Federal Urban Driving Schedule drive cycles using ORNL's vehicle simulator.
- Determined that benefits can be obtained in reduced torque ripple, reduced copper losses, and increases in efficiency with IPM concentrated winding machines; however, the power demands of the US6 cycle required increasing the gear ratio above the baseline gear ratio.

Amorphous core material evaluation

- Performed evaluations of amorphous core materials, and determined that the unavailability of bulk manufacturable amorphous core material and high material costs will continue to prevent radial-gap motors from meeting cost targets.
- Performed FEA simulations with amorphous core material in existing motor designs, yielding low saturation flux densities.
- Determined that use of amorphous core materials will require specific motor designs developed to optimize and realize the gains potentially available from them.

Wide bandgap materials

- Continued efforts to characterize, model, and simulate new wide bandgap devices as they became available from various vendors.
- Developed a novel integrated motor/inverter packaging concept using silicon carbide devices. Further work on the design will be continued into the next fiscal year.

Advanced converter systems for high-temperature HEV environments

- Designed, assembled, and tested a 30 kW continuous, 55 kW peak power buck/boost dc-dc converter to prove the benefits of the topology.

- Achieved efficiencies in the 97–98% range during laboratory testing of the prototype.
- Achieved a power density of 8.5 kW/kg and 17.8 kW/l with the low-temperature prototype.
- Developed and tested a second-generation silicon-on-insulator gate driver chip.

Current source inverter for HEVs and FCVs

- Designed, built, and successfully tested a 55 kW prototype.
- Achieved the following with the prototype:
  - a reduction in total capacitance to 195 μF,
  - a voltage boost ration of up to 3.47, and
  - an output voltage total harmonic distortion factor lower than 12.5%.

Traction drive power electronics system to provide plug-in capability for HEVs

- Designed, fabricated, and tested a prototype of a 55 kW PHEV traction drive inverter with a charging capability of 20 kW.
- Conducted tests with the prototype over a load range of 1–14 kW, achieving the following:
  - measured efficiencies between 92 and 97% and
  - total harmonic distortion of the ac current of less than 10% over a wide range of charging power.

Benchmarking competitive technologies

- Successfully benchmarked the Toyota Lexus LS 600h.
- Generated efficiency maps for the modules, and completed destructive teardowns of the modules to determine manufacturing, packaging, and thermal design issues.
- Analyzed the bus capacitors and motor magnets over a temperature range as part of the teardown.

RELATED WFO

ORNL worked with an automotive original equipment manufacturer (OEM) and a Tier 1 supplier to develop inverter and converter topologies and assess new device technologies for HEV, PHEV, and FCV applications. Promising technologies will be built into prototypes and evaluated.

Work was also performed throughout the year with a wide bandgap device manufacturer to test and characterize new devices suitable for elevated temperature operation.

LABORATORY DIRECTED R&D

ORNL is sponsoring a 2-year Laboratory Directed R&D (LDRD) project to conduct research on developing modular power electronic converters for utility applications entitled “Modular Utility-Scale Power Converters and Controllers for the Next Generation Grid.” The goal of this ORNL LDRD is to design high power modules that can be combined to make a flexible converter that can be used for a variety of utility-scale applications such as an interface with distributed generation (solar cells, fuel cells, microturbines, etc.) or a static VAR compensator or active filter. The modules and converter will have an intelligent controller so that units can be multifunctional. In addition, the modules will have protection against faults and can reset or bypass themselves if needed.

Clean Cities, Fuel Economy, Policy and Analysis

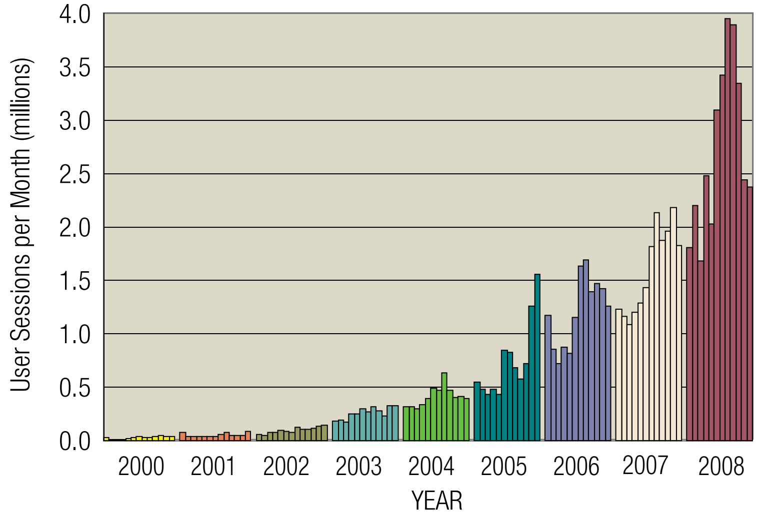
Through the Clean Cities, Fuel Economy, Policy and Analysis program, ORNL provides research, analysis, and technical support to VTP to do the following:

- Improve the federal fuel economy information program.
- Update, enhance, and distribute the *Fuel Economy Guide* (FEG).
- Enhance and improve the joint DOE-EPA fuel economy Web site.
- Conduct a variety of information and research projects related to the use of fuel economy information by consumers and the marketing of fuel economy information to consumers.

www.fueleconomy.gov

Over the years, www.fueleconomy.gov has become the predominant tool the Fuel Economy Information project uses to reach consumers with fuel economy information. Traffic on the Web site has increased by nearly 50% each year since its inception, reaching more than 2 million users (each visiting the site for approximately 10 minutes) per month in 2008 **(Figure 5)**. In 2008, total user sessions exceeded 32 million.

The most important task of FY 2008 was the model year (MY) 2008 rollout and preparation for the MY 2009 update of www.fueleconomy.gov. This required processing fuel economy data provided by EPA, adding emissions data, collecting and formatting vehicle photographs, and updating related data including tank size, estimated GHG emissions, and annual petroleum consumption estimates. The fuel economy data were reviewed in collaboration with EPA and the automotive manufacturers to correct errors and fill in missing information. The team updated the 2008 MPG



Model Year: 2008

Total User Sessions: 32,744,641

Average Daily User Sessions: 89,466

Total Hits: 4,428,279,866

Total Page Views: 345,037,440

Figure 5. User sessions at www.fueleconomy.gov by year, showing dramatic increase in 2008.

(miles per gallon) data throughout the year to add models that were not available at the time of the initial MY 2008 rollout. Preliminary fuel economy data for MY 2009 were added in three installments (May, July, and September). The gasoline and diesel fuel price information used in the "Find and Compare Cars" section (and the FEG) was updated weekly to match the national average fuel prices reported by the Energy Information Administration (EIA). The E85 (85% ethanol with 15% gasoline) prices were updated as available to match the prices in the *Alternative Fuel Price Report* produced by DOE's Clean Cities Program.[6]

"Your MPG" is a tool which helps fueleconomy.gov visitors calculate and track their fuel economy. They can also share their MPG with other users. The shared information provides consumers and researchers with a valuable and unique source of real-world fuel economy data. The shared Your MPG information was analyzed and updated each week on www.fueleconomy.gov. All new shared information was checked using automated error checking routines; the shared information was also reviewed manually by the Your MPG team. As of September 23, 2008, 59,343 registered and 222,899 guest drivers had visited Your MPG. It had 25,337 shared MPG records for 8,026 vehicles in EPA's database. As a bonus, 15,000 fueleconomy.gov bumper stickers were produced for distribution to anyone who enters data in Your MPG. A contract is in place with Direct Mail Services to distribute the bumper stickers beginning in FY 2009.

In 2008, the fueleconomy.gov team established an agreement with the automotive Web site Edmunds.com to provide them the EPA fuel economy data in a convenient format and to provide updates on a regular basis. In return, they have agreed to provide us with tank size and manufacturer's suggested retail price (MSRP) data for use on the fueleconomy.gov Web site. The tank size data are used to calculate cost of a fill-up and miles on a tank in fueleconomy.gov's "Find and Compare Cars" section. The MSRP data will also be used to improve the search options in the Find and Compare Cars section. Edmunds.com also requested assistance in updating their MPG estimates for used cars to be consistent with EPA's new method of calculating MPG. The team provided Edmunds with revised MPG estimates for 1985—2007 vehicles.

The proliferation of hand-held wireless communication devices with connection to the internet (PDAs, mobile phones etc.) creates a new opportunity for bringing fuel economy information to consumers in a convenient and timely way. We completed development of a version of www.fueleconomy.gov's Find and Compare Cars formatted for mobile communication devices. This new Web site allows consumers to take www.fueleconomy.gov with them to the new or used car dealership or wherever they need it. The mobile Web site, fueleconomy.gov/m was launched in conjunction with the 2008 Washington, D.C., Auto Show.

Online market research conducted in the summer of 2008 indicated that fueleconomy.gov users would like more options for searching the Find and Compare Cars database. In response to their comments we developed an "Advanced Search Tool." This tool allows users to choose from up to 34 different options including model year, market class, vehicle or fuel type, transmission, drive, cylinders, and MPG. The Advanced Search Tool will be installed with the October launch of the 2009 Fuel Economy Web site.

The team completed development of a new "Find and Compare Cars" feature that shows consumers the carbon

[6]The *Clean Cities Alternative Fuel Price Report* is a quarterly newsletter (January, April, July, and October) designed to keep readers updated on the prices of alternative fuels and conventional fuels in the United States. It can be accessed online at http://www.afdc.energy.gov/afdc/price_report.html.

footprint of each vehicle in the database. The carbon footprint provides a new measure of the GHG emissions produced by each vehicle.

Maintaining consumer interest on the Internet requires constant updating of information. The following components of the Web site were updated and improved in FY 2008.

- Statistics for pages in the "Why Is Fuel Economy Important?" section were updated.
- The fueleconomy.gov home page features links to news articles on fuel economy. We continued to update these links each weekday.
- In response to questions from fueleconomy.gov users regarding high gas prices in the spring of 2008, the "Frequently Asked Questions" page of the "Gas Prices" section was updated to include new information from EIA.
- The "Hybrid Vehicles" section, including the "Tax Incentives" page, was updated to include information on 2008 and 2009 hybrid models.

GAS MILEAGE TIPS

In 2008, DOE authorized the ORNL Fuels, Engines, and Emissions Research Center (FEERC) to initiate studies to validate and improve the driving and maintenance tips on fueleconomy.gov. The site currently includes some information that dates back to the 1970s and 1980s. Given the changes in vehicle technology that have occurred over the past three decades, this information needs to be updated. Experiments were initiated in late FY 2008 to examine the effect of clogged engine intake air filters on fuel economy. Experiments will examine modern closed-loop vehicles as well as a vintage carbureted example from the precontrol era. In FY 2009, these experiments will be completed and reported. Also, the team will assemble a panel of experts to advise and assist in planning follow-on studies to continue to improve the driving and maintenance tips.

FUEL ECONOMY GUIDE

Distribution and printing

In collaboration with EPA and DOE, the 2008 FEG was finalized and distributed as scheduled on October 11, 2007. With the cooperation of the National Automobile Dealers Association, the FEG is now being distributed electronically via e-mail to most dealers. Any dealer requesting a shipment of hardcopy guides receives copies from the EERE Information Center, as does any individual requesting a hard copy.

Hardcopy guides were also mailed to all public libraries and all federal credit unions.

The EPA officially incorporated this distribution method into its rules for automobile dealers in 2007.

2009 FEG—Design and review

In collaboration with EPA and DOE, we designed, reviewed, and finalized a new cover for the 2009 FEG. The textual content of the FEG was comprehensively reviewed and revised as appropriate, and new material and updates were incorporated. Drafts were distributed for review and proofreading; comments were incorporated.

In FY 2007, software was developed which allows automatic creation of the FEG from the "Find and Compare Cars" database. This software allowed the team to update the annual fuel cost data for the 2008 FEG each week based on up-to-date national average fuel prices.

WEB SITE PROMOTION AND MARKET RESEARCH

The fueleconomy.gov team worked with the Alliance to Save Energy (ASE) to provide assistance in their Transportation Energy Efficiency Campaign, the Drive Smarter Challenge. In support of their campaign, we provided fuel savings tips, fuel economy data and GHG emissions information for the Fuel Savings Calculator on ASE's campaign Web site, http://drivesmarterchallenge.org/. The calculator not only computes savings due to an individual's actions, but also keeps a running tally of savings by everyone who has taken the challenge.

In FY 2008, work was initiated to add Spanish versions of selected pages to the fueleconomy.gov Web site. In conjunction with the Spanish translations, the fueleconomy.gov team worked with Rosa M. Toledo to launch a class project in her "Spanish for Marketing Majors" class at the University of Tennessee. The class was divided into five teams of five students each, and each team developed a plan with specific recommendations for marketing the Spanish-language pages on fueleconomy.gov to the Spanish-speaking population in the United States.

The fueleconomy.gov team worked with DOE headquarters and Argonne National Laboratory (ANL) to develop fact sheets and other materials for the 2008 Washington, D.C., Auto Show, including a stand-alone version of the fueleconomy.gov Web site on a laptop to be used as a "demo," and features for the fueleconomy.gov home page which ran during the D.C. and Detroit Auto Shows.

The program's productive relationship with MotorWeek, which is our principle means of reaching the public via television, was continued in 2008. In FY 2008, the team worked with Maryland Public Television to complete the following four segments for the MotorWeek television show.

- **MotorWeek Clean Power Drive**—A real-world fuel economy and emissions comparison test comparing three types of vehicles and various fuel/power sources: Mercedes-Benz E320 Bluetec diesel versus the E350 gasoline, Honda Civic Hybrid versus the Civic Gasoline, Chevrolet Tahoe 2-mode Hybrid versus the gasoline and E85 FFV Tahoe. The segment included a 160-mile economy drive with guest test drivers from DOE and measured on-the-road emissions with the SEMTECH mobile emissions analyzer from Sensors, Inc. The results were presented with actual test numbers as well as conclusions drawn about which fuel/power source would give the most benefit to consumers in various driving situations.
- **Argonne National Laboratory**—This segment included a behind-the-scenes tour of Argonne's advanced vehicle technology laboratories to see the work being done on developing lithium-ion batteries, PHEVs, and hydrogen internal combustion engines.
- **Challenge X**—This segment highlighted the conclusion of the 3-year Challenge X competition[7], including the results of comparative benchmark testing, team presentations, and ultimately the judging and awarding of prizes to the best student-designed alternative fuel vehicle.
- **MotorNews Segment**—This MotorNews segment featured fueleconomy.gov/m, a mobile version of fueleconomy.gov's Find and Compare Cars Tool.

These MotorWeek segments are available to the public on www.fueleconomy.gov.

Media contacts

The team updated electronic mailing lists (e.g., American Automobile Association's nationwide, previous media contacts, top U.S. newspapers, online media, television affiliates nationwide, college newspapers, alternative newspapers) and continued an ongoing effort to add new addresses as they become available and remove obsolete addresses as needed.

Market research

Feedback from users is essential to improving the fueleconomy.gov Web site. We contracted with the Looking Glass Group to conduct online market research discussions with users of the fueleconomy.gov Web site. The goal of the research was to improve fueleconomy.gov based on user input. The focus group participants were recruited from visitors to the fueleconomy.gov Web site. One group comprised registered users of Your MPG. This group primarily focused on the Your MPG portion of the Web site. The other group was recruited from visitors to the Find and Compare Cars section of the Web site. The second group reviewed the entire Web site including Find and Compare Cars and the mobile version of fueleconomy.gov. The online focus groups were conducted in late July and early August 2008, and Looking Glass Group submitted the final report in September. Based on comments from the research participants, several improvements will be made to the Web site in FY 2009.

Energy Storage

Lithium ion battery technology is projected to be one of the energy storage leapfrog technologies for the electrification of automotive drivetrains and to provide stationary storage solutions to enable the effective use of renewable energy sources. This technology is already in use for low-power applications such as consumer electronics and power tools.

Extensive research and development has enhanced the technology to a stage where it seems very likely that safe and reliable lithium ion batteries will soon be on-board hybrid-electric and electric vehicles and connected to solar cells and windmills. However, safety of the technology is still a concern, service life is not yet sufficient, and costs are too high.

ORNL has performed a thorough technical assessment of materials and processing for energy storage devices and developed partnerships with leading battery developers, the automotive industry, and utility companies. Parts of the assessment and cost estimates have been published in an overview article. Based on the assessment, ORNL has identified characterization and process development as the key components of a new, enabling research and development program at ORNL.

[7]Since 1987, DOE and various other organizations have sponsored competitions challenging engineering students to develop vehicle technologies for better fuel economy and lower emissions while maintaining or improving safety, performance and other features. In 2003, General Motors, DOE, and other government and industry leaders developed the Challenge X: Crossover to Sustainable Mobility competition to give engineering schools an opportunity to participate in hands-on research and development with leading-edge automotive technologies. More information is available on the official Web site, http://www.challengex.org/.

Fuels Technology and Advanced Combustion Engines

The ORNL FEERC, located at NTRC, conducted R&D for multiple VTP subprograms in 2008, including Advanced Combustion Engines, Fuel Technologies, Vehicle Systems, and Health Impacts. Strong industry collaboration in FEERC was evidenced by the seven formal Cooperative Research and Development Agreements (CRADAs) in fuels/engine/emissions technology. Less-formal, yet very active collaborations with about 15 additional private-sector organizations and non-DOE agencies continued. In addition to the CRADAs, eight private-sector firms and other federal agencies sponsored R&D at the center in FY 2008.

FEERC staff are highly engaged in supporting FreedomCAR and 21st Century Truck Partnership (21CTP) programmatic activities such as the Advanced Combustion and Emission Control tech team, the Diesel Crosscut Team, and the 21st Century Truck "Lab Council." ORNL provides coleadership with industry of the Cross-Cut Lean Exhaust Emissions Reduction Simulation (CLEERS) activity. In fuels utilization, FEERC staff have worked with industry, the National Renewable Energy Laboratory (NREL), and EPA to carry out tests of intermediate ethanol blends (iBlends) on legacy vehicles, which is a strategic component of satisfying the biofuels utilization target of the Energy Independence and Security Act (EISA). The iBlends project is cosponsored by VTP and the EERE Biomass Program.

KEY TECHNICAL ACCOMPLISHMENTS

Completion of 2008 milestone for light-duty engine efficiency (on the path to the 2010 45% efficiency goal). The path to the 2010 goal makes use of key discoveries in advanced combustion, emission controls, and fundamental thermodynamics at ORNL and at other DOE laboratories, universities, and industry.

- Demonstrated a brake thermal efficiency (BTE) of 43% on a light-duty diesel engine.
- Investigated advanced engine technologies, including thermal energy recovery (TER), electrification of auxiliary components, lubricants and fuel properties. (TER was not used to meet the 43% BTE.)
- Explored and analyzed several TER approaches.
- Constructed a Rankine bottoming cycle system for on-engine experiments.

Progress in high efficiency clean combustion (HECC). ORNL has used an experimental multicylinder engine with combined low-pressure and high-pressure exhaust gas recirculation (EGR) to generate data for improved understanding of the influence of intake charge preparation, cylinder/cyclic dispersion. and emissions formation/reactivity on reducing engine-out emissions while maintaining or improving overall engine efficiency (SAE 2008-01-0645). This mixed source EGR approach provides the greatest reduction in nitrogen oxide (NO_X) emissions without harming efficiency. This activity makes use of more fundamental single-cylinder engine research at Sandia National Laboratories (SNL) and modeling activities at the University of Wisconsin **(Figure 6)**.

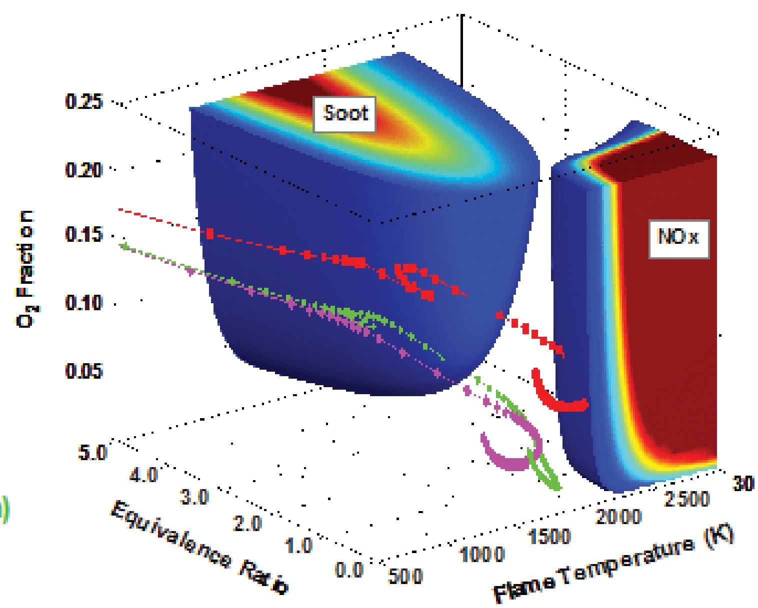


Figure 6. Model illustration of combustion paths of conventional, high dilution, and HECC modes.

Progress in the practical implementation of spark ignition-homogenous charge compression ignition (SI-HCCI) combustion

ORNL simulation and controls experience has been combined with Delphi Automotive Systems Corporation's component and subsystem experience to overcome barriers to SI-HCCI control under a CRADA for the development of advanced gasoline engines **(Figure 7)**.

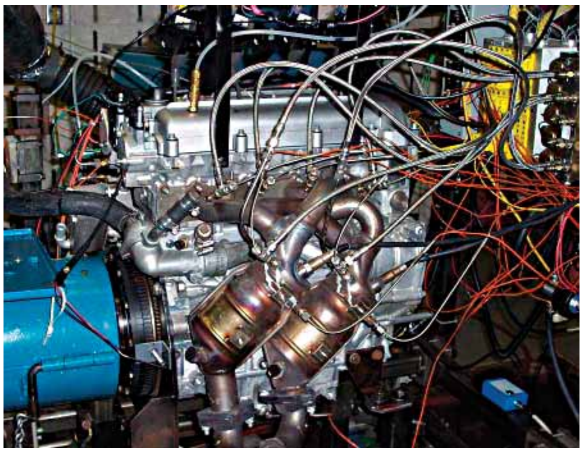


Figure 7. SI-HCCI multicylinder engine developed under Delphi CRADA.

- Developed a low-order dynamic model to predict the complex cycle-to-cycle interactions of spark assisted HCCI that have been observed in experiments.
- Developed a new combustion metric for use with feedback control to provide rapid characterization of the spark assisted HCCI combustion event. Control concepts which make use of the predictive model and combustion metric are in development for use on a multicylinder direct-injection gasoline engine. A patent for aspects of the control concepts being used in this CRADA was issued in October 2008 (US 7,431,011).

Impact of lean emission controls and advanced combustion on hybrid vehicle efficiency

- Carried out integrated systems simulations of hybrid and plug-in hybrid vehicles using aftertreatment device models adapted from CLEERS and engine maps including advanced combustion modes. These simulations have been the first made by any national lab to reveal the impacts of these technologies on hybrid vehicle fuel efficiency and emissions under realistic drive cycle conditions. One key contribution from ORNL in this area has been the development of algorithms for simulating the transient temperature and emissions produced by engines operating under highly variable drive cycle conditions where aftertreatment catalysts are subjected to repeated engine starts and shutdowns. Under these conditions, the performance of both lean exhaust aftertreatment devices and conventional three-way catalysts can be significantly degraded. This degradation can in turn result in failure to meet emissions regulations or increases in fuel consumption in order to maintain emissions compliance.
- Using this simulation capability, quantified the expected impact of replacing conventional gasoline engines with diesel engines in hybrid and plug-in hybrid vehicles.

Commercialization of SpaciMS and 2008 R&D 100 Award

A research team led by ORNL personnel (Partridge, Choi, Storey, Lewis) with collaborating industry partner Cummins Inc. (Currier, Yezerets) received an R&D 100 award for the development of a spatially resolved capillary inlet mass spectrometer (SpaciMS), shown in **Figure 8**. This

Figure 8. R&D 100 winning technology—SpaciMS.

technology is capable of obtaining gas samples inside the confined spaces of reactors like automotive catalysts, fuel reformers, or fuel cells, measuring changes in chemical composition in both space and time within the reactors. This technology was used in the optimization of the groundbreaking 2007 Dodge Ram heavy-duty pickup truck, which met 2010 emissions control standards 3 years ahead of schedule. More recently, the technique has been modified to make intracatalyst NH_3 measurements. The SpaciMS has been commercialized by Hiden Analytical, also a member of the R&D 100 team.

New diagnostic method for fuel dilution in oil transferred to partner

In a CRADA with Cummins, ORNL has developed and validated a diagnostic method for measuring the fuel dilution into the lubricating oil in near real time. The method is based on laser-induced fluorescence and uses an optical fiber probe inserted in the engine system to make near-real-time measurements for rapid determination of oil dilution rates. Intended primarily for R&D use, this instrument will enable engine developers to calibrate the timing and amount of fuel injection to minimize the oil dilution. The method was evaluated at Cummins and has been licensed to them. Other firms have expressed interest in the method.

First-of-kind data on EGR cooler fouling

- In studies of biodiesel effects on EGR cooler fouling, determined the mass and chemistry of the deposits and also their thermal conductivity **(Figure 9)**. Deposit thermal conductivity is a key parameter in modeling the relation of the deposit formation process to the performance of the EGR cooler. These data are characteristically absent from the literature because of the difficulty in accomplishing the conductivity measurement. ORNL used a flash diffusivity method at the High Temperature Material Laboratory.
- Developed a new industry collaboration on this subject under the Diesel Crosscut Team.

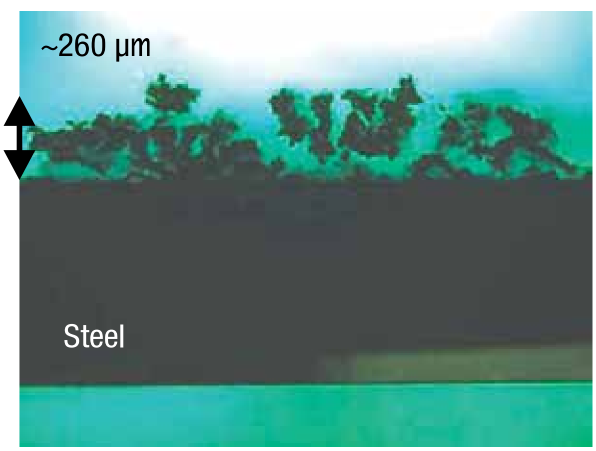


Figure 9. Photograph of deposit layer in surrogate EGR cooler tube. Thermal conductivity found to be essentially that of air, hence loss of heat transfer effectiveness.

Development and demonstration of unique emissions and catalyst diagnostics

- Demonstrated the first intracatalyst measurements of NH_3.
- Developed and demonstrated methods for nondestructive imaging of soot, ash, and catalyst monoliths using a commercial X-ray machine.
- Acquired the first neutron imaging visuals of a diesel particular filter.
- Developed and demonstrated a fast fiber-optic-based backscatter probe which is able to measure cycle and cylinder resolved particulate emissions.

Efficient emission controls via improved catalyst fundamentals

- Integrated catalysis research has led to an improved understanding of correlations between spatio-temporal distributions of reactions and surface species which dictate global LNT (lean NO_X trap) performance.
- ORNL's direct measurements of the water-gas-shift reaction in LNTs created a foundation for a Cummins patent application on a method of monitoring LNT degradation.
- The role of NH_3 formation and utilization during regeneration of an LNT has been clarified and leads to better (more fuel efficient) reductant utilization.
- In the area of NO_X reduction performance, which relates directly to cost of implementation, the kinetics of nitrate release and regeneration were shown to limit low temperature performance more than NO oxidation.
- Cerium was shown to be effective in improving low temperature NO_X and sulfur management performance.
- Gained knowledge of sulfur degradation mechanisms during experiments on the CLEERS reference LNT.
- Quantified desulfation activation energies, and mapped the distribution and stability of sulfur species along the flow axis.

Impacts of intermediate ethanol blends on legacy vehicles and engines (an ORNL-NREL-VTP-EERE Biomass Program collaboration)

- Completed and published a review and assessment of prior work indicating the need for a broad test program on intermediate ethanol blends, which was started in summer 2007.
- Under subcontract to ORNL, Battelle assisted with data analysis and experimental design of the intermediate blends program, and the detailed vehicle test program plan was completed with industry and EPA input.
- Placed three vehicle testing contracts, two at the Transportation Research Center, Inc., to augment vehicle tests at ORNL and to test cars originally assigned to ANL, and one at the Colorado Department of Public Health, Aurora Emissions Technical Center, for testing of NREL vehicles. Contracts for purchase of thousands of gallons of fuel were placed and the fuel delivered.
- Completed the screening study, running hundreds of test operations **(Figure 10)**.

- Published a joint ORNL-NREL report describing studies of 13 vehicles and 28 small nonroad engines in October 2008. An updated report, with results for three additional vehicles, was released in February 2009

Figure 10. ORNL vehicle dynamometer laboratory and one of the intermediate blends test vehicles.

Fuel property effects on engine efficiency and emissions performance

- ORNL has played a leadership role in resolving issues related to the release of the Coordinating Research Council's Fuels for Advanced Combustion Engines Group (FACE) fuels for purchase by interested researchers.
  - All nine of the diesel fuels have been formulated and are available for purchase. ORNL has worked to provide samples of the fuels for experimentation and analyses to other interested laboratories, including Pacific Northwest National Laboratory (PNNL), NREL, SNL, and the National Centre for Upgrading Technology (NCUT) (Canada). At least five additional organizations are acquiring the FACE fuels for research.
  - ORNL has worked with PNNL and NCUT to provide an exceptionally thorough characterization of the chemical makeup and physical properties of the fuels that will be critical in establishing the impact of fuel properties on advanced combustion processes. Many of these analyses have been publicly released to foster interest in the use of the fuels by combustion researchers.
  - ORNL has completed experiments with all nine fuels in a single-cylinder HCCI engine and will conduct studies in a General Motors (GM) 1.9-liter multicylinder engine in premixed charge compression ignition (PCCI) modes in early FY 2009.
- A new CRADA was initiated in FY 2008 with Reaction Design in support of the Model Fuels Consortium. This effort supports development of surrogate fuel data for determination of kinetic reaction mechanisms associated with advanced combustion modes.
- As a team member to Cummins High Efficiency Clean Combustion research contract, ORNL conducted an experimental and data analysis project to define the effects of fuel properties on HECC.

Fundamental thermodynamic approach to stretch engine efficiency

- ORNL continues to lead research on advanced concepts to understand and reduce thermodynamic combustion losses as well as develop paths for redirecting and/or recovering thermal energy discarded to the environment.
- Concepts for reducing fundamental combustion losses, such as staged or unmixed combustion, have been formed based on extensive modeling and are being considered for future experimental evaluation.
- Thermodynamic analysis routines have also been developed and integrated into full engine models at ORNL. This work has been incorporated into two commercial engine simulation codes (WAVE and GT Power). This research has also involved the development of a detailed thermodynamic analysis for experimental data and consequently new insight (with visual mapping) into the potential of TER across the speed/load range of a light-duty engine.

Investigations of concerns and potential improvements posed by increased biodiesel use

- A study was completed examining the impacts of biodiesel formulation on efficiency and emissions when used in an HECC combustion mode. The results showed that biodiesel formulated from soybean and coconut feedstocks produced similar efficiency and emissions when used in a PCCI-type HECC mode.
- Studies of particulate oxidation kinetics conducted by ORNL have shown that particulate produced when using some biodiesel blends exhibits a lower ignition temperature and faster oxidation rates than particulate produced when using ultralow sulfur diesel fuel. This phenomenon is a potential benefit to the performance of diesel particle filters. Ongoing studies are underway to fully describe the characteristics of the particulate that result in this behavior. This project also produced first-of-their kind neutron tomographic images of full-size particle filters loaded with particulate. This technique produces detailed cross-sectional images and opens a new pathway to studies of fuel and aftertreatment system compatibility.

Studies to resolve issues and demonstrate potential benefits of increased ethanol use

- Responded rapidly to a need for data in support of Underwriters' Laboratory (UL) recertification of E85 fuel dispensers. (UL briefly withdrew their certification in 2007.)

- An experimental apparatus was developed and operated extensively to complete E85 and E25 (25% ethanol with 75% gasoline) long-term exposure studies, meeting the aggressive UL timetable for data availability.
- The project has recently focused on dispenser materials compatibility with E20 (20% ethanol with 80% gasoline).

- Developed a means to operate a Saab BioPower in closed-loop lean mode so that the potential for silver-alumina lean-NO_X catalysts could be investigated. The vehicle was successfully operated at lean air : fuel equivalence ratios (as much as 40% lean). The silver-alumina catalyst technology was shown to provide more than 90% NO_X reduction.
- Continued work with Delphi under a CRADA for maximizing the efficiency of engines/vehicles using E85.
- Prepared a draft Report to Congress on flexible fuel vehicle optimization, helping DOE comply with an EISA requirement.

Health impacts—real-world emissions studies
ORNL-FEERC conducts experimental investigations of unregulated emissions of new engine and fuel technologies to ensure that there are no unintended consequences of future fuel-saving technologies. Generally termed mobile source air toxics (MSATs), the emissions constituents of concern include particulate matter and volatile and semivolatile organics. Recent studies included measurement of MSATs when using intermediate ethanol blends in legacy vehicles and determination of MSAT differences between conventional diesel combustion and PCCI. For modern vehicles, MSAT emissions are very low, but it was found that intermediate blends decrease benzene, xylene, toluene, and ethylbenzene in the exhaust. Acetaldehydes increased, but were still at very low levels. Particle emissions from PCCI were found to be generally smaller than with conventional diesel combustion but more laden with heavy hydrocarbons. ORNL collaborated with the University of Maryland in these studies, using a unique instrument, the aerosol particle mass analyzer.

IMPROVEMENTS IN FACILITIES AND CAPABILITIES

Flexible microprocessor-based engine control system operational
The control system on one of two GM 1.9-liter engines has been upgraded to a flexible microprocessor-based system and is now fully operational.

Additional engine cell construction near completion
This engine cell has 600 hp dc and 230 hp ac double-ended motoring dynamometers (industry-donated or purchased with non-VTP funds) and is able to accommodate up to three engine setups simultaneously. The engine cell is also approved for and equipped to handle a variety of fuels including diesel, ethanol/gasoline, and natural gas. Three industry partners are supplying engines and/or controls to accommodate multiple work-for-others and CRADA projects in this engine cell. ORNL has provided about $1,100k of internal funding to support the development of this capability. Engines to be installed in the near future include a Caterpillar C15 ACERT (advanced combustion emissions reduction technology) engine to support a potential CRADA with Caterpillar Inc. **(Figure 11)** and an ethanol-fueled GM Ecotec engine with advanced technologies from Delphi Automotive Systems including direct fuel injection, a flexible production viable intake/exhaust system, and a pressure based control system.

Figure 11. Caterpillar ACERT engine at ORNL-FEERC.

Bench-scale–microscale flow reactor for catalyst research
The new combination bench is capable of the characterization of catalytic materials ranging in size from powders to monolith core samples. The reactor incorporates automated controls and safety interlocks that enable unattended 24-hour-per-day operation.

Vehicle dynamometer upgrade
During the intense campaign of vehicle studies with ethanol blends, the much-used and aging dynamometer absorber unit sustained a coupling/bearing failure. Spare parts were located and the laboratory was returned to operation with only 3 days of downtime. Subsequently, a new dynamometer has been acquired and is being commissioned.

Soot kinetics microreactor
The microreactor system can be used to measure several fundamental properties of soot (or catalysts) including, surface area, volatile content, O_2 storage capacity, and kinetic parameters for oxidation by O_2 or NO_X. Using this small-scale system is essential for accurately measur-

ing these parameters in the absence of heat and mass transfer effects; the small samples help to ensure uniform temperature and gas concentrations across the reactor.

The system consists of a one or two stage quartz U-tube plug flow reactor, with reaction products analyzed by a quadrupole mass spectrometer. It is equipped with a switching valve and two independent gas manifolds supplied by digital mass flow controllers flowing bottled gases and capable of humidified flow. Each stage of the reactor is outfitted with external and internal thermocouples to monitor the gas or bed temperature and a digitally controlled furnace capable of reaching temperatures up to 1,100°C. A second reactor containing an oxidation catalyst can be bypassed or used to completely convert oxidation products or oxidize volatiles evolving from the sample **(Figure 12)**.

Figure 12. Microreactor experiment for soot oxidation studies.

Three new single-cylinder engines. The following engines have been added for research purposes

- Light-duty gasoline- and diesel-based single-cylinder engine stands have been developed for use in DOE and industry funded investigations. The gasoline engine has a Sturman hydraulic-actuated variable valve timing system **(Figure 13)**. The diesel was provided by industry for a proprietary project.
- A natural gas single-cylinder engine based on a Waukesha Advanced Power Generation engine will be used for investigation of opportunity fuels such as landfill gases and for fundamental combustion studies.

Fuel storage facility expansion

To generate large volumes of data in a wide range of projects, our engine and vehicle laboratory uses many drums of fuel of many different compositions. To provide safe storage, a prefabricated conditioned fuel storage container has been acquired.

DIRECT SUPPORT TO INDUSTRY (WFO)

ORNL FEERC performed direct industry-funded research for nine firms in FY 2008. These efforts are typically proprietary and not discussed in public forums.

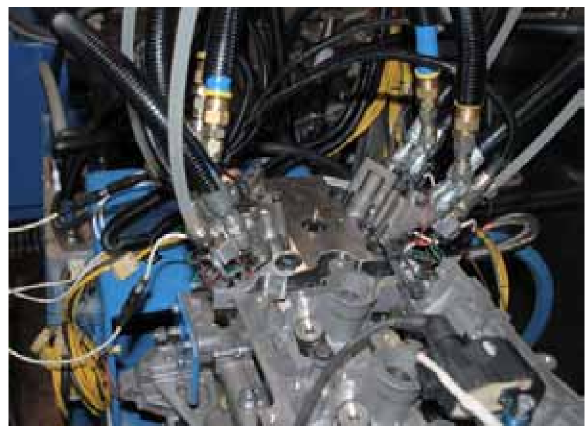


Figure 13. Single-cylinder direct-injection, spark-ignition engine with hydraulic actuation valve system.

High Temperature Materials Laboratory User Program

The High Temperature Materials Laboratory (HTML) User Program supports the missions of DOE, EERE and VTP by working with industry, universities and other national laboratories to enable the development of energy-efficient technologies that will help the United States use less oil. These technologies include batteries and other energy storage devices, which are essential for the electrification of transportation. During FY 2008, the HTML User Program received 61 new proposals: 19 from industry, 40 from universities, 2 from others.

New HTML User Program projects were established in 2008 with the University of Michigan, Ohio State University, Brookhaven National Laboratory, Motorola, and the Massachusetts Institute of Technology to study various aspects of lithium ion batteries, from the development of better electrodes to understanding the mechanisms that are responsible for the stability and durability of batteries.

During FY 2008, researchers from industry, academia, and other national laboratories participated in the HTML User Program to characterize graphite fibers, fiber-reinforced composites, magnesium and aluminum alloys, and other structural materials. An especially significant user project with Metalsa, which is a leading tier 1 supplier of chassis and body structures for light and heavy vehicles, will result in 30 million pounds of steel saved per year, along with associated energy and fuel savings.

Consistent with its goal to become a world-leading laboratory for the characterization of materials, the HTML User Program made significant investments to upgrade and acquire new instruments for thermophysical property characterization and for surface chemical analysis. The program also made important investments to develop tools for in situ characterization of materials and processes. Some of these tools have already produced remarkable results.

For example, through user projects with the University of Texas-Austin and the University of Missouri-St Louis, it has become possible to study in real time at the atomic level how catalytic nanoparticles behave at high temperature. These observations will enable the development of improved technologies for exhaust aftertreatment and the production of hydrogen and biofuels. These same tools will also allow real-time characterization at the atomic level of how the microstructure of lithium ion battery electrodes changes during charging-discharging cycles. Such experiments will provide important understanding of the mechanisms that limit the durability of these batteries.

Lightweighting Materials

As a major component of DOE's VTP, Lightweighting Materials (LM) focuses on the development and validation of advanced materials and manufacturing technologies to significantly reduce automotive passenger-vehicle body and chassis weight without compromising other attributes such as safety, performance, recyclability, and cost.

LM is pursuing five areas of research: cost reduction, manufacturability, design data and test methodologies, joining, and recycling and repair. Because the single greatest barrier to the use of lightweight materials is cost, priority is given to activities aimed at reducing costs through development of new materials, forming technologies, and manufacturing processes.

In August 2008, GM, Ford, Chrysler, Cosma, and Camanoe completed the first design iteration of the magnesium front end and technical cost modeling for the unibody steel front end (baseline). Gaps with respect to crash performance and meeting weight-reduction targets were identified. These are the first milestones in a joint effort between the United States, Canada, and China on developing and validating the front end, thereby demonstrating cost-effective weight reductions of 50% or more. ORNL provides technical advice and progress monitoring in support of the DOE program manager. ORNL is also supporting the project by developing joining methods and nondestructive evaluation (NDE) techniques and performing fundamental research into the processing and performance of magnesium alloys.

Selection of the material and process system and preliminary design for a structural-composite underbody were completed in December 2007 by the Automotive Composites Consortium, one of the consortia of the United States Council for Automotive Research. This is an initial milestone in an approximately 5-year effort aimed at developing and validating technology for cost-effective weight reductions of 30% or more in a large, monolithic, safety-critical component. ORNL provides technical advice and progress monitoring in support of the DOE program manager. ORNL is also conducting a project to evaluate and develop techniques for joining the composite underbody to other dissimilar vehicle materials that interface with the underbody.

By the end of FY 2008, ORNL had established a partnership with FISIPE S.A. in Lisbon, Portugal, for producing commodity textile polyacrylonitrile (PAN) fiber precursor for lower cost carbon fiber suitable for automotive body and chassis applications. ORNL and FISIPE evaluated multiple PAN compositions and down-selected the most promising formulation. ORNL developed a chemical pretreatment process for in-line modification of the precursor during the wet-spinning stage of processing, and ORNL established the stabilization, oxidation, and carbonization time-temperature-tension profiles for conversion of the precursor into carbon fiber. ORNL processed multiple 26,600 filament tows into carbon fiber using the ORNL carbon fiber pilot line, exceeding program strength and modulus requirements **(Figure 14)**.

Figure 14. FISIPE precursor during processing (yellow). Conventional precursor is white.

By the end of 2008, mechanical properties of 31 Msi modulus, and 380 Ksi strength (program goals: 25 Msi, 250 Ksi) had been obtained. Being able to use lower cost precursors, produced in high volume, is a critical step toward lower cost carbon fiber composites which are capable of effecting body and chassis weight reductions of 50% or more.

During FY 2008, the Auto/Steel Partnership fabricated and tested 10 Phase-1 (materials substitutions) prototypes of a rear chassis structure using advanced high-strength steels (AHSSs) and addressed the technology gaps related to fabricating AHSS structures. They developed a methodology to determine the fatigue resistance of a chassis structure by virtual testing and prepared a Phase-2 design (complete redesign) which reduced the mass by 27% through use of AHSS, new architectures, and manufacturing innovations. Corrosion tests were passed successfully with coated substrates. ORNL is supporting this portion of the program by the development of joining technologies and an understanding of strain rate sensitivity in AHSSs.

During FY 2008 PNNL, ORNL, the University of Illinois at Urbana-Champaign and Moldflow Corporation developed, validated, and implemented a new fiber orientation model (by Moldflow) for long fiber thermoplastic composites. The model successfully predicted fiber orientation tensor components for a glass-polypropylene ISO-plaque. This is part of a larger effort involving the above participants, the American Chemistry Council Plastics Division (formerly known as the American Plastics Council of the "Plastics Makes It Possible" TV commercials), and six other U.S. universities jointly funded by LM and the National Science Foundation. This larger effort is aimed at improving the ability to predict the properties of fiber-reinforced composites and is an example of integrated computational materials engineering (ICME), described below.

In April 2008, a blue-ribbon panel of the National Materials Advisory Board of the National Research Council, partially supported by the VTP LM technology area, completed an 18-month study of ICME, the use of modern computational methods for the processing-structure-properties relationships in materials. The study recognized that the materials field lags other engineering fields in the use of computerized modeling and made recommendations to overcome deficiencies.[8] ORNL is using ICME to develop diffusion databases for magnesium alloys in order to understand and model the casting, forming, and in-service properties of magnesium for potential automotive applications.

[8]National Research Council, National Materials Advisory Board, Committee on Integrated Computational Materials Engineering. *Integrated Computational Materials Engineering; A Transformational Discipline for Improved Competitiveness and National Security.* National Academies Press, Washington, D.C., 2008; available online at http://www.nap.edu/catalog.phpNOrecord_id=12199.

Propulsion Materials

The Propulsion Materials program is a partner and supporter of the VTP Hybrid and Vehicle Systems, Energy Storage, APEEM, Advanced Combustion Engines, and Fuels and Lubricants R&D programs. Projects within the Propulsion Materials program address materials concerns that directly impact the critical technical barriers in each of these programs—barriers such as fuel efficiency, thermal management, emissions reduction, and reduced manufacturing costs. The program engages only the barriers that involve fundamental, high-risk materials issues.

ENABLING TECHNOLOGIES

The Propulsion Materials program focuses on enabling and innovative materials technologies that are critical in improving the efficiency of advanced engines. The program provides enabling materials support for combustion, hybrid, and power electronics development, including the following.

- Materials for low-temperature combustion (e.g., HCCI).
- Materials for hydrogen engine fuel systems.
- Materials for 55% thermal efficiency heavy-duty diesel engines.
- Materials for waste heat recovery via thermoelectric (TE) modules (with the potential for a 10% increase in fuel efficiency).
- Materials for efficient and effective reduction of tailpipe emissions.

The program supports these core technology areas by providing materials expertise, testing capabilities, and technical solutions for materials problems. The component development, materials processing, and characterization that the program provides are enablers of the successful development of efficient and emissions-compliant engines.

PROGRAM ORGANIZATION

The Propulsion Materials program consists of five R&D projects which support the VTP propulsion technologies. Each project consists of several related R&D agreements.

- Materials for Electric and Hybrid Drive Systems—developing materials appropriate for power electronics and other hybrid system applications.
- Combustion System Materials—developing materials for HCCI engines and fuel injection systems.
- Materials for High Efficiency Engines—developing materials for efficient engine components, such as valve-train components, fuel injectors, and turbochargers.
- Materials for Control of Exhaust Gases and Energy Recovery Systems—developing materials for exhaust aftertreatment and TE exhaust heat recovery applications.
- Materials by Design—developing advanced materials for NO_X catalysts, lithium ion batteries, and thermoelectric generators (TEGs) through adoption of a computational materials–atomic-scale characterization protocol.

R&D projects and agreements are evaluated annually using strategic objectives. Agreements are evaluated based on relevance to VTP and supported team's priorities, strength of industrial support for the activity, and perceived value of the R&D activity to VTP. To keep the program fresh and up-to-date, more than 10% of agreements are retired annually. New projects are selected in accordance with identified VTP needs, including the following.

- Advanced Combustion Team
  - Internal combustion engine materials
  - TE materials
  - Catalysts and aftertreatment materials
  - Materials for engine sensors
- Hybrid Electric Systems Team
  - Power electronics materials
  - Materials for energy storage
- Fuels Team
  - Alternative fuels materials compatibility

KEY TECHNICAL ACCOMPLISHMENTS

Materials for electric and hybrid drive systems

The goal of the APEEM program is to reduce the size, weight, and volume of the power electronics without increasing the cost or reducing the reliability. Many, if not most, technical barriers are directly linked to the contemporary material limitations of subcomponents found within devices that comprise inverters, converters, and motors. The material limitations include the following.

- Insufficient temperature capability.
- Excessive thermal insulations.
- Excessive electrical insulation.
- Insufficient power density in permanent magnets.
- Insufficient bandgap.

Many of these issues are already being addressed in the APEEM Program, but there is interest in additional means to overcome some of those material limitations through the application of advanced materials science and engineering. In 2008 we conducted modeling and analysis of a new concept for a direct-cooled power electronics substrate. The concept of the direct-cooled substrate is shown in **Figure 15**.

A finite element model of stress and temperature was constructed. Experimental strength data for an alumina ceramic substrate were used with the finite element model and the Cares/Life computer code to predict the probability of survival of the direct-cooled substrate, **Figure 16**. The probability of survival was predicted to be greater than 99.999%. The direct-cooled ceramic substrate could be of interest for use in hybrid vehicle inverters because it has the potential to substantially reduce both the volume and weight of the inverter. A prototype will be fabricated in FY 2009.

The strength of several candidate substrates and silicon chips was measured for use in probabilistic analyses; biaxial flexure strengths are shown in **Table 4**.

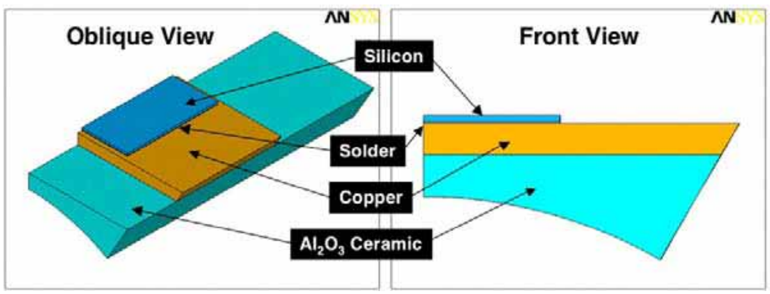


Figure 15. Model of a direct-cooled ceramic substrate.

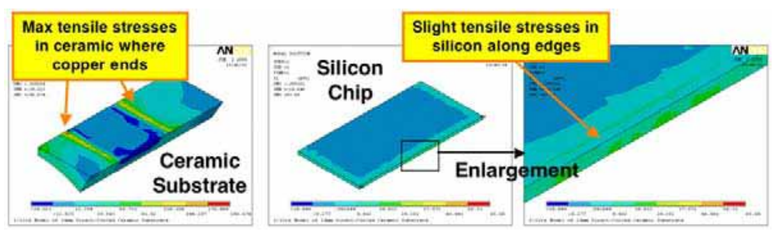


Figure 16. First principal stresses in the ceramic substrate and the silicon.

Table 4. Comparison of Weibull strength distributions for anticlastically fractured silicon and silicon carbide chips

Material	Descriptor	Number of Specimens	Characteristic Equibiaxial Strength[a] (MPa)	Weibull Modulus
Aluminum nitride	As fired	15	665	33.0
Aluminum nitride	Lapped	10	452	13.0
Aluminum oxide	AD96	10	595	12.7
Aluminum oxide	AD995	10	692	16.9
Boron nitride		15	50	12.8
Silicon carbide	Sintered alpha	10	518	4.8
Silicon nitride	SN460	15	1,097	17.7

[a]*Test fixture: Ball on ring (15 mm ring, 1/2 in. WC ball, XHD=0.5 mm/min)*

Materials for high efficiency engines

To enable the improved selection and use of materials, surface treatments, and lubricating strategies for components like exhaust valves and seats in energy-efficient diesel engines, researchers at ORNL designed and built a specialized high-temperature, repetitive impact apparatus **(Figure 17)** to investigate the combined effects of mechanical contact, high temperatures, and oxidizing environments on the durability of high-performance diesel engine valve materials. The testing system is capable of testing actual valves as well as simpler specimens of promising materials not currently available as valves. A set of diesel engine exhaust valves was provided by Caterpillar Inc. to serve as best-practice commercial materials for benchmark testing and to ensure that the apparatus would properly fit commercial valves. Initial experiments used a specimen holder inclined at 45 degrees to mimic the actual seat angle and produce a combination of impact plus slip on the contact surfaces.

Figure 17. High temperature, repetitive impact testing machine with the furnace door open to reveal the specimen holders.

Engine manufacturers have recognized several key needs that must be addressed for heavy duty diesel engines to achieve a national efficiency goal of 55% by the year 2012. These include (1) improved structural materials to accommodate higher cylinder pressures and temperatures (associated with advanced combustion methodologies), (2) improved thermal management and waste heat recovery technologies, (3) improved durability, (4) improved transient performance, and (5) better aftertreatment performance. These needs address barriers associated with high parasitic losses, HECC, and thermal management of the cylinder and exhaust.

A CRADA between Caterpillar Inc. and ORNL brings together the comprehensive expertise in engine design and testing and materials development within both organizations to address these critical barriers. Caterpillar provided ORNL with two 600 hp motoring dynamometers and a C15 ACERT engine for testing of engine components and materials **(Figure 18)**. Working with ORNL, Caterpillar will develop and provide prototype components to be evaluated on the engine platform. ORNL engine research staff will evaluate the engine performance with emphasis on combustion diagnostics, optimization, and modeling. Materials scientists at ORNL will examine material performance and provide guidance on materials development.

Figure 18. Photograph showing mounted Caterpillar engine and dynamometer in ORNL engine test cell. The engine will be used for testing advanced component designs and materials.

The development of new emission-treatment catalytic systems is still largely dominated by trial and error, which is often slow and expensive. A knowledge gap between theory and experiment has been a major contributing factor: traditional computational approaches have been significantly simplified in comparison to real materials, and experimental studies, especially on emission treatment catalysts, have primarily focused on fully formulated systems that can treat engine-out emissions in vehicles.

ORNL researchers are developing a protocol that combines the power of theory and experiment for atomistic design of catalytically active sites that can contribute directly to complete catalyst systems suitable for technical deployment. The protocol includes theoretical modeling of catalyst systems via density functional theory, synthesis of experimental catalyst systems, exposure of catalysts under simulated operating conditions (including an ex-situ reactor, which permits duplication of the reaction conditions in a bench-top reactor and facilitates high-resolution scanning transmission electron microscopy), and characterization of the catalyst performance and changes that occur in the catalysts during operation. In 2008, we conducted theoretical and experimental studies of the oxidation and reactivity of CO, NO_X, and hydrocarbons on platinum clusters supported on alumina, which are a common constituent of a variety of emission treatment catalysts, including three-way, NO_X trap, oxidation, and hydrocarbon selective catalytic reduction (SCR) catalysts.

The durability of diesel particulate filters (DPFs) is being evaluated by ORNL research staff and Cummins, Inc., via application of probabilistic design tools, NDE, and refinement and use of lifetime-prediction models. Mechanical and thermal shock characterization test procedures developed previously were used to rank the relative thermal shock resistance of several candidate DPF substrate materials. The properties used to measure the thermal shock resistance included the fracture toughness, elastic modulus, and coefficient of thermal expansion. The porosity of the cordierite substrate was the most important variable that determined the elastic and fracture mechanical properties of the substrate. The effect of porosity on the fracture toughness of cordierite substrates was quantitatively identified. In addition, the effect of catalytic "washcoating" and soot loading on the high temperature elastic properties of DPF substrates was characterized. A field returned DPF was thoroughly characterized **(Figure 19)** and its properties compared to that of virgin, uncoated filters. The difference in the properties of field returned filters was explained based on microstructural observations.

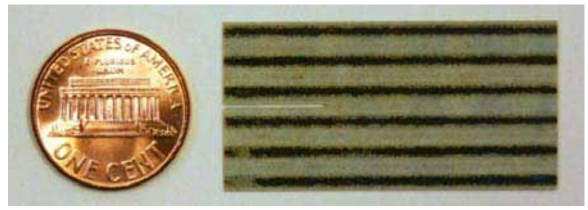


Figure 19. Double-torsion specimen prepared from a high mileage filter. The alternate dark lines are due to soot loading on the inlet channels of the filter.

Materials by design

Researchers in the ORNL Propulsion Materials program are developing design strategies for TE materials based on first principles calculations of electronic, vibrational, and transport properties to identify potentially low cost, high performance TE materials suitable for application in vehicles. New insights into TE materials performance have emerged from density functional calculations in conjunction with transport theory. Promising new potentially low cost TE materials, especially $YCuO_2$ **(Figure 20)** have been identified, and a mechanism for thermal conductivity reduction in PbTe has been elucidated.

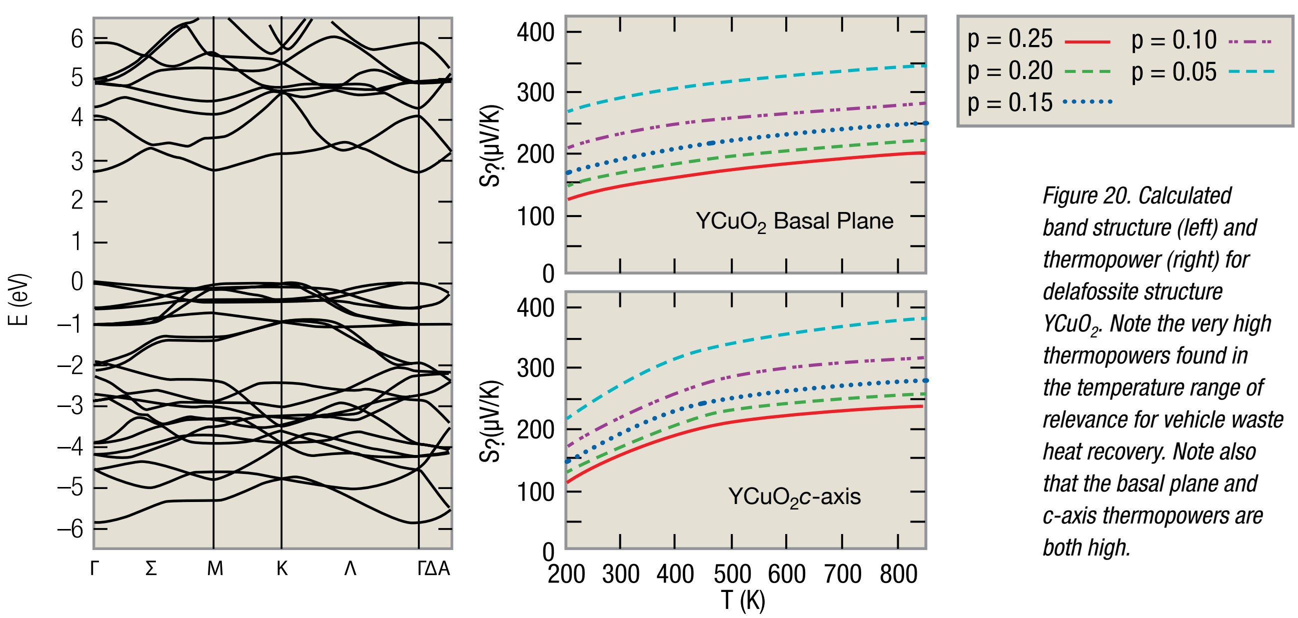


Figure 20. Calculated band structure (left) and thermopower (right) for delafossite structure $YCuO_2$. Note the very high thermopowers found in the temperature range of relevance for vehicle waste heat recovery. Note also that the basal plane and c-axis thermopowers are both high.

SUMMARY OF FY 2008 ACTIVITIES

The use of TE devices to convert waste heat in vehicle exhaust to electricity offers the potential for significant energy savings. In particular, a fuel savings of 10% would be enabled by manufacturable TE materials with figure of merit, ZT, values greater than 2 over the appropriate temperature range. Among the requirements for the effective use of such devices in vehicles is the availability of high performance, low cost TE materials. We are therefore developing improved materials using a science-based approach. Specifically, we are using materials design strategies based on first principles calculations of electronic, vibrational, and transport properties to identify potentially low cost, high performance TE materials suitable for application in vehicles. We are also calculating properties of existing materials as a function of doping and other parameters to obtain information needed for optimization of these materials. The emphasis is on the TE figure of merit, ZT, at temperatures relevant to waste heat recovery and materials properties of importance in engineering TE modules (e.g., anisotropy and mechanical properties). The calculations are done using state-of-the-art computational tools such as the linearized augmented plane wave method and the BoltzTraP code.

NDE development for ACERT engine components

The objective of this project is to develop and assess various NDE methods for characterization of advanced engine components in valve train, fuel-injection, and turbo systems in a Caterpillar heavy-duty ACERT experimental engine at ORNL. Work in FY 2008 was focused on development of optical methods for advanced valve train materials and evaluation of X-ray, ultrasonic, and infrared thermal imaging NDE methods for ACERT engine components/materials. The optical NDE development was focused on detection and characterization of fracture initiation flaws that limit the strength of ceramic engine valves **(Figure 21)**. For ACERT applications, we identified thermal imaging suitable for inspection of thermal barrier coatings (TBC) to be evaluated in initial engine tests **(Figure 22)**. Advanced thermal imaging methods are being developed for prediction of coating thermal properties and for 3D imaging of subsurface coating structures. This work is a collaboration between Caterpillar Inc. and ORNL.

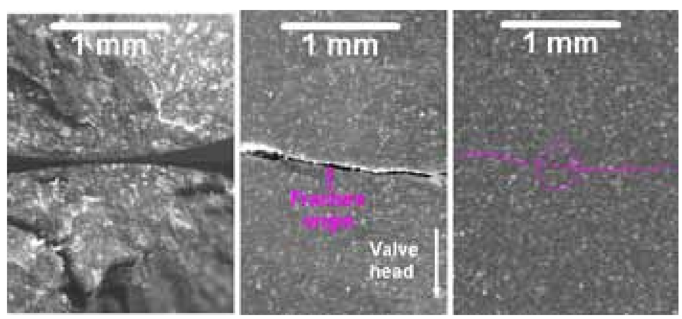


Figure 21. NDE detection of fracture origin (a large inclusion) in a ceramic valve stem.

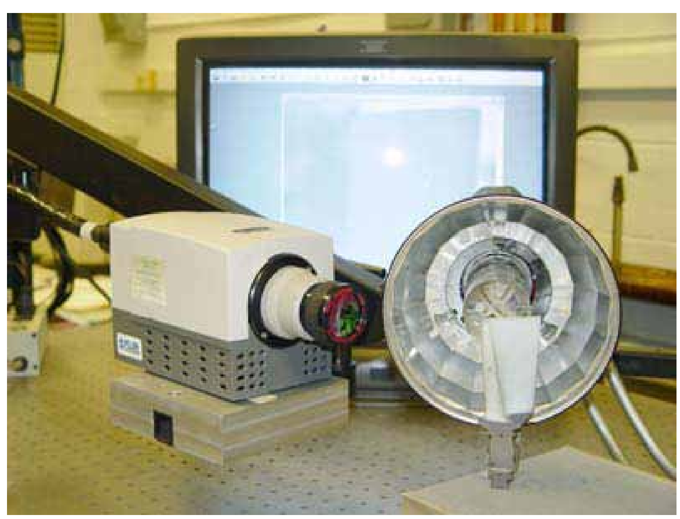


Figure 22. One-sided flash thermal imaging setup for testing of a turbine blade with TBC coating.

Validation of approach for oxide TE materials

We performed detailed calculations of transport properties of the TE oxide Na_xCoO_2, including the effects of magnetic field, and compared the results with experimental data. This showed that the Boltzmann transport calculations based on electronic structure calculations can be used to predict the TE power of oxide materials. Oxides offer significant advantages in applications. In particular they have potentially low cost and high stability. This validation provides confidence in the mechanisms for TE performance found based on our calculations and in predictions of new oxide TE materials based on them.

Materials design rules for oxide TE materials

We used the calculated results for Na_xCoO_2 as well as several other oxide materials to identify the reasons for the high TE performance of Na_xCoO_2 in terms of the basic bonding and electronic structure. These design rules allow us to identify other candidate oxide TE compounds with properties that are more amenable to vehicular applications. The following were among our findings.

- The high thermopower of Na_xCoO_2 at metallic carrier densities is due to the combination of very narrow bands and the absence of carrier localization.
- The conductivity of Na_xCoO_2 is due to the mixed valence of the cobalt (Co) ions and strong hybridization between the Co and oxygen in this compound.
- The combination of narrow bands and strong hybridization is a consequence of the bonding topology: in particular, near 90° Co-O-Co bonds combined with a substantial Co-Co distance that precludes direct metal-metal electron hopping.

Application of materials design rules to find new candidate materials

We used the above design rules to identify other potential TE compositions. The focus was on materials that are more amenable to vehicular applications than Na_xCoO_2. One particular problem with Na_xCoO_2 is that it is highly anisotropic, so high TE performance is only realized in oriented single crystal form. In particular, we looked for compositions that would have potentially low materials cost and that would have more isotropic properties than Na_xCoO_2. We performed electronic structure calculations for tetragonal ordered spinel type Zn_2TiO_4 and Mg_2TiO_4, finding that their band structure does indeed show narrow conduction bands comparable to those in Na_xCoO_2 that will lead to high thermopowers when subjected to n-type doping (e.g., with niobium). In addition we identified $YCuO_2$ as a potentially low cost p-type oxide TE material with much more isotropic properties than Na_xCoO_2. These predictions have been communicated to experimental groups that are synthesizing the materials in preparation for testing.

Mechanisms for TE performance in tellurides

Tellurides, in particular lead telluride- (PbTe-) based materials and the so-called LAST phases (PbTe-$AgSbTe_2$), are currently the most popular materials for TE waste heat recovery. These materials offer good performance combined with other properties that make them amenable to vehicle applications. However, tellurium (Te) is a rare element whose limited availability may limit large scale deployment of TE systems based on tellurides. Therefore it is important to identify the origins of the favorable properties of tellurides so that alternative materials can be identified.

Partially in response to a request from GM, we investigated the lattice vibrations of PbTe to determine why the thermal conductivity of this material is favorable in spite of its simple crystal structure, which has a small unit cell and no rattling ion or possibility of disorder induced phonon scattering. We found that PbTe has a very soft transverse optical phonon branch that is strongly anharmonic itself and additionally is very strongly coupled to the heat carrying longitudinal acoustic branch. This provides a basis for the low thermal conductivity of PbTe and PbTe-based materials and, more importantly, provides another mechanism for thermal conductivity reduction that can be used in searching for new TE materials. We also performed calculations for lanthanum telluride. This was initiated in part to determine whether this isotropic cubic material, which has the highest known *ZT* at very high temperatures, could be adapted for use at lower temperatures for waste heat recovery and also to determine the mechanism for the high performance of an n-type material in spite of the fact that it has large concentrations of lanthanum vacancies, which might be expected to lead to carrier localization and poor performance. We found that two bands are involved in conduction, a heavy band and a light band, and used this to predict the doping dependence and provide understanding of conduction in this material.

ORNL contributed to new knowledge discovery in several key areas relevant to the VTP mission: reduced petroleum consumption, use of nonpetroleum fuels, and emission compliance.

KEY TECHNICAL ACCOMPLISHMENTS

PHEV Value Proposition Study

ORNL, with the support of Sentech, Inc., the Electric Power Research Institute, and General Electric, will conduct a study of the benefits, barriers, technical and infrastructure requirements, opportunities, and challenges of grid-connected PHEVs to establish potential value propositions that will lead to commercially viable PHEVs. Accomplishments to date include the following.

- Held a PHEV Value Proposition Workshop with stakeholders from automotive suppliers, OEMs, utilities, transmission and distribution companies, government, regulators, and automotive dealerships.
- Integrated data and models that are highly regarded by industry. These data and models aggregated the technical and economic impact of 17 PHEV value propositions on vehicle components and systems, facility owners, transmission and distribution systems, and utility power generation plants for a baseline case study of Southern California in 2030.
- Coordinated laboratory meetings for collaborating PHEV activities among the DOE national laboratories.
- Reported on the findings of the PHEV Value Proposition Study Workshop, data and model building, and assessment results.

Enabling high efficiency ethanol engines (Delphi PHEV CRADA)

The objective of this CRADA with Delphi Automotive Systems Corporation is to explore the potential of ethanol-based fuels for improvements in drive-cycle efficiency and emissions based on simulation and experiments. Accomplishments to date include the following.

- Multicylinder engine cell for evaluating ethanol efficiency potential and enabling technologies is near completion.
- Ethanol engine build is under way with expected delivery to ORNL in early FY 2009.
- Engine maps from a Saab BioPower vehicle were validated for gasoline and ethanol fuels.
- Parallel HEV and PHEV vehicle model development is underway for use with Saab data.
- Models are being used to simulate conventional and advanced powertrains over relevant drive cycles.

Development of models for advanced engines and emission control components

The objective of this project is to ensure that computer simulations using the Powertrain Systems Analysis Toolkit (PSAT) have the necessary components to accurately reflect the drive performance, cost, fuel savings, and environmental benefits of advanced combustion engines and aftertreatment components as they could potentially be used to optimize leading-edge HEVs and PHEVs. Apply the above component models to help DOE identify the highest HEV and PHEV research and development priorities for reducing U.S. dependence on imported fuels. Accomplishments to date include the following.

- Generated Saab 2-liter BioPower flex-fuel engine maps for both gasoline and ethanol fueling.
- Validated the Saab engine maps with cold and hot start vehicle chassis dynamometer data.
- Generated the first public map for the GM 1.9-liter research diesel engine that is capable of HECC combustion and is being used as a common reference engine by the national laboratories and several universities.
- Added and validated external heat loss and thermal transient models to PSAT that can account for these effects on hybrid vehicle performance.
- Documented the LNT PSAT model as a template for future lean-exhaust aftertreatment components.
- Constructed a new three-way catalyst model for PSAT to be used to account for catalyst light-off and extinction on stoichiometric hybrid vehicles.
- Tested preliminary DPF and SCR lean exhaust aftertreatment models for PSAT.
- Demonstrated a preliminary TEG model for simulating TE exhaust heat recovery.
- Demonstrated comparisons between stoichiometric and lean-engine-based HEVs using PSAT.
- Demonstrated the usefulness of PSAT for making leading-edge integrated engine aftertreatment concepts evaluations to the CLEERS Focus Groups and the DOE Diesel Cross-Cut Team.
- Disseminated research results via publications and presentations (e.g., the Society of Automotive Engineers, CLEERS Workshop, DOE annual reports, and FreedomCAR and Fuel Partnership Technical Team meetings).

In FY 2009, ORNL will continue its emphasis on after-treatment solutions for PHEVs. Additionally, ORNL heavy-duty research activities will focus on drive cycles for Class 6 vehicles and the evaluation of Class 8, 2007 emissions-compliant engine technologies.

HEAVY TRUCK DUTY CYCLE PROJECT

The Class-8 Heavy Truck Duty Cycle (HTDC) project (Phase 3 of the Heavy and Medium Truck Duty Cycle Program) was the precursor effort to this Class-6/Class-7 Medium Truck Duty Cycle (MTDC) project (Phase 4). As the Phase 3 efforts came to an end in FY 2008, we segued into efforts related to the Class-6/Class-7 MTDC project. It involves efforts to collect, analyze, and archive data and information related to Class-6/Class-7 medium truck operation in real-world driving environments. Such data and information will be useful to support technology evaluation efforts and provide a means of accounting for real-world driving performance within medium class truck analyses. The project is being led by ORNL and involves private industry partners from various trucking enterprises and organizations representing Class-6/Class-7 vehicles currently in use **(Figures 23 and 24)**. Additionally, ORNL is collaborating with the Federal Motor Carrier Safety Administration (FMCSA; part of DOT), and in the future possibly with EPA, to determine whether there is possible synergy between this Class-6/Class-7 duty cycle data collection effort and that agency's needs to learn more about the operation and duty cycles of these significant fuel consuming commercial vehicle classes. The EPA is specifically interested in duty cycle data collection in concert with key emissions data to support their SmartWay Transport Partnership, which seeks to improve energy efficiency while reducing GHG and air pollutant emissions. The FMCSA is primarily interested in collecting safety data relative to the driver, carrier, and vehicle. Furthermore, FMCSA, through ORNL and other industry partners, is in the process of developing and testing requirements to "wirelessly" transfer data from a commercial vehicle, to the roadside. ORNL will work to establish partnerships with these agencies to leverage scarce resources to better accomplish these national goals.

This MTDC project is a critical element in DOE's vision for improved truck energy efficiency. It will collect real-world data for various situational characteristics (rural/urban, freeway/arterial, congested/free-flowing, good/bad weather, etc.) and look at the unique nature of Class-6/Class-7 vehicles' drive cycles (stop-and-go delivery, power-take-off, idle time, short radius trips), to provide a rich source of data and information that can contribute to the development of new performance evaluation tools, provide DOE a sound basis upon which to make technology investment decisions, and provide a national archive of real-world-based medium truck operational data that will support truck energy efficiency research. The MTDC project will be conducted over a 36-month period of time (February 1, 2008, through January 31, 2011).

This project will result in real-world MTDC data that

- supports ANL's continued development of PSAT,
- provides data to conduct an independent evaluation of PSAT,
- provides a source of real-world Class-6/Class-7 medium-truck performance data that can be used by DOE for making decisions related to future technology research,
- provides a baseline of data that can be used to gauge 21CTP technology advances, and
- provides a national source of real-world data for the Class-6/Class-7 medium-truck research community.

Figure 23. An H. T. Hackney vehicle currently active in the MTDC effort.

Figure 24. A Knoxville Area Transit vehicle currently active in the MTDC effort.

Technical Project Highlights

The remainder of this report comprises technical highlights describing significant achievements or milestones attained during the reporting period. Each highlight provides a brief programmatic context, a description of the R&D activity, and the benefits expected to accrue to VTP and the transportation industry. The highlights also address, as appropriate, commercialization activities or future R&D plans to address technical barriers and challenges.

Advanced Power Electronics and Electric Machines

Advanced Converter Systems for High Temperature Environments

Background

The Oak Ridge National Laboratory is developing an innovative power conversion system for hybrid electric vehicles that employs the concept of modular multilevel voltage converters with small magnetic components. The proposed multilevel power conversion technology makes it possible to use available silicon power semiconductor devices and capacitors as well as future silicon carbide (SiC) devices and high temperature capacitors to reach any voltage and current levels and, when compared to the existing power conversion technology, to provide the most efficient, least weight, most compact power conversion system operable at underhood temperature limits of 200°C or higher.

Technology

The goal of this project was to develop a new and unique bidirectional direct current (dc-dc) power converter that minimizes magnetics and incorporates high temperature power devices, capacitors, and a gate driver that will enable the converter and gate drive to operate in high ambient temperatures.

During the course of this project, a high temperature gate driver was fabricated with silicon-on-insulator (SOI) material that is capable of operating at temperatures of up to 225°C. The gate drive chip has dimensions of only 2.2 mm^2 (Figures 1 and 2).

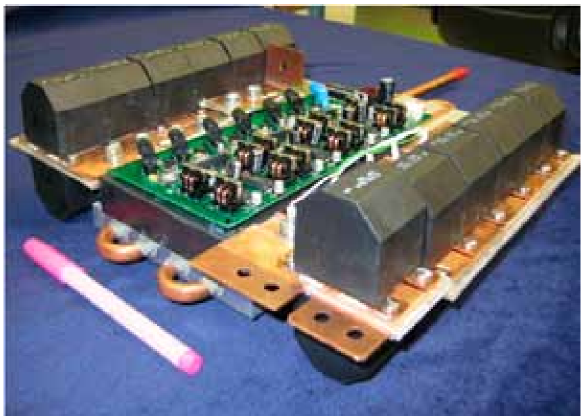


Figure 1: Prototype 55 kW dc-dc converter.

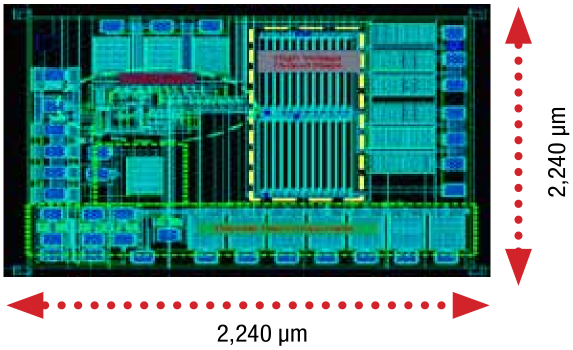


Figure 2: SOI gate drive chip layout.

Benefits

- *High efficiency converter has low power losses.*
- *Gate drive chip can tolerate high temperatures with minimal cooling requirements.*
- *Liquid cooling loop for power electronics can be eliminated.*
- *Smaller thermal management systems increase peak power to weight ratio of converter system.*

Status

A high temperature gate driver integrated circuit (IC) was designed and fabricated using an 0.8 micron, three-metal, two-poly bipolar complementary metal-oxide semiconductor and diffusion metal-oxide semiconductor (BCD) on SOI process. Testing of the chip was completed for switching frequencies of up to 40 kHz with no cooling at temperatures of up to 175°C, but with some chip failures. Modifications and simulations of the gate driver circuit for a second generation of the chip were completed. The SOI gate drive chip with dimensions of 2.2 mm^2 was fabricated and tested at temperatures of up to 225°C.

High temperature packaging of SiC junction gate field effect transistors was demonstrated and tested at up to 175°C.

A 55 kW, 200 V/600 V multilevel dc-dc converter was fabricated and tested at low temperatures. The efficiency was in the 96–98% range.

Gains made from this project will likely impact other power electronics projects that need high temperature packaging, gate drives, or modular conceptual designs.

Figure 3: Three SOI gate driver ICs.

Contacts

Laura D. Marlino
Technical Program Manager
Oak Ridge National Laboratory
(865) 946-1245
marlinold@ornl.gov

Susan Rogers
Technology Development Manager
U.S. Department of Energy
(202) 586-8997
susan.rogers@ee.doe.gov

A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

Advanced Power Electronics and Electric Machines

Application of Concentrated Windings to Electric Motors without Surface Mounted Permanent Magnets

Background

Application of fractional-slot concentrated windings (FSCWs) to electric motors supports achieving goals of increased power density, specific power, efficiency, and reliability and decreased cost. FSCWs have been applied mainly to surface-mounted permanent magnet motors in the past. Oak Ridge National Laboratory (ORNL) researchers extended FSCWs to two types of internal permanent magnet motors (1) interior permanent magnet (IPM) motors and (2) embedded permanent magnet motors. FSCWs have the potential to reduce motor fabrication cost, size, and weight and increase efficiency through the use of concentrated winding bobbin cores.

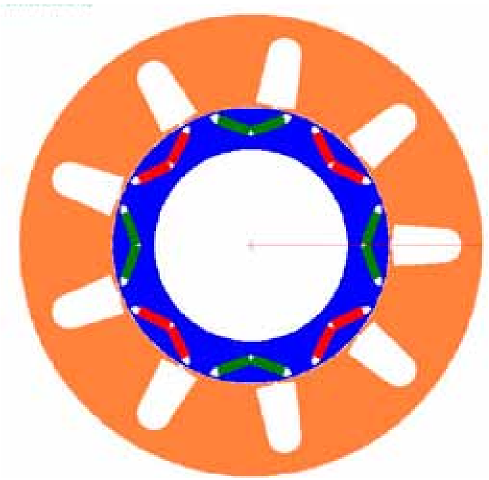


Figure 1: Outline of IPM configuration with 9 slots and 8 poles.

Technology

The objective of this research was to determine whether there were electric motor configurations using IPMs that benefit from using FSCWs instead of distributed windings, specifically for use in electric vehicle or hybrid electric vehicle traction drives. Early motor development began with concentrated windings but changed to distributed windings because concentrated windings produced sinusoidal back electromotive forces. However, recently there has been renewed interest in concentrated windings for a number of reasons, including their increased fault tolerance at higher operating speeds, elimination of most of the end turns, improved packing of wires in the stator slots, and reduced fabrication costs.

Status

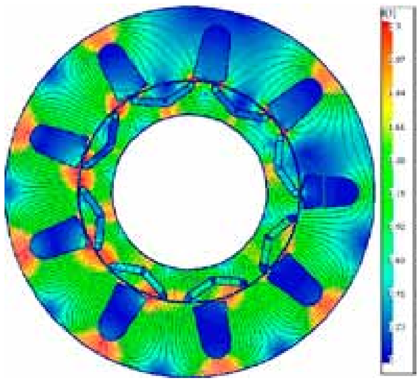
Performance simulations of IPM motors using integral-slot distributed windings and FSCWs were performed as a baseline and shown to deliver up to 55 kW for short bursts and 30 kW continuously. The simulated power delivered at base speed for two FSCW-modified cases above 80 kW achieved 97 and 93% efficiencies. Assessment shows that a 9-slot stator configuration (Figure 1) is not symmetric, which causes flux variations much larger than normal in the rotor, resulting in high eddy current losses.

Benefits

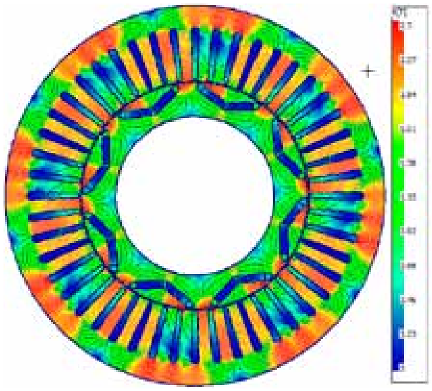
Fractional-slot concentrated windings potentially offer significant advantages.

- *Larger inductance for increased low speed traction and high speed fault tolerance.*
- *More effective use of copper–wound on bobbin, no end windings–reduced I^2R losses and reduced size.*
- *Manufacturing advantages–stator segments (old cut-core technology).*

Analysis of a 9-slot, 8-pole IPM with concentrated windings was completed and compared with a 48-slot, 8-pole baseline IPM with distributed windings. Both motor designs were simulated, and a comparison was performed of their performance running the US6 and Federal Urban Driving Schedule drive cycles using ORNL's vehicle simulator (Figure 2). It was concluded that benefits can be obtained in reduced torque ripple, reduced copper losses, and increases in efficiency with IPM concentrated winding machines. However, the power demands of the US6 cycle required increasing the gear ratio above the baseline gear ratio.



9-8 configuration with concentrated windings



Baseline configuration with distributed windings

Figure 2: Flux density maps showing asymmetric flux linkages of the 9-8 motor during operation at 5,800 rpm compared with the axisymmetric flux linkages of a baseline motor.

Contacts

Laura D. Marlino
Technical Program Manager
Oak Ridge National Laboratory
(865) 946-1245
marlinold@ornl.gov

Susan Rogers
Technology Development Manager
U.S. Department of Energy
(202) 586-8997
susan.rogers@ee.doe.gov

A Strong Energy Portfolio for a Strong America

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Advanced Power Electronics and Electric Machines

Benchmarking Competitive Technologies

Background

The Oak Ridge National Laboratory is performing research to benchmark competitive technologies. This research will determine the status of nondomestic hybrid electric vehicle (HEV) technologies through assessment of design, packaging, fabrication, and performance during comprehensive evaluations. The results will be compared with other HEV technologies and findings in the open literature. The effort supports the Vehicle Technologies Program (VTP) in planning and assisting in guiding research efforts by confirming the validity of the program technology targets, providing insight for program direction, and producing a technical basis that aids in modeling/designing. The effort also fosters collaborations between the FreedomCAR Electrical and Electronics Technical Team (EETT) and Vehicle Systems Analysis Technical Team (VSATT) by identifying unique motor/inverter/converter/drive-train technologies and ascertaining what type of additional testing is needed to support research and development.

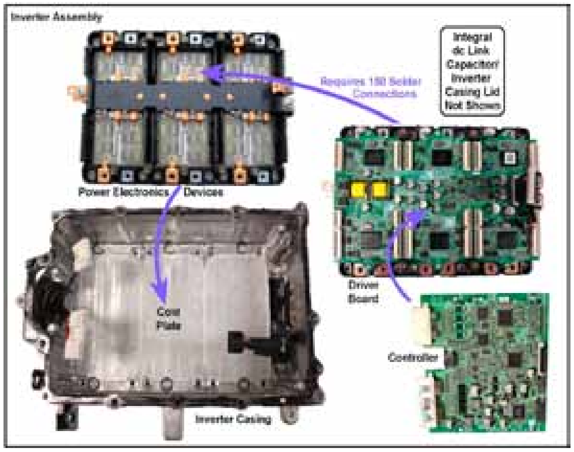

Figure 1: Example of PCU teardown: Analysis of power electronics design, layout, and packaging.

Technology

The 2008 Lexus LS 600h system was selected to benchmark based on anticipated automotive manufacturer interest due to the novel double-sided cooling technique that accompanies the most powerful HEV drivetrain currently on the market. Design/packaging studies were conducted on the LS 600h power control unit (PCU) and electronic continuously variable transmission (ECVT), revealing significant improvements over Toyota Prius and Camry designs. The LS 600h PCU motor inverter controls were bypassed to allow full control over testing conditions. Key components within the PCU/ECVT were disassembled and evaluated (Figure 1). Mass, volume, power density, and specific power of various PCU/ECVT components were assessed. The efficiency, performance, and continuous operational capabilities of the LS 600h subsystems were evaluated.

Benefits

- *Determine effectiveness and value of new technologies.*
- *Provide support to VTP planning and guidance of research efforts.*
- *Determine performance and operational parameters and publish findings.*
- *Confirm validity of the program technology targets.*
- *Render insight for program direction.*
- *Produce a technical basis that aids in modeling/designing HEV systems meeting FreedomCAR targets.*

Status

The Toyota Lexus LS 600h was successfully benchmarked. Efficiency maps for the modules were generated and destructive teardowns of the modules were completed to determine manufacturing, packaging, and thermal design issues (Figure 2). The bus capacitors and motor magnets were analyzed over extended temperature ranges as part of the teardown. A technical report was completed detailing the work.

Future benchmarking efforts will focus on technologies of interest to VTP, EETT, and VSATT.

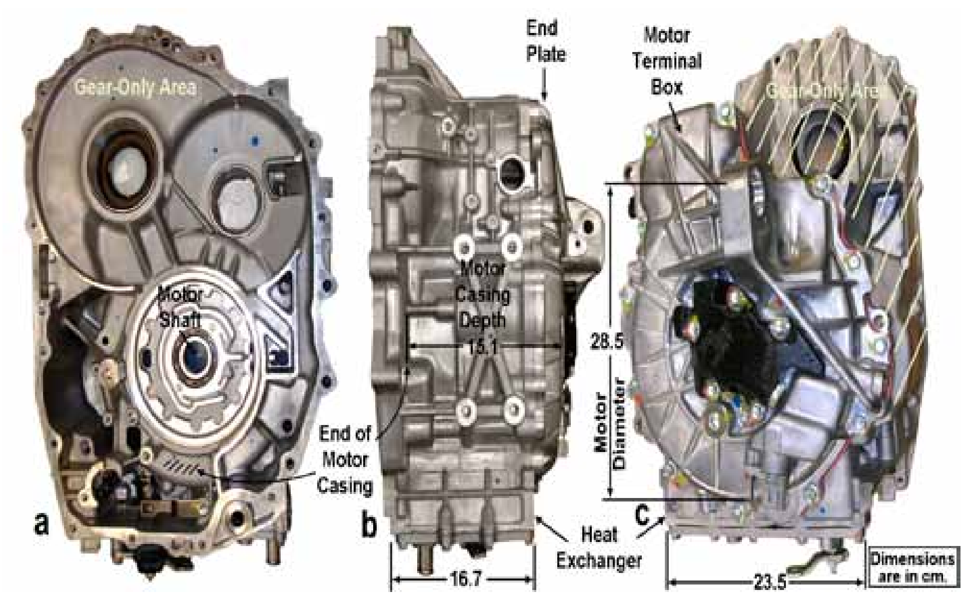

Figure 2: Example of transaxle teardown.
- *Evaluation of drive characteristics*
  - *– Planetary/drive gears, motor volume, etc.*
- *Assessment of cooling system functionality*
  - *– Oil flow and heat exchange*

Contacts

Laura D. Marlino
Technical Program Manager
Oak Ridge National Laboratory
(865) 946-1245
marlinold@ornl.gov

Susan Rogers
Technology Development Manager
U.S. Department of Energy
(202) 586-8997
susan.rogers@ee.doe.gov

A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

Advanced Power Electronics and Electric Machines

Current Source Inverter

Background

Current electric vehicles (EVs) and hybrid EVs (HEVs) use inverters that operate off a voltage source because the most readily available and most efficient energy storage devices are voltage sources. These voltage source inverters (VSIs) can easily be integrated with energy storage devices, such as batteries. The VSI, however, possesses several drawbacks that make it difficult to meet the FreedomCAR Partnership goals in terms of volume, lifetime, and cost for the inverter. It requires a very-high-performance direct current (dc) bus capacitor bank to maintain a near-ideal voltage source. Also, currently available capacitors that can meet the demanding requirements are costly and bulky, taking up one-third of the inverter volume and cost. The reliability of the inverter is also limited by the capacitors and further hampered by the possible shoot through of the phase legs making up a VSI. In addition, steep rising and falling edges of the output voltage in the form of pulse trains generate high electromagnetic interference noises, impose high stress on the motor insulations, produce high frequency losses in the copper windings and iron cores of the motor, and generate bearing leakage currents that erode the bearings over time. Furthermore, the capacitor presents the most difficult hurdle to operating a VSI in automotive high temperature environments.

Technology

A new inverter topology based on the current source inverter (CSI) is offered to eliminate or significantly relieve the aforementioned problems. The CSI significantly reduces the amount of capacitance required, using only three alternating current (ac) filter capacitors of a much smaller capacitance; the total capacitance of the ac filter capacitors is estimated at about one-fifth that of the dc bus capacitance in the VSI. The CSI offers many other advantages important for HEV applications, including that (1) it doesn't need antiparallel diodes in the switches, (2) it can tolerate phase-leg shoot through, (3) it provides sinusoid-shaped voltage output to the motor, and (4) it can boost the output voltage to a higher level than the

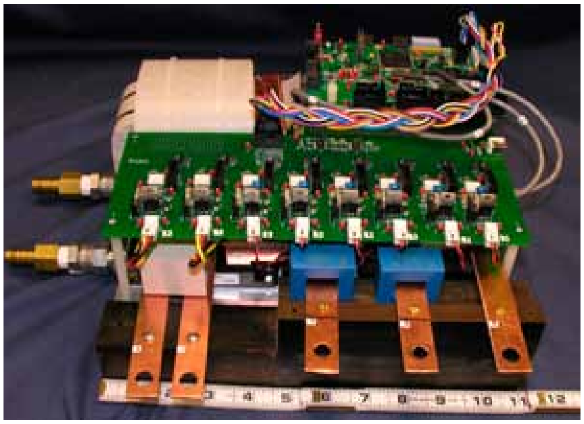

Figure 1: ORNL's high speed, interior permanent magnet reluctance motor with brushless field excitation.

Benefits

- *High reliability due to elimination of dc bus capacitors and endurance of phase-leg shoot through.*
- *Improved motor efficiency and lifetime by providing sinusoid-shaped voltage and current to the motor.*
- *Increased constant-power speed range.*
- *Reduced requirements for battery storage capacity in plug-in HEVs.*
- *Inherent boost capability.*

source voltage to enable the motor to operate at higher speeds. These advantages translate into a significant reduction in inverter cost and volume with increased reliability, a much higher constant-power speed range, and improved motor efficiency and lifetime. Further, the CSI's capability to boost the output voltage could lead to a smaller battery storage capacity in PHEVs because the inverter can output the rated voltage over a wider discharge window. In other words, more energy can be drawn from the battery by discharging it to a deeper level. In comparison, the output voltage of the VSI drops with the decrease in the battery voltage as discharging proceeds.

By significantly reducing the amount of capacitance required, the CSI-based inverter with silicon insulated gate bipolar transistors can substantially decrease the requirements for cooling the capacitors in a 105°C coolant environment and could further enable air-cooled power inverters in the future when silicon-carbide-based switches become commercially viable.

The proposed CSI includes a novel interfacing circuit for incorporating energy storage devices such as batteries and ultracapacitors. The interfacing circuit transforms the voltage source of a battery or ultracapacitor bank into a current source to the inverter bridge by providing the capability to control and maintain a constant dc bus current. More importantly, the interfacing circuit also enables the inverter to charge the battery during dynamic breaking without the need for reversing the direction of the dc bus current.

Status

Oak Ridge National Laboratory (ORNL) has designed, fabricated, and successfully tested a 55 kW CSI prototype. The total capacitance was reduced to 195 μF. Test results confirmed a voltage boost ratio of up to 3.47. An output voltage total harmonic distortion factor lower than 12.5% was achieved.

Future work will continue to design, fabricate, and test a 55 kW inverter prototype that can operate with a 105°C coolant.

Contacts

Laura D. Marlino
Technical Program Manager
Oak Ridge National Laboratory
(865) 946-1245
marlinold@ornl.gov

Susan Rogers
Technology Development Manager
U.S. Department of Energy
(202) 586-8997
susan.rogers@ee.doe.gov

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Advanced Power Electronics and Electric Machines

Utilizing the Traction Drive Power Electronics System to Provide Plug-in Capability for Hybrid Electric Vehicles

Background

Plug-in hybrid electric vehicles (PHEVs) are emerging as a pre-fuel-cell technology that offers a greater potential to reduce oil consumption and carbon dioxide pollutants than other hybrid electric vehicles (HEVs) currently available. To achieve a substantial reduction in oil consumption during daily commuting, the PHEV's battery energy storage capacity needs to be increased significantly to enable a driving distance of at least 40 miles in an all-electric mode. A charger is also required to replenish the battery, which is typically done overnight to leverage energy costs by taking advantage of off-peak electricity rates. Stand-alone battery chargers impose extra cost to the already expensive HEVs. Further, to lower their cost, typical stand-alone battery chargers have a limited charging capacity and thus require a long charging time, which could negatively impact the acceptance of the PHEVs.

Figure 1: A 55 kW motor inverter and a 30 kW generator inverter with plug-in charging capability of 20 kW.

Technology

To minimize the cost of the charger, this project aims at investigating novel ways to use the already onboard power electronics and motors for fulfilling the charging requirements. A significant reduction (90%) in the battery charging related cost and volume compared to a stand-alone battery charger is expected.

The proposed approach is to integrate the battery charging function into the traction drive system and to eliminate or minimize the number of additional components (Figure 1). Because traction power inverters have a greater current-carrying capability than stand-alone chargers, whose charging capacity is limited by their cost and volume, the integrated charger can reduce the charging time significantly. Another added benefit with this approach is the capability of making PHEVs function as mobile generators at no additional or minimal extra cost.

Benefits

- *Significantly reduce the cost and volume of battery chargers in HEVs.*
- *Provide rapid charging capability.*
- *Enable PHEVs as mobile generators.*

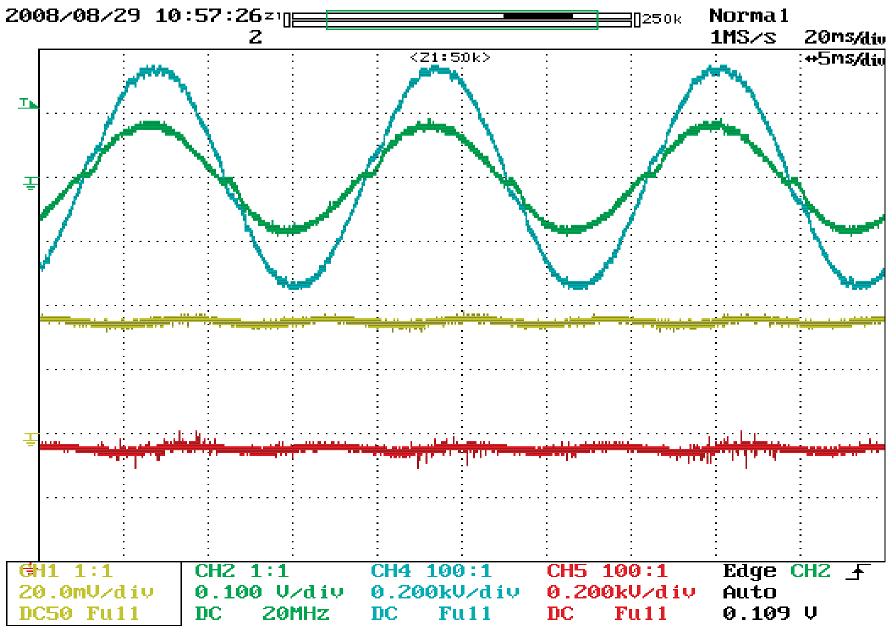

Figure 2: Complete layout of the gate driver chip.

Status

Oak Ridge National Laboratory has completed modeling of the proposed charging schemes. Simulation results have shown that the onboard electric propulsion systems can be used to provide rapid charging capabilities and enable HEVs to function as mobile power generators at no additional or minimal extra cost (Figure 2).

Future work includes assessing any safety issues with the design concept and demonstrating the design's capabilities to perform mobile power generation. Also, smart charging schemes that involve utilities in deciding the best time and the amount of power to charge the batteries will be investigated using the prototype as a test bed.

Contacts

Laura D. Marlino
Technical Program Manager
Oak Ridge National Laboratory
(865) 946-1245
marlinold@ornl.gov

Susan Rogers
Technology Development Manager
U.S. Department of Energy
(202) 586-8997
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Automotive Lightweighting Materials

Advanced Preforming Technologies

Background

Because significant automobile weight reduction and corresponding increases in fuel economy can be achieved by replacing dense materials such as metals with strong, lightweight materials, the Oak Ridge National Laboratory (ORNL), with the assistance and direction of the U.S. Department of Energy (DOE) Office of vehicle Technologies, is conducting research and development into lightweight materials for transportation applications.

Carbon fiber reinforced (CFR) composites, because of their remarkably high strength, high modulus, and low density, have the potential to reduce automotive component weight by as much as 50 to 60%. However, broader use of CFR composites in automotive applications is currently inhibited because of the high cost of carbon fiber and the processes used to make composite components. In addition to a major effort to reduce the cost of carbon fiber itself, the ORNL-DOE program is addressing manufacturing technologies including advanced preforming.

Technology

ORNL and the Automotive Composites Consortium (ACC) of the United States Council for Automotive Research are collaborating to advance the development and implementation of automated preforming processes for creating lightweight composite structures for automotive applications. The goal of this effort is to better understand preforming technology to optimize its impact on meeting DOE goals for weight/energy savings in vehicle applications.

The preforming process is the first step in creating polymer composite structural and semistructural auto parts that are lightweight and cost competitive with the metal parts they would replace. Researchers in ORNL's Polymer Matrix Composites Group are currently using a machine originally developed by Aplicator System AB as a baseline for evaluating and pushing development of advanced preforming. This machine is commonly referred to as P4, short for "programmable powdered preform process." The process features a robotically actuated machine that sprays reinforcing fiber (typically carbon fiber

Figure 1: Robotic preforming machine at ORNL.

Benefits

- *Increased fuel economy potential of 20–25% through weight savings.*
- *Variable thickness sections ranging from 1.5 mm to 8 mm.*
- *Fiber volume fractions to 40%.*
- *Carbon, glass, or mixed fiber reinforcement.*
- *Thermoset or thermoplastic composite matrices .*
- *Increased design flexibility, resulting in improved structural performance.*
- *Excellent durability characteristics.*

or fiberglass) along with a matrix material [either a binder (currently in powder form) or thermoplastic fiber] onto a screen shaped like the final part to create fiber preforms.

The objective of this next generation program is to develop processing techniques based on current P4 technology that will enable high volume, cost effective processing of carbon fiber, hybrid glass and carbon fiber, and reinforced thermoplastic preforms.

Hybrid preforms are especially attractive as they may be the best way to introduce carbon fiber to automotive production by lowering the overall cost of materials in a part versus use of all carbon fiber. ORNL has demonstrated the capability to blend, chop, preconsolidate, and mold in situ blends of hybrid glass and carbon fiber with polypropylene; however, molding limitations have hindered detailed product evaluation. Plans are underway to procure a combination convection-infrared heating system for preheating thermoplastic charges and to implement a recently acquired urethane injection machine for structural reaction injection molding of thermosets to facilitate evaluation of hybrids.

Working with ACC, ORNL has also made improvements in chopping techniques, including introducing and upgrading an alternative prototype chopper to chop fiber at a rate roughly 4 times faster than the chopper on the original machine. Alternative blade coatings for this machine have reduced blade wear in initial testing.

Status

Although this technology is still under development, a limited number of components produced using this and related processes have been commercialized for low-production-rate parts and specialty vehicles. Products produced in this manner have met technical goals but have not yet achieved widespread implementation.

Figure 2: ORNL press and mold for evaluating preform developments.

Contacts

Robert E. Norris
Group Leader/Project Leader
Polymer Matrix Composites Group
Oak Ridge National Laboratory
(865) 576-1179
norrisrejr@ornl.gov

C. David Warren
Field Technical Manager
Transportation Composites
Oak Ridge National Laboratory
(865) 574-9693
warrencd@ornl.gov

Joseph Carpenter
Technology Development Manager
U.S. Department of Energy
(202) 586-1022
joseph.carpenter@ee.doe.gov

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Automotive Lightweighting Materials

Dynamic Characterization of Spot Welds

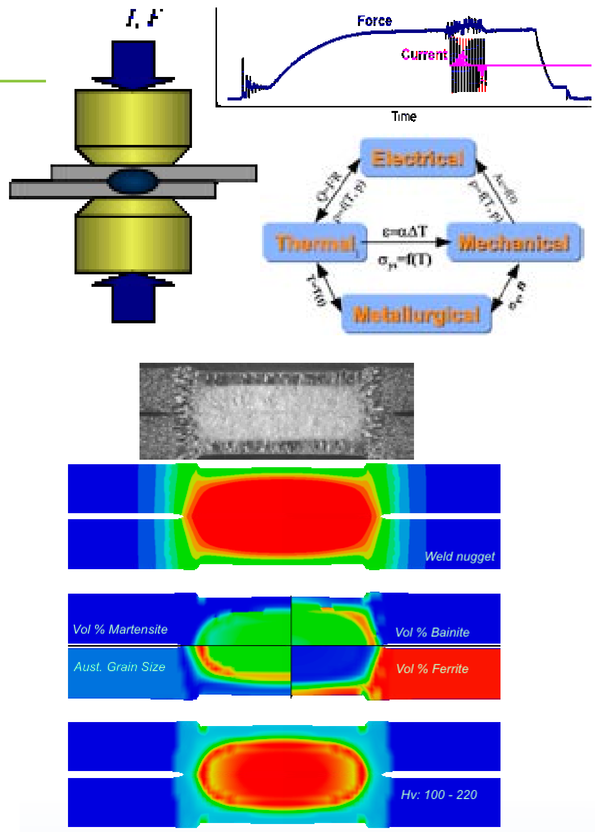

Figure 1: The integrated RSW process model predicts the weld microstructure and property gradients in a steel weld.

Background

A primary driver for increased use of advanced high-strength steels (AHSSs) and other high-strength, lightweight materials such as aluminum and magnesium alloys in auto-body structures is their ability to improve crash performance while reducing vehicle weight. Resistance spot welding (RSW) is by far the most common joining process used in automotive manufacturing. Typically, there are several thousands of spot welds in a vehicle. Because the separation of spot welds can affect the crash response of welded components, the dynamic behavior of spot welds is a critical factor in vehicle design and manufacturing.

Computer-aided engineering (CAE) has become an indispensable tool that enables rapid and cost-effective design and engineering of crash resistant auto- body structures. Currently, CAE crash prediction of spot weld behavior in AHSSs and other lightweight materials is generally unsatisfactory, which impedes effective use of these materials in auto-body structures to achieve the balance of fuel efficiency, safety, performance, and cost target metrics.

Technology

Under the sponsorship of the U.S. Department of Energy Office of Vehicle Technologies and Auto/Steel Partnership, Oak Ridge National Laboratory and the University of South Carolina are developing a robust spot weld modeling approach, supported by experimental data, that can be implemented in crash simulation finite element analysis codes used by automotive crash modelers. A three-pronged development approach was used: (1) develop a spot weld element (SWE) formulation with the complexity to incorporate weld geometry and microstructure effects and the associated constitutive models for use in CAE simulations (Figure 1); (2) develop a physics based integrated electrical-thermal-mechanical-metallurgical spot weld process model to generate the weld geometry, microstructure, and residual stress results needed for the SWE model; and (3) develop a companion weld characterization and impact test

Benefits

- *Support rapid and optimal insertion of AHSSs and other lightweight materials in auto-body structures through advanced crashworthiness CAE.*
- *Enable widespread use of high-strength, lightweight materials in auto-body structures to achieve the 20% vehicle weight reduction target for petroleum displacement.*

database for validation of the new spot weld modeling approach (Figure 2).

Status

We have successfully completed phase I (concept feasibility) of the project. The effectiveness of the spot weld modeling framework has been demonstrated for two steel grades. The initial version of simulation software has been licensed for industry applications. Phase II of the project will extend the model to cover the range of materials, weld configurations, welding conditions, and loading modes required for industry CAE implementation

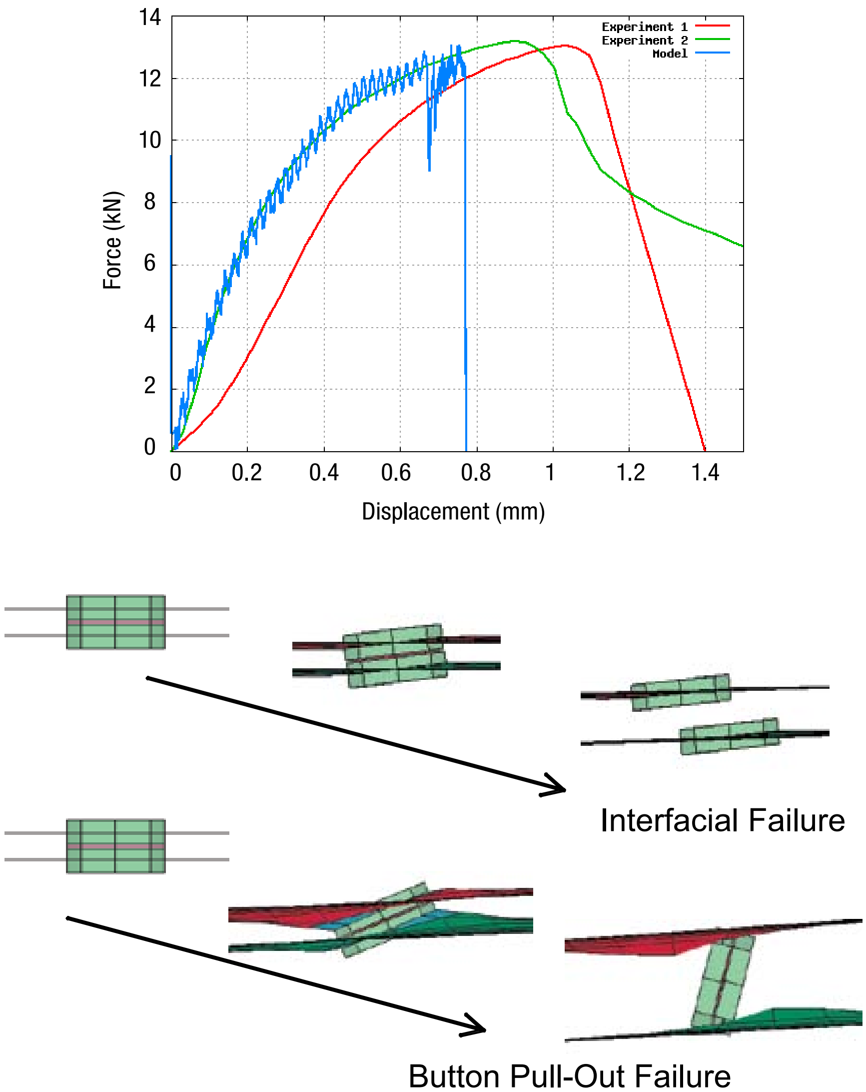

Figure 2: SWE model predicts the deformation, failure load and failure mode of spot weld during impact tests.

Contacts

Zhili Feng
Principal Investigator
Oak Ridge National Laboratory
(865) 576-3797
fengz@ornl.gov

Philip S. Sklad
ORNL Program Manager
Oak Ridge National Laboratory
(865) 574-5069
skladp@ornl.gov

Joseph A. Carpenter
Technology Development Manager
U.S. Department of Energy
(202) 586-1022
joseph.carpenter@ee.doe.gov

Automotive Lightweighting Materials

Infrared Inspection of Resistance Spot Welds: Nondestructive Inspection of Automotive Structures

Background

With the assistance and direction of the U.S. Department of Energy Office of Vehicle Technologies, the Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for transportation.

Welding is the most widely used technology for assembling auto body structures. Despite extensive research and development efforts over the years, nondestructive weld quality inspection is still a critical issue for the auto industry, largely due to the unique technological and economical constraints of the auto production environment. Any weld quality inspection technique must be fast, highly economical, and extremely low in false rejection rate and must not interfere with the highly automated welding fabrication process (i.e., roughly 20,000 cars a day for GM, Ford, or Chrysler). This project addresses this critical industry need through the development of infrared (IR) based online weld quality monitoring technology.

Technology

Heat generated during the resistance spot welding process can be used to monitor weld quality. Working with the United States Council for Automotive Research and using preliminary results supported by ORNL High Temperature Materials Laboratory user projects, we have successfully developed an online inspection technique using IR thermography. A well designed test matrix was prepared at ORNL, and spot weld coupons were made at ArcelorMittal Steel. Postmortem IR inspections using several heating and cooling techniques were carried out to assess weld quality.

Benefits

- *Noncontact inspection and potential to be developed into turn-key system.*
- *No interference with assembly-line production.*
- *Low false call rate because of high heat input to differentiate welds of varying quality.*
- *Uses heat generated during welding so no extra heating or cooling steps are needed.*
- *Potential to reduce the cost and waste of destructive tests.*
- *Integration with robots and machine vision software to allow rapid feedback and control.*
- *Applicable to high strength steels where some more traditional tests do not work well and may cause injuries.*

Cold welds, small, undersized and just below expulsion welds, were carefully prepared by ArcelorMittal Steel. The selected cooling and heating methods clearly distinguished these welds and allowed them to be grouped according to the heat flow through the weld nuggets. Then the IR camera was taken to the ArcelorMittal Global Research and Development Laboratory in East Chicago, Indiana. The spot welds were reproduced with the IR camera recording the temperatures (Figure 1). Thermal images of the electrodes and steel plates were recorded and played back. "Thermal signatures" of welds with different quality were captured and analyzed by the software. It was found that the heat input during welding is very different when making a cold weld versus a normal weld. Similar to postmortem inspection, different quality welds could be grouped together according to the temperature time-profiles. This concept feasibility project has shown the promising potential of this online IR inspection technique.

Figure 1: IR imaging of resistance spot welding.

Status

The IR inspection technique and image analysis software are pending in invention disclosures that will likely be commercialized together. Prospective commercialization partners should contact C. David Warren at the address shown below.

Contacts

C. David Warren
Field Technical Manager
Transportation Composites
Oak Ridge National Laboratory
(865) 574-9693
warrencd@ornl.gov

Joseph A. Carpenter
Technology Development Manager
U.S. Department of Energy
(202) 586-1022
joseph.carpenter@ee.doe.gov

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Automotive Lightweighting Materials

Low Cost Carbon Fiber Production: Advanced Oxidation of Carbon Fibers

Background

With the assistance and direction of the U.S. Department of Energy Office of Vehicle Technologies, the Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for transportation.

Significant automobile weight reduction and corresponding increases in fuel economy can be achieved by replacing dense materials such as metals with strong, lightweight materials. Carbon fiber reinforced composites are an excellent candidate for this lightweight material. Carbon fibers, as the load-bearing components in these composites, offer significant weight saving potential because of their remarkably high strength, high modulus, and low density. The use of carbon fibers is currently restricted because of their high cost. Carbon fibers with the properties needed for automotive applications currently sell for $8 to $15 per pound.

Technology

The conversion of precursor fibers into finished carbon fibers requires four major heat treatment steps: stabilization (cross-linking), oxidation, carbonization, and graphitization. Oxidation is the most time-consuming, and therefore rate-limiting, step in the conversion process. It limits the material throughput and thus significantly controls the economics of carbon fiber production. ORNL researchers, with the assistance of an industrial partner, Sentech, are developing atmospheric-pressure plasma processing techniques to oxidize polyacrylonitrile precursor fibers (Figure 1). The technical target is to produce carbon fibers costing $5 to $7 per pound, with uniform mechanical properties of at least 25 Msi tensile modulus and 1% ultimate tensile strain.

Preliminary results suggest that the technical targets are well within reach; in fact, they have nearly been satisfied with no tow tension and only partial carbonization heat treatment. Oxidation has been

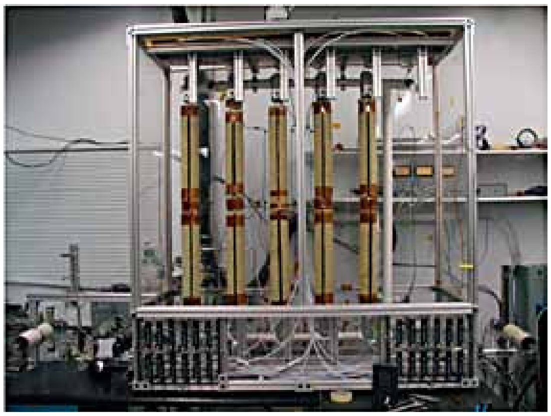

Figure 1: Single-tow, multiple zone plasma oxidation unit.

Benefits

- *A likely reduction in carbon fiber direct production costs of slightly more than $1 per pound.*
- *Faster processing speeds.*
- *Lower processing temperature.*
- *Reduced energy demand per unit mass throughput.*
- *Reduced unit footprint (compact equipment and plant layout) for both capital equipment and real estate.*
- *Reduced unit investment cost.*
- *A high degree of equipment modularity in all processing stages.*

achieved with a residence time roughly one-third of that required for conventional thermal oxidation. The current experimental scale is 3,000 filaments running at ~0.3 m/min. A new reactor has been constructed and commissioned to enable a severalfold increase in the number of filaments treated and increased line speed. The researchers plan to scale to hundreds of thousands of filaments and several meters per minute, which would reduce the estimated fiber production cost by more than $1 per pound

Status

Advanced oxidation is part of a suite of patented or patent pending carbon fiber conversion technologies that will likely be commercialized together.

Currently efforts are focused on scaling the process up to industrial production levels, improving the properties of the carbon fibers, integrating the plasma processing technology with the other main stages of the production process, and seeking industrial partners for commercialization.

Contacts

C. David Warren
Field Technical Manager
Transportation Composites
Oak Ridge National Laboratory
(865) 574-9693
warrencd@ornl.gov

Joseph A. Carpenter
Technology Development Manager
U.S. Department of Energy
(202) 586-1022
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Automotive Lightweighting Materials

Low Cost Carbon Fiber Production: Lignin Based Precursors for Lower Cost Carbon Fibers

Background

With the assistance and direction of the U.S. Department of Energy (DOE), Office of Vehicle Technologies, the Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for transportation. Carbon fiber reinforced composites are excellent candidates. Carbon fibers offer significant weight saving potential because of their remarkable high strength, high modulus, and low density. The use of carbon fibers is currently restricted because of their high cost ($8 to $15 per pound). Forty to fifty percent of that cost is attributable to the cost of the precursor. ORNL has developed the baseline technology necessary to use lignin (a coproduct of the paper making process) as a very low cost feedstock for making carbon fiber precursors. The key to using lignin precursors, however, is the ability to purify the lignin to a satisfactory level and spin it into a suitable precursor fiber.

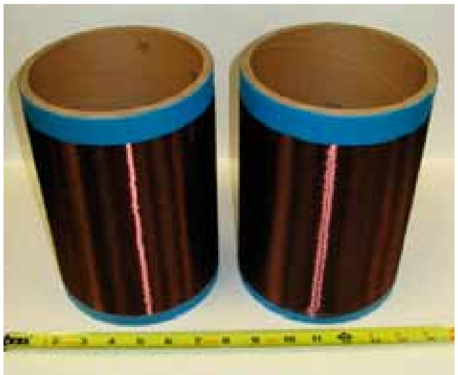

Figure 1: Spools of 100% lignin fibers.

Technology

After demonstrating that organic-purified hardwood lignin can be continuously melt spun into fiber form without the need for any additives (Figure 1), the focus in FY 2008 has been on the evaluation of various sources of lignin and their conversion into carbon fibers. Unpurified kraft softwood lignin (mixed with a purified kraft hardwood lignin as a plasticizer) and Alcell lignin (from a biomass refinery) have been successfully melt spun into fibers. The fibers have been processed and converted into carbon fibers and their mechanical properties measured. Although the current properties are still short of the DOE target values (50–60% of target), work is progressing toward the optimization of processing conditions and evaluation of alternative conversion methods to improve the carbon fiber properties.

The processing facilities for the lignin based carbon fiber project have been expanded recently, and they now include a compounding/ pelletizer line (Figure 2). This line will play a key role when mixtures of lignin and additives are studied, which will be the focus of the experimental work next year. This line will improve compounding and

Benefits

- *Lignin based precursors cost less than half the cost of traditional precursors.*
- *Melt spinning is less expensive than solution spinning (used with traditional precursors).*
- *Solvents used in solution spinning are eliminated.*
- *Total saving in carbon fiber cost could exceed $2/lb ($4.50/kg).*
- *Reduced unit investment cost.*
- *Lignin is a sustainable, renewable resource readily available from domestic forest products and increasingly from biorefineries for cellulosic ethanol production.*

Figure 2: Compounding/pelletizer line.

will speed up the evaluation process for the various mixtures.

Spinning speed is one of the most important process parameters with respect to the economics of carbon fiber production from lignin. Melt spinning trials have confirmed that the spinning speed of lignin can be increased to at least 2 times the Kline economic model baseline speed. Alcell lignin fibers of the target diameter of 10 μm were successfully spun at a winding speed of 1,200 m/min.

Status

We hope to bring this technology to the marketplace through collaborations with industrial, government, and/or academic partners and welcome all inquiries. To date, collaborative agreements have been established between ORNL and the following.

- Kruger Wayagamack, Inc, Canada (supplier of kraft softwood lignin).
- Lignol Innovations Ltd., Canada (supplier of Alcell and biomass-derived lignin).
- STFI-Packforst, Swedish Research Institute (supplier of kraft lignin from the LignoBoost process).

Contacts

C. David Warren
Field Technical Manager
Transportation Composites
Oak Ridge National Laboratory
(865) 574-9693
warrenCD@ORNL.gov

Joseph A. Carpenter
Technology Development Manager
U.S. Department of Energy
(202) 586-1022
joseph.carpenter@ee.doe.gov

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Automotive Lightweighting Materials

Low Cost Carbon Fiber Production: Textile Based Precursors

Background

With the assistance and direction of the U.S. Department of Energy (DOE) Office of Vehicle Technologies, the Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for transportation and particularly into the use of lower cost carbon fiber which would be available at a target price of $5 to $7 per pound.

Significant automobile weight reduction and corresponding increases in fuel economy can be achieved by replacing dense materials such as metals with strong, lightweight composite materials. Carbon fiber reinforced composites are excellent candidates for this lightweight material. Carbon fibers, as the load-bearing components in these composites, offer significant weight saving potential because of their remarkably high strength, high stiffness, and low density. Carbon fiber strength is higher than that of steel at approximately the same stiffness and ~ 1/5 of steel's density. It is estimated that vehicle structure weights could be reduced from 50% to 70% if carbon fiber composites were used in passenger automobiles.

While carbon fiber composites have proven themselves in high performance aircraft and other high performance applications, they are typically not used in passenger vehicles due to their high cost. The most significant component of their cost is the cost of the carbon fiber itself, and slightly more than half of that cost is the cost of the precursor (starting material) from which the fiber is made. Carbon fiber is made by the slow pyrolysis of a relatively expensive precursor.

Carbon fibers with the properties needed for automotive applications currently sell for $8 to $15 per pound. About 50% of that cost is attributable to the cost of the precursor used to make the carbon fiber. Recently, Hexcel and ORNL developed the baseline technology necessary to use textile based polyacrylonitrile (PAN) fiber as a very low cost precursor for making carbon fiber. The key to using textile PAN precursors is the application of a chemical pretreatment during manufacture of the precursor fiber. ORNL and FISIPE S.A. (Portugal) are working to complete development and commercialization of this precursor to make it available to current and potential carbon fiber manufacturers.

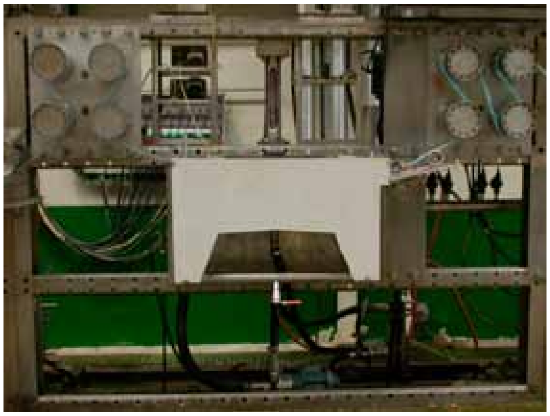

Figure 1: Chemical pretreatment station for chemical modification of textile grade PAN precursors installed at a FISIPE facility.

Benefits

- *Textile based PAN precursors cost less than half of the cost of traditional carbon fiber precursors.*
- *Chemical pretreatment is easily incorporated into existing textile mills.*
- *Textile mill volumes can support the large increases in fiber quantity required for automotive applications.*
- *Total saving in carbon fiber cost could exceed $2/lb.*
- *Higher speed conversion of the precursor into carbon fiber yields additional cost savings.*

Technology

A collaborative international program under ORNL and FISIPE S.A. in Portugal is working to render textile based polyacrylonitrile suitable for conversion into carbon fiber. Textile fiber sells for half the cost of conventional carbon fiber precursors and would result in a savings of more than $2.00 per pound in the finished carbon fiber manufacturing costs.

Recently the two organizations have defined several textile formulations that could yield suitable carbon fibers. They are modifying materials that can be oxidized at temperatures below 330°C. In addition, they have developed a way to modify the chemistry of the starting materials by the addition of a small amount of a third component and have defined a chemical pretreatment protocol for further altering the fiber chemistry while the fiber is still in the uncollapsed state. Different levels and conditions of the pretreatment were also evaluated. Key to incorporating these changes has been the ability to perform the chemical modification in current production facilities and at current production speeds and temperatures (Figure 1). Mechanical properties now well exceed the program requirement as shown in Figure 2.

The oxidative stabilization of the modified textile precursors requires only ~50 minutes compared to a time of 80–100 minutes for conventional carbon fiber precursors. Oxidative stabilization is the low speed bottleneck in the carbon fiber conversion process. As a result, modified textile precursors may be carbonized at much higher speeds and a significant production cost reduction achieved

Status

FISIPE, a commercial manufacturer and distributor of acrylic fiber, intends to offer this new fiber as a lower cost precursor to current and future carbon fiber manufacturers. ORNL has other parallel efforts to develop new production technologies that will enable manufacturers to develop high volume, commercial carbon fiber plants that use textile based PAN precursors along with other advanced manufacturing methods and is looking for additional commercial partners.

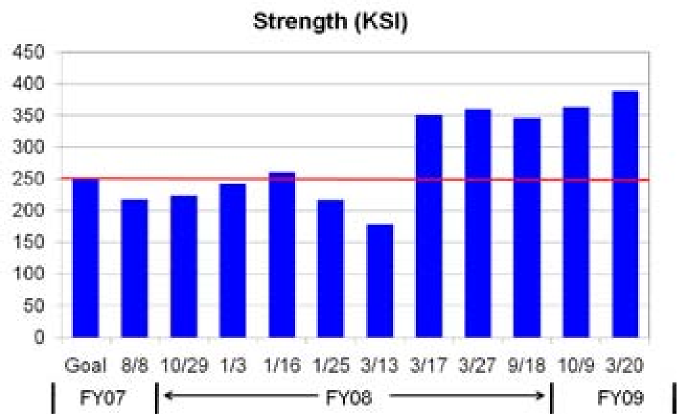

Figure 2: Improvement in fiber strength during the project.

Contacts

C. David Warren
Field Technical Manager
Transportation Composites
Oak Ridge National Laboratory
(865) 574-9693
warrencd@ornl.gov

Joseph A. Carpenter
Technology Development Manager
U.S. Department of Energy
(202) 586-1022
joseph.carpenter@ee.doe.gov

A Strong Energy Portfolio for a Strong America

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Automotive Lightweighting Materials

Predictive Modeling of Polymer Composites: Injection Molded Long Fiber Thermoplastics

Background

With the assistance and direction of the U.S. Department of Energy Office of Vehicle Technologies, Automotive Composites Consortium, and American Plastics Council, the Oak Ridge National Laboratory (ORNL) and Pacific Northwest National Laboratory (PNNL) are conducting research and development into lightweight materials for transportation.

Long fiber reinforced thermoplastics have generated great interest within the automotive industry due to their low production cost and good mechanical properties. These materials have already been used for semi-structural applications and are now candidate materials for automotive structural applications to reduce vehicle weight. Because conventional injection molding equipment can be modified to produce long fiber thermoplastics (LFTs), most injection molding operations can be converted to LFT production at little or no additional cost.

The application of reinforced plastics and polymer composites in automotive structures is currently limited by the inability to accurately predict the stiffness, strength, long-term durability, and service life of these materials based on their constitutive properties and processing parameters. Enhanced process models to accurately predict the as-formed composite microstructure and predictive modeling tools that capture the nonlinear behaviors due to residual stresses, damage, fatigue, creep, and impact of complex shapes are being developed to address this shortcoming

Technology

A collaborative program involving ORNL, PNNL, Moldflow Corporation, and a group of universities is implementing coupled process and structural modeling tools. Moldflow software simulating the injection molding process can provide fiber architecture and other material microstructure information based on enhanced process models being developed as part of this program. The structural analysis code ABAQUS is interfaced with Moldflow to use the material microstructure

Benefits

- *Increased confidence in design of reinforced thermoplastic materials.*
- *Reduced component weight.*
- *Reduced manufacturing cost.*
- *Low tooling fabrication costs.*
- *Accelerated process development.*
- *Coupled process and structural models.*
- *Elimination of excessive knockdown factors used in design of reinforced plastics.*

information for mechanical property prediction of molded components. New processing as well as structural models are being incorporated in the coupled processing-structural predictive framework.

Development and validation of models relies on accurate experimental data. Experimental techniques for fiber length distribution and fiber orientation measurement have been refined and used to obtain data for comparison with models. A novel technique allowing measurement of fiber length distribution as a function of thickness was developed. Using this technique, the researchers were able to verify that fiber length distribution varies as a function of thickness, which is at odds with the common assumption of uniform fiber length distribution. Larger glass fiber-PA66 plaques were molded and investigated. Mechanical tests were performed at –40°C, 25°C, and 80°C to evaluate the effect of temperature on mechanical response. The nature of fracture surfaces differed depending on test temperature (Figure 1). Detailed scanning electron microscope images have shown that appropriate sizing allowed a residuum of PA 66 to remain on exposed fibers on the fracture surface (Figure 2).

Status

Predictive models are being implemented in commercially available and supported packages. Current and future work is focused on development and validation of models for creep, fatigue, and impact response of LFTs. The resulting suite of tools will accelerate the use and reduce the cost of use of lightweight composite components in automotive applications.

Moldflow Corporation is an active team member in this project, but inquiries from other parties interested in commercializing this technology are welcome.

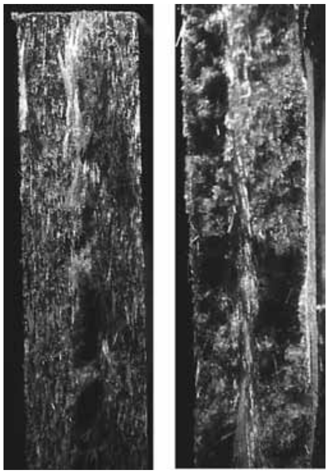

Figure 1: Fracture surfaces with core-shell structure vVisible.

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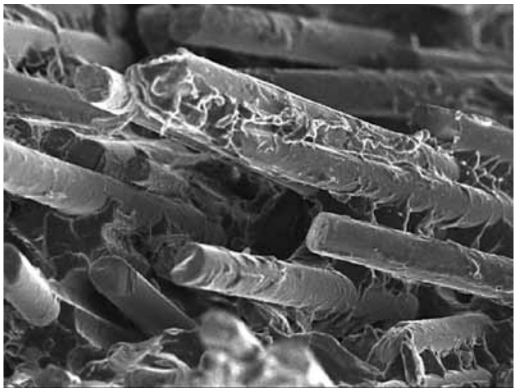

Figure 2: Matrix material residuum on exposed fibers after fracture.

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Contacts

C. David Warren
Field Technical Manager
Transportation Composites
Oak Ridge National Laboratory
(865) 574-9693
warrencd@ornl.gov

Mark T. Smith
Energy Materials
Pacific Northwest National Laboratory
(509) 375-4478
mark.smith@pnl.gov

Joseph A. Carpenter
Technology Development Manager
U.S. Department of Energy
(202) 586-1022
joseph.carpenter@ee.doe.gov

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Clean Cities, Fuel Economy, Policy and Analysis

Fuel Economy Information Program: Helping Consumers Choose Energy Efficient Vehicles

Background

The United States depends on foreign oil for more than half (60%) of its petroleum needs, costing the country $270 billion in imports annually. The transportation sector is especially dependent. It relies on petroleum for 96% of its energy needs and accounts for 68% of the petroleum that Americans use. The mission of the Fuel Economy Information Program is to reduce U.S. oil dependency by promoting highway vehicle fuel economy and helping consumers make informed fuel economy choices when they purchase a vehicle.

The Oak Ridge National Laboratory estimates that the Fuel Economy Information Program will reduce U.S. petroleum consumption by more than 400 million gallons in 2008 (Figure 1).

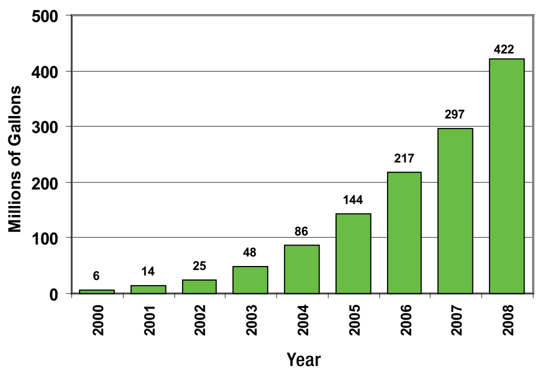

Figure 1: Estimated fuel savings by year from fuel economy information program.

Technology

The Fuel Economy Information Program, funded by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy, provides information to consumers through two primary products: fueleconomy.gov and the *Fuel Economy Guide*. Fueleconomy.gov is an online resource that provides the following information.

- U.S. Environmental Protection Agency (EPA) fuel economy ratings for passenger cars and trucks, 1985–present.
- User-provided, real-world fuel economy estimates.
- Energy impact scores (petroleum consumption).
- Fuel economics.
- Carbon footprint and air pollution ratings.
- Information on vehicles that can use alternative fuels (e.g.,E85 and compressed natural gas).
- Fuel-saving tips.
- Information on tax incentives for hybrids and alternative fuel vehicles.
- Downloadable Fuel Economy Guide.

Benefits

- *Provides fuel economy information to millions of consumers each year (32 million user sessions in 2008).*
- *Estimated to have reduced U.S. petroleum consumption by more than 400 million gallons in 2008.*
- *In 2008, more than 1,200 television, Internet, and radio articles featured the site or information from the site, including CNN, CBS News, and USA Today.*

The *Fuel Economy Guide,* accessible on fueleconomy.gov, is an annual publication produced by DOE and EPA that lists the miles per gallon, both city and highway estimates, for all new model year vehicles. It is distributed to all new car dealerships in the United States, as well as libraries, credit unions, and several other entities.

Status

Fueleconomy.gov is beginning its 10th year of providing fuel economy data to the public. The visibility and influence of the site have increased dramatically since it was introduced in October 1999. As of October 2008, the site had hosted more than 85 million user sessions. In 2008 alone, the site hosted more than 32 million user sessions (Figure 2). The site is a nationally established resource for fuel economy information. In 2008, more than 1,200 television, Internet, and radio articles featured the site or information from the site, including CNN, CBS News, and USA Today.

In 2008 fueleconomy.gov/m, a version of the fueleconomy.gov Web site formatted for mobile communication devices, was launched in conjunction with the Washington, D.C., Auto Show. With this new Web site, consumers can access the fuel economy ratings and other information from cell phones and PDAs.

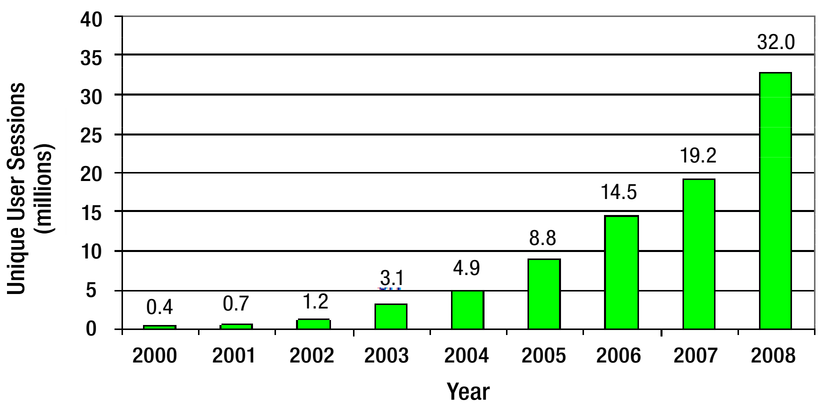

Figure 2: Fueleconomy.gov user sessions by year, showing dramatic increases in use since its launch in 1999.

Contacts

Dr. David L. Greene
Project Manager
Oak Ridge National Laboratory
(865) 946-1310
dlgreene@ornl.gov

Dennis Smith
Technology Development Manager
U.S. Department of Energy
202-586-1791
dennis.a.smith@ee.doe.gov

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Energy Storage Materials and Processing

Advanced Characterization and Process Development for Energy Storage Materials

Background

Lithium ion battery technology is projected to be one of the energy storage leapfrog technologies for the electrification of automotive drivetrains and providing stationary storage solutions to enable the effective use of renewable energy sources. This technology is already in use for low-power applications such as consumer electronics and power tools. Extensive research and development (R&D) has enhanced the technology to a stage where it seems very likely that safe and reliable lithium ion batteries will soon be on board hybrid electric and electric vehicles and connected to solar cells and windmills. However, safety of the technology is still a concern, service life is not yet sufficient, and costs are too high.

Technology

Oak Ridge National Laboratory (ORNL) has performed a thorough technical assessment of materials and processing for energy storage devices and developed partnerships with leading battery developers, the automotive industry, and utility companies. In this assessment ORNL worked together with many battery developers, original equipment manufacturers, automotive suppliers, and automotive companies. Parts of the assessment and cost estimates have been published in an overview article.[1] Based on the assessment, ORNL has identified characterization and process development as the key components of a new, enabling R&D program at ORNL.

Status

To benchmark our newly developed materials and processes, a shared battery test laboratory has been set up and equipped with state-of-the-art characterization instruments such as a 32-channel Maccor battery cycler with temperature control chambers, an 8-channel Solartron frequency response analyzer, a portable Gamry potentiostat, and a large glove box with a video microscope. Each of these can be expanded to accommodate a larger number of test stations as demand grows. The portable potentiostats will be used for experiments at ORNL's Spallation Neutron Source and High Temperature Materials Laboratory electron microscopy, synchrotron, and X-ray diffraction laboratories. The video microscope will be

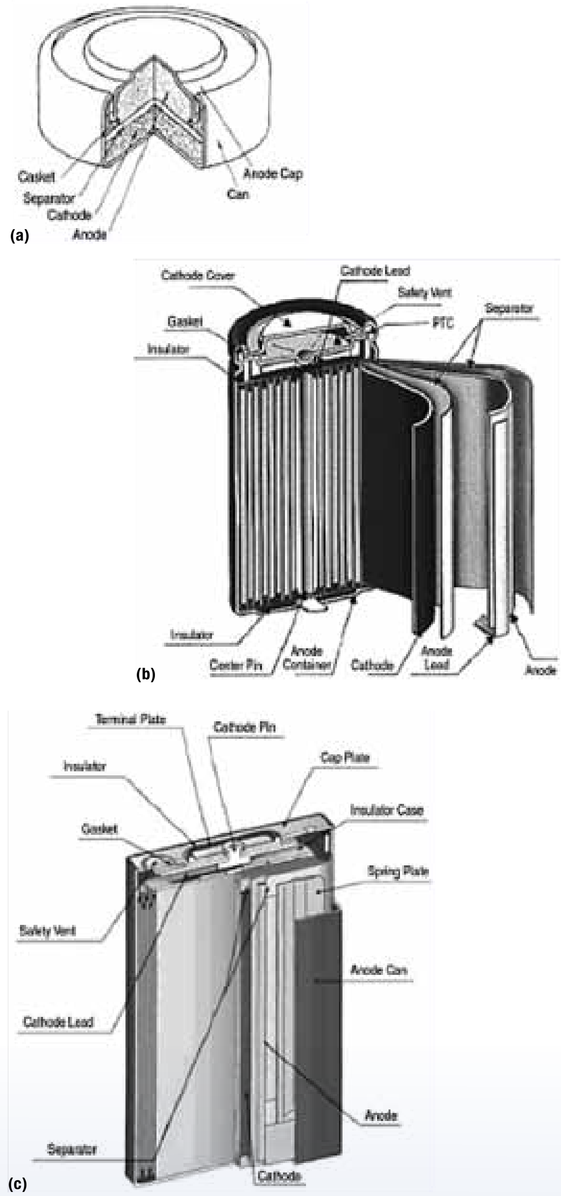

Figure 1: A schematic of cell forms as found from a multitude of sources: (a) button cell, (b) cylindrical cell, and (c) prismatic cell. [From JOM, 60 (9), 43–48.]

Benefits

- *Establish and strengthen domestic manufacturing.*
- *Reduce dependence on foreign oil imports.*
- *Increase energy security.*
- *Understand failure mechanisms.*
- *Enable the effective use of intermittent renewable energy sources.*

used to assemble liquid flow cells for transmission electron microscope and scanning electron microscope characterization of critical battery materials and interfaces. Basic battery fabrication equipment and materials, such as a coin cell crimping machine, will also be available. About a dozen likely users attended a 1.5 day training session conducted by a Maccor representative in February 2009.

For the characterization efforts, ORNL is focusing on elucidating life-limiting structural and compositional phenomena in operating batteries in order to propose new and advanced materials for the future. To this end, ORNL is developing in-situ characterization tools such as in-situ microscopy and in-situ fatigue testing.

Scientists from ORNL and colleagues at Vanderbilt University have developed a new nanoscale imaging technique for micrometer thick specimens in liquid that can be used to image whole cells in biological experiments and for the imaging of operating energy systems. The new technique–liquid scanning transmission electron microscopy (STEM)–uses a microfluidic device with electron transparent windows to enable the imaging of materials in liquid[2] and will be used for in situ microscopy of energy storage materials and battery cells. The fundamentals of the liquid STEM technique have been the basis for designing a specialized holder for the in situ microscopy testing of micrometer-size (miniaturized) batteries in the Hitachi HF-3300 high-resolution scanning/transmission electron microscope. For the in situ battery testing and the concurrent live-time observation (and recording) of the solid electrolyte interface formation (and other microstructural changes) during rapid charge-discharge events, the liquid flow cell will "contain" the liquid electrolyte as well as the battery anode and cathode materials (forming the miniature battery). Recently we started testing the holder, and the study will require chip/window (which form flow cell) redesign and extensive baseline characterization of "known" battery materials and correlation of the in situ tests with actual laboratory tests of full-size batteries.

In the coming year's effort, we will focus on working directly with battery developers and their suppliers and customers to scale the technology, establish domestic manufacturing, and understand performance limiting barriers. In addition, ORNL has established an extensive internally funded effort on materials, processing, and modeling for electrical energy storage.

Refs:

1. Daniel, C., "Materials and processing for lithium-ion batteries," *JOM*, 60 (9), 43–48.
2. de Jonge, N., et al., "Electron microscopy of whole cells in liquid with nanometer resolution," *Proc. Natl. Acad. Sci.* (2009).

Contacts

Claus Daniel, Ph.D.
Oak Ridge National Laboratory
(865) 241-9521
danielc@ornl.gov

Dave Howell
Team Leader
Hybrid Electric Systems Subprogram
U.S. Department of Energy
(202) 586-3148
david.howell@ee.doe.gov

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Fuels, Engines, and Emissions

Achieving & Demonstrating the FreedomCAR Efficiency Milestones for Advanced Combustion Engines

Background

The FreedomCAR roadmap has established efficiency and emissions goals for the next several years, with a 45% peak brake thermal efficiency (BTE) being demonstrated in 2010 while meeting the Tier 2 Bin 5 emissions levels. The objective of this activity is not to develop all the necessary technology to meet these goals but rather to serve as a focus for the integration of technologies into a multicylinder engine platform and to provide a means of identifying pathways for improved engine efficiency.

Technology

Substantial improvements in engine efficiency will require a reduction in thermal energy losses to the environment and a better understanding of thermodynamic loss mechanisms associated with the combustion process. With less than half of fuel energy converted to useful work in a modern engine, opportunity exists for significant advancements in engine efficiency. A fundamental thermodynamics perspective in combination with simulations and laboratory experiments is being used toward this purpose to provide guidance on developing and evaluating a path for meeting 2010 and intermediate milestones and to provide longer term insight into the potential of future high efficiency engine systems.

A peak BTE of 43% and a part-load BTE of 27% were demonstrated on a light-duty diesel engine. These accomplishments are interim milestones on the path to 2010 FreedomCAR goals of 45% peak BTE and Tier 2 Bin 5 emissions (see Figure 1). Advanced engine technologies identified and investigated in FY 2008 include thermal energy recovery, electrification of auxiliary components, advanced lubricants, and fuel properties. In addition, a flexible microprocessor-based control system was used for reoptimization of engine parameters to make better use of these technologies.

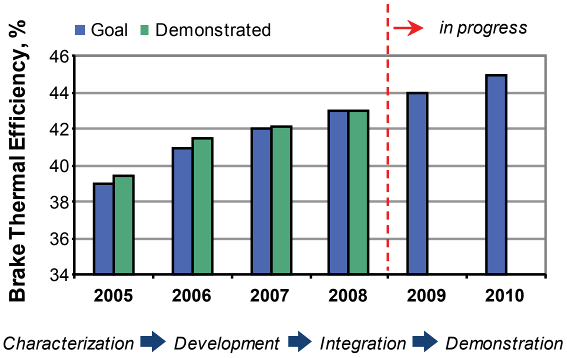

Figure 1: On path to demonstrating FY 2010 FreedomCAR engine and efficiency milestones including 45% peak BTE.

Benefits

- *Improved fundamental understanding of fuel efficiency losses in internal combustion engines and the identification of promising strategies for reducing these losses.*
- *Demonstration of U.S. Department of Energy FreedomCAR fuel efficiency and emissions milestones.*
- *New insight into systems integration of advanced transportation technologies to expand the boundaries of engine efficiency and emissions improvements.*

Thermal energy recovery was not used to meet the FY 2008 milestones, but significant progress was made in developing this technology for light-duty applications, including modeling and on-engine experiments under conditions consistent with a light-duty vehicle drive cycle. An example of the thermodynamic availability (i.e., the potential to do useful work) of the exhaust system is shown in Figure 2. The potential impact of recovering this discarded thermal energy on fuel economy improvements over a light-duty vehicle drive cycle was investigated using composite modal experiments and simulated thermal energy recovery on the exhaust system. These approximations indicate potential fuel savings on the order of 8% with conservative thermal energy recovery estimates.

This activity makes use of knowledge from internal ORNL activities, other national laboratories, universities, and industry. Internal activities include those focused on advanced combustion operation, aftertreatment, fuels, and unconventional approaches to improve combustion efficiency. The progress and results of this activity are regularly shared with external sources through government-industry technical meetings, professional conferences, and one-on-one interactions with industry teams.

Status

The path forward to the demonstration of FY 2010 efficiency and emissions milestones has been developed through extensive modeling, experiments, and interactions with the scientific community. The path will make use of several efficiency enabling technologies including thermal energy recovery in combination with advanced combustion operation and the integration of appropriate aftertreatment systems. Demonstration and verification will be accomplished with on-engine experiments and vehicle system modeling.

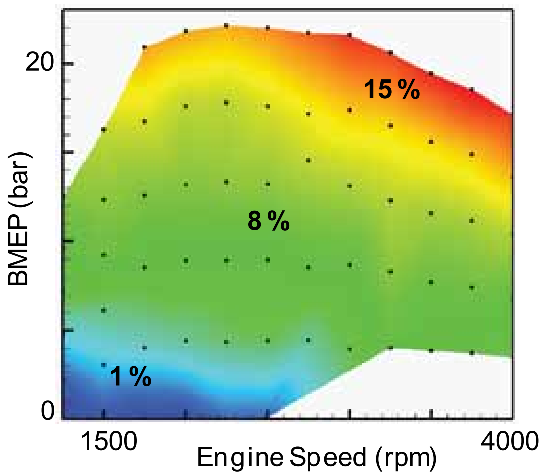

Figure 2: Thermodynamic availability (in terms of percentage of fuel availability) shows a significant amount of fuel energy is discarded to the environment and potentially available for recovery.

Contacts

Ronald Graves
Project Manager
Oak Ridge National Laboratory
(865) 946-1226
gravesrl@ornl.gov

Gurpreet Singh
Team Leader
Advanced Combustion Engine R&D Subprogram
U.S. Department of Energy
(202) 586-2333
gurpreet.singh@ee.doe.gov

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Fuels, Engines, and Emissions

Efficient Emissions Control for Multimode Lean Direct Injection Engines

Background

New combustion regimes are being investigated in ongoing work at the Oak Ridge National Laboratory (ORNL) as a way to improve the efficiency of diesel engines. Reduced nitrogen oxide (NO_X) emissions can remove some of the burden from postcombustion emissions controls and can thereby reduce the fuel penalty associated with NO_X reduction. However, the current consensus is that these nontraditional low-emissions combustion regimes will not supplant the need for postcombustion emissions controls, and to date, these ultralow NO_X combustion regimes have only been realized at light engine loads. Because power density is also critical to the engine of the future, it is possible that new engines will run in multiple modes, depending on the load, running in more conventional modes at high loads.

One of the advanced combustion modes demonstrated as an effective means of simultaneously reducing engine out NO_X and particulate matter is high efficiency clean combustion (HECC). HECC is a type of premixed charge compression ignition combustion mode that uses advanced timing and high exhaust gas recirculation (EGR) rates to enable dramatic reductions in engine out NO_X and particulate matter with relatively small fuel efficiency penalty. HECC becomes increasingly more difficult to attain at higher loads as EGR levels and cooling become challenging. Thus, HECC at low and medium loads is often combined with conventional combustion at higher loads for multimode engine operation.

Technology

The emphasis of this project is on using combinations of advanced combustion regimes and/or emissions control devices to demonstrate the feasibility of combining technologies to achieve U.S. Department of Energy goals for efficiency and emissions (Figure 1). The work is carried out at ORNL on modern compression ignition direct injection engines with advanced catalysts provided by the Manufacturers of Emission Controls Association. Of particular focus are catalytic technologies for lean NO_X reduction such as lean NO_X trap (LNT)

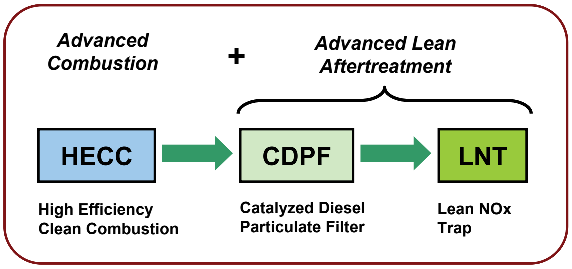

Figure 1: Schematic demonstrating integration of advanced combustion technologies with advanced emissions control technologies.

Benefits

- *Understanding integration of advanced engines with advanced emissions control technologies.*
- *Enables cost-effective meeting of emission regulations for efficient engine technologies.*

and selective catalytic reduction catalysts. Diesel particulate filter (DPF) technology is used as well for control of particulate matter emissions.

Results from a recent study focused on the LNT catalyst technology are shown in Figure 2. Here the engine was operated at various steady-state load and speed conditions in two conventional combustion modes, with and without EGR. A DPF and LNT system enabled reduction of the NO_X and particulate matter emissions in the exhaust. Then, the engine was operated with multimode combustion where HECC was used at low and medium loads to reduce engine out NO_X and particulate matter. Figure 2 shows the reduction in engine out emissions from multimode operation, and subsequently, lower tailpipe emission levels are achieved for the combination of multimode operation with the DPF-LNT catalyst system.

Status

This project is continuing to study combinations of advanced combustion techniques and emission control strategies. It is anticipated that as advanced combustion regimes are discovered and/or further refined, this project will further incorporate those combustion techniques and analyze their potential under multimode operation and with emission control devices.

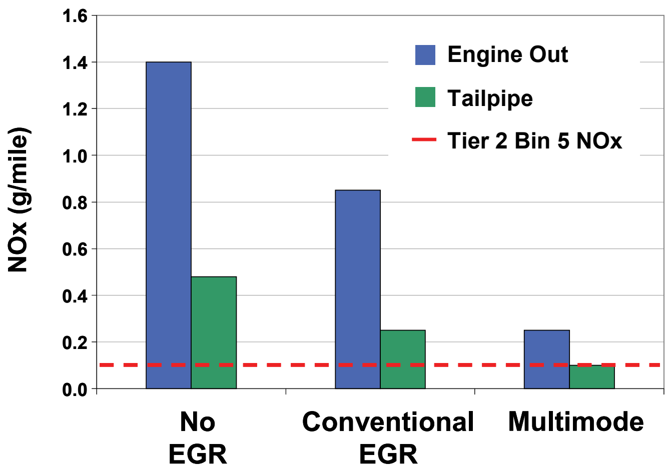

Figure 2: NO_X emissions for conventional vs multimode operation with a DPF-LNT emission control system.

Contacts

Jim Parks
Project Manager
Oak Ridge National Laboratory
(865) 946-1283
parksjeii@ornl.gov

Ken Howden
Combustion & Emission Controls
U.S. Department of Energy
(202) 586-3631
ken.howden@ee.doe.gov

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Fuels, Engines, and Emissions

Fuel Property Effects on High Efficiency Clean Combustion Technologies

Background

Compression ignition, or diesel, engines have long been known for their relatively high efficiency compared with spark ignition engines. Diesels have also historically suffered from higher nitrogen oxides(NO_X) and particulate matter (PM) emissions. High efficiency clean combustion (HECC) techniques offer the promise of very low NO_X and PM emissions simultaneously but suffer from increased hydrocarbon and carbon monoxide emissions.

Currently there are a number of HECC techniques and hardware that may be sensitive to fuel properties such as the cetane number (for diesel-like processes), octane number (for gasoline-like processes), fuel volatility, and fuel chemistry (Figure 1). Identifying key fuel properties and their effects on HECC processes is a key to meeting U.S. Department of Energy goals for petroleum displacement through enabling market use of these technologies.

This activity includes a number of specific projects spanning both diesel-like and gasoline-like applications with engines ranging from single-cylinder research engines to production-like platforms. The projects focus on generating a more in-depth understanding of the importance of fuel properties on the performance, efficiency, and emissions of engines using HECC processes. This is particularly important for emerging fuels such as those derived from oil sands and renewable sources.

Technology

The Oak Ridge National Laboratory (ORNL) has examined the effects of fuel properties through direct engine-based experiments on engines ranging from single-cylinder research engines to multicylinder production-like engines. Studies of the impact of test fuels from the Coordinating Research Council's Fuels for Advanced Combustion Engines Group (FACE) on homogenous charge compression ignition (HCCI) in a single-cylinder fumigated-charge engine and on premixed charge compression ignition (PCCI) in a 4-cylinder GM 1.9-liter diesel

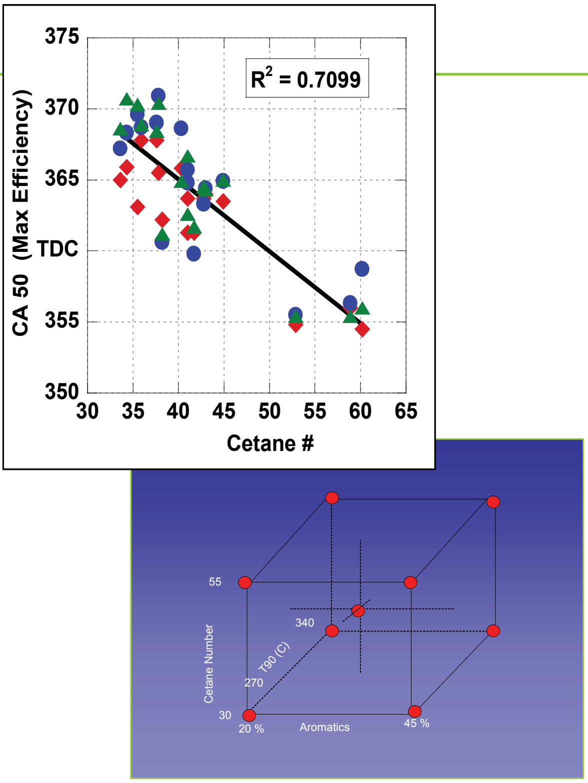

Figure 1: HECC speed/load range expansion achieved with improved control of intake mixture temperature. Efficiency similar for conventional and HECC operation.

Benefits

- *Better understanding of the impacts of marketplace fuel variations on HECC processes*
- *Opportunities for improved use of renewable fuel streams in advanced engine platforms*
- *Improvements in engine performance through better codevelopment of engines and fuel formulations*

were completed this year. The data are being examined using traditional analysis techniques and advanced statistical methods. Early results from both of these studies showed that cetane number continues to play an important role in advanced combustion performance. Data analyses are ongoing; publication of more in-depth results from the FACE fuel matrix is anticipated later this year. Experiments with biodiesel blends in PCCI modes to examine potential connections between biodiesel fuel quality and oil dilution are planned for later this year.

A new single-cylinder engine equipped with a Sturman variable-valve actuation system was commissioned at ORNL this year to study fuel property effects on combustion and to investigate high efficiency engine concepts. The new engine is based on a GM spark-ignited engine and is equipped with both port fuel injection and direct injection capabilities. The controller used with this engine is designed to facilitate cycle-to-cycle feedback combustion control, a very useful capability for controlling HCCI.

ORNL has also been participating in multiorganization efforts to identify and formulate surrogate fuels for use in numerical simulations and working to provide combustion kinetics data through the use of a single-cylinder HCCI engine to aid in matching the combustion properties of surrogates with those of commercial fuels. This work has also incorporated Chemikin modeling alongside the engine-based research to maximize the impact of the experiments.

Status

ORNL continues to engage with other organizations to further the understanding of fuel property impacts on engine efficiency and performance including actively participating in stakeholder groups such as FACE, the Advanced Engines and Combustion working group, and the Model Fuels Consortium.

Contacts

Ronald Graves
Project Manager
Oak Ridge National Laboratory
(865) 946-1226
gravesrl@ornl.gov

Kevin Stork
Team Leader
Fuel Technologies Subprogram
U.S. Department of Energy
(202) 586-8306
kevin.stork@ee.doe.gov

A Strong Energy Portfolio for a Strong America

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Fuels, Engines, and Emissions

Fuel Property Impacts on Exhaust Gas Recirculation Cooler Fouling

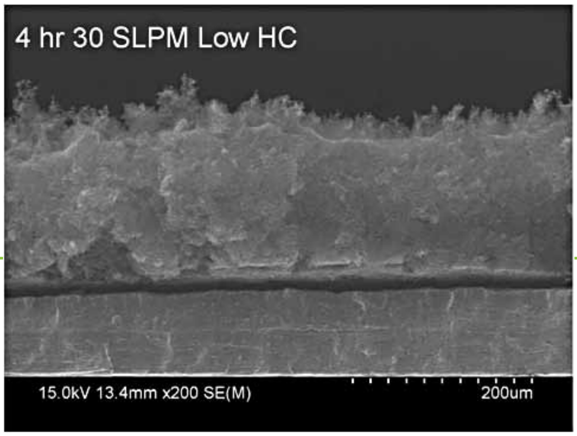

Figure 1: Electron microscope image of deposit attached to stainless steel tube wall (bottom).

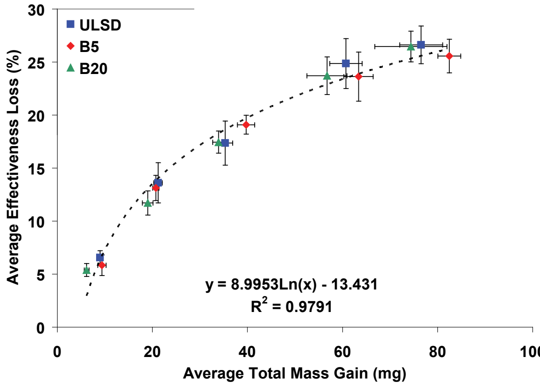

Figure 2: Relationship between EGR cooler effetiveness loss and deposit mass gain for ULSD, B5, and B20 fuels at low HC concentration.

Background

Compression ignition, or diesel, engines have long been known for their relatively high efficiency compared with spark ignition engines. Exhaust gas recirculation (EGR) and, more recently, the use of EGR coolers have been instrumental in continuing to reduce nitrogen oxide (NO_X) emissions while maintaining high engine efficiency. The EGR cooler contributes to lower NO_X emissions and improved efficiency through cooling the EGR stream before it reenters the engine intake manifold. The cooled gases allow the engine to induct fresh charge into the cylinders more efficiently and provide for decreased in-cylinder temperatures during combustion. This allows the engine to operate at an efficient condition while producing low levels of NO_X.

Over time, EGR coolers experience fouling of the heat exchanger surfaces. Fouling is caused by the presence of particulate matter (PM) and hydrocarbons (HCs) in the exhaust gases and results in the formation of deposits in the EGR cooler that reduce the effectiveness of the cooler in removing heat from the gases. Historically, systems were over-designed both to avoid conditions that cause accelerated fouling and to be tolerant of some degradation in performance from fouling. However, the demand for lower engine-out NO_X emissions and trade-offs in engine and emissions control system designs have resulted in fouling becoming a much more important issue in newer engine system designs. If the fouling issue cannot be successfully resolved or avoided, it often results in the engine operating condition changing to maintain low NO_X levels while sacrificing engine efficiency.

Fuel formulations may have significant impacts on EGR cooler fouling because of differences in fuel chemistry. These differences can manifest themselves through the combustion process as changes in PM characteristics as well as through unburned HCs in the exhaust. This is of particular concern for biodiesel as there is little information available to address this potential issue.

Benefits

- *Better understanding of the impacts of fuel formulations on the EGR cooler fouling issue.*
- *Fundamental data to support models of the fouling process in an effort to reduce the impact of fouling on engine efficiency and performance.*

Technology

The Oak Ridge National Laboratory (ORNL) has developed a capability for studying EGR cooler fouling through the use of individualized shell-and-tube heat exchangers fed with exhaust from a 2008 model year 6.4-liter diesel engine from a Ford Superduty pickup truck. The heat exchangers are individual surrogates for EGR cooler tubes and feature removable tubes to enable studies of the thermal, chemical, and physical characteristics of the deposits in situ (Figure 1). This design also allows different tube geometries as needed to support experimental efforts. In recent studies, the engine was fueled with ultralow sulfur diesel (ULSD) as a baseline fuel and with a 20% biodiesel blend (B20). Studies investigated the EGR cooler fouling process at near-zero HC level and with a higher level of HCs and three coolant temperatures. The exhaust gas temperature and particulate levels were kept constant. Assessments of the degradation in heat exchanger performance were accomplished and correlated to both the mass and the volatile fraction of the deposits (Figure 2). Researchers also successfully demonstrated a capability to measure the thermal conductivity of the deposits in situ. The thermal conductivity of a deposit is a key parameter in attempts to model the performance of EGR coolers where fouling is occurring.

The results to date have shown that short-term EGR cooler fouling behavior of engines running on ULSD and B20 are similar for the conditions studied. Studies are also underway to investigate potential impacts of fuel distillation properties in combination with coolant temperature effects.

Status

ORNL continues to perform research in this area to identify and resolve potential barriers to the broad use of nonpetroleum-based fuels. The information and results gleaned from this work have been published through SAE International, reviewed during U.S. Department of Energy (DOE) Annual Merit Reviews, and discussed with industry stakeholders. These efforts are also performed in close collaboration with a related project at ORNL that is tasked with examining EGR cooler deposit properties. The deposit properties study is funded through the DOE Propulsion Materials Program and is coordinated through the Diesel Crosscut Team.

Contacts

Ronald Graves
Project Manager
Oak Ridge National Laboratory
(865) 946-1226
gravesrl@ornl.gov

Kevin Stork
Team Leader
Fuel Technologies Subprogram
U.S. Department of Energy
(202) 586-8306
kevin.stork@ee.doe.gov

Fuels, Engines, and Emissions

Spark-Assisted Hybrid Combustion Experiments and Modeling for Improved Control

Background

An improvement in the fuel efficiency of gasoline engines is necessary to realize a significant reduction in U.S. energy usage. Homogeneous charge compression ignition (HCCI) in internal combustion engines is of considerable interest because of the potential reductions in nitrogen oxide and particulate emissions and the potential for fuel economy improvements resulting from unthrottled operation, faster heat release, and reduced heat transfer losses. Unfortunately for many transportation applications, HCCI may not be possible or practical under the full range of speed and load conditions, and thus the ability to switch between HCCI, conventional spark ignition (SI) operation, and hybrid (spark assisted HCCI) combustion modes will be required.

Technology

Delphi Automotive Systems Corporation and the Oak Ridge National Laboratory (ORNL) have established a Cooperative Research and Development Agreement (CRADA) on the control of HCCI combustion for gasoline engines. ORNL has extensive experience in the analysis, interpretation, and control of dynamic engine phenomena, and Delphi has extensive knowledge and experience in powertrain components and subsystems which have been used in the development of an advanced engine for this CRADA (see Figure 1). The partnership of these knowledge bases is critical to overcoming the critical barriers associated with the realistic implementation of HCCI and enabling clean, efficient operation in the next generation of transportation engines.

A single-cylinder research engine was used in the preliminary phase of this activity to improve the fundamental understanding of SI-HCCI combustion dynamics. To achieve the transition from SI to HCCI combustion, this engine made use of a full-authority hydraulic variable valve actuation system that allowed high levels of exhaust gas to be retained in the cylinder through manipulation of the intake

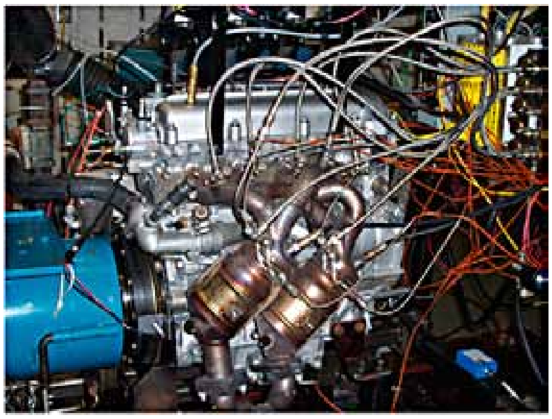

Figure 1: Mutlicylinder direct-injection gasoline engine with Delphi advanced components installed at the Delphi Technical Center in Rochester, New York. This engine will be used to demonstrate advanced control algorithms for enabling expanded HCCI operation.

Benefits

- *Improved controls for enabling combustion modes with high efficiency and low emissions across an expanded engine operating range.*
- *Development of simplified cyclic combustion models for rapid simulation, diagnostics, and controls.*

and exhaust valve events. All of these experiments were performed at stoichiometric fueling conditions and provided data for model development.

The current experimental phase of this activity is being performed using a multicylinder research engine developed by Delphi and installed at the Delphi Technical Center in Rochester, New York. Specific tasks for the multicylinder effort include (1) development and baselining of engine management systems; (2) mechanistic and physical modeling and control algorithm development for an improved understanding of hybrid combustion physics; (3) steady-state experiments for conventional, HCCI, and hybrid operation; and (4) transient experiments to maneuver within the HCCI envelope and switch between SI and HCCI operation.

A conceptual model has been developed based on fundamental physics, chemistry, and experimental data to explain the dynamics of the SI-HCCI transition and hybrid combustion modes. The concept is based on competition between the SI and HCCI combustion modes within the same cycle. This competition is driven by the presence or absence of sufficient concentrations of intermediate fuel species, which accumulate through internal exhaust recirculation. A graphical example of the model concept is shown in Figure 2.

Status

Multicylinder experiments are now in progress at the Delphi Technical Center. In addition, a new single-cylinder engine setup has been developed at ORNL and will be used in FY 2009 to further explore hybrid combustion modes and to provide new information for improved models and control algorithm development. Progress on this activity has been presented in several forums including meetings of the Society of Automotive Engineers, the Combustion Institute, and the American Society of Mechanical Engineers. Also, a patent on related control concepts was awarded to ORNL in FY 2009.

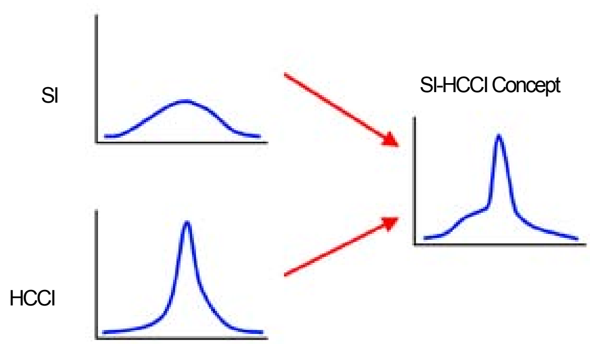

Figure 2: Conceptual diagram of the combining of two combustion rate profiles (SI and HCCI) into a composite hybrid combustion mode.

Contacts

Ronald Graves
Project Manager
Oak Ridge National Laboratory
(865) 946-1226
gravesrl@ornl.gov

Gurpreet Singh
Team Leader
Advanced Combustion Engine R&D
Subprogram
U.S. Department of Energy
(202) 586-2333
gurpreet.singh@ee.doe.gov

Heavy Vehicle Propulsion Materials

Life Prediction for Diesel Engine Components

Background

There has been considerable interest in the potential use of advanced ceramics and intermetallic alloys for applications in next generation diesel engine systems because of their superior thermomechanical properties and corrosion and oxidation resistance at elevated temperatures. The implementation of components fabricated from these advanced lightweight materials would lead to significant improvement in engine efficiency up to 50%, long-term durability, and reduction in nitrogen oxide and carbon monoxide exhaust emissions as required in the 21st Century Truck program. Interest has focused primarily on research aimed at characterization and design methodology development (life prediction) for silicon nitride (Si_3N_4) ceramics and TiAl alloys in order to manufacture consistent and reliable complex-shaped components for diesel engine applications. The valid prediction of mechanical reliability and service life is a prerequisite for the successful implementation of these materials as internal combustion engine components, which is the primary research objective of this subtask.

Figure 1: Photos showing Caterpillar G3406 natural gas engine and Si_3N_4, TiAl, and steel valve locations in the engine.

Technology

Caterpillar Inc. has been working with Oak Ridge National Laboratory (ORNL) to carry out valve train component design and testing to introduce advanced lightweight materials (i.e., Si_3N_4 ceramics and TiAl alloys) for heavy-duty diesel engine applications (Figure 1). Implementation of these advanced lightweight components will decrease reciprocating inertial, enabling more efficient engine operation and also operation in extreme combustion conditions that would lead to significant improvement in engine efficiency and emission reduction. Also, the superior high temperature mechanical performance and corrosion/oxidation resistance of these materials would allow a much longer service interval (durability) and thus lower maintenance cost. Success of engine field testing will ultimately lead to successful development of lightweight, wear- and corrosion-resistant valve train materials for applications in heavy-duty diesel engines with excellent long-term reliability and durability.

Benefits

- *Engine field test will enable the verification of probabilistic valve component design and life prediction model.*
- *Characterization results of tested valves will generate the component property database for further engine and valve design optimization.*
- *Engine component testing will provide the materials, design, manufacturing, and economic information to bring these advanced lightweight valves and the related technologies to commercialization.*

Status

The mechanical strength of the airfoils of a TiAl turbo wheel was measured (Figure 2). Results showed that the specimens with as-processed surfaces exhibited strength that was 30% lower than those with as-machined surfaces. The mechanical data generated would enable an engine company to verify the probabilistic component design and life prediction models.

Mechanical testing at room temperature of both Si_3N_4 and TiAl valve stems and heads following 555 h engine testing showed little or no mechanical strength degradation arising from oxidation/corrosion attack in engine environment. Detailed fractography and scanning electron microscopy (SEM) analysis revealed the strength limiting flaw to be the critical transverse flaws introduced during valve machining (Figure 3). The measured retained mechanical strength indirectly confirmed the life prediction (i.e., very high probability of survival) of these lightweight materials.

A 3-year ORNL-Caterpillar Cooperative Research and Development Agreement was officially approved by the U.S. Department of Energy to enable the use of engine/combustion and materials expertise at Caterpillar and ORNL to provide new insights into the integration of these technologies through a materials-by-design approach to high temperature, high pressure engine operation, and thus achieve 55% engine efficiency by 2012.

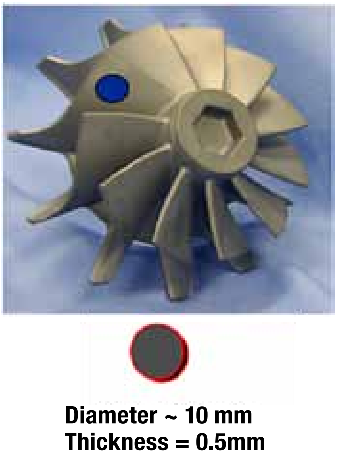

Figure 2: As-received TiAl turbo wheel for component mechanical database study.

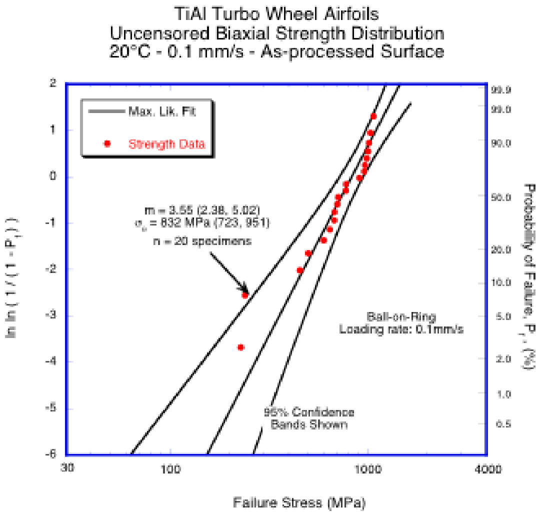

Figure 3: SEM micrographs showing the strength limiting flaw of machining grove.

Contacts

D. Ray Johnson
Field Technical Manager
Oak Ridge National Laboratory
(865) 576-6832
johnsondr@ornl.gov

Jerry L. Gibbs
Technology Development Manager
U.S. Department of Energy
(202) 586-1182
jerry.gibbs@ee.doe.gov

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Heavy Vehicle Propulsion Materials

Mechanical Reliability of PZT Piezoelectric Stack Actuators for Fuel Injectors

Background

The use of piezoelectric stack actuators as diesel fuel injectors has the potential to reduce injector response time, provide greater precision and control of the fuel injection event, and lessen energy consumption (Figures 1 and 2). Though piezoelectric function is the obvious primary function of lead zirconate titanate (PZT) ceramic stacks for fuel injectors, their mechanical reliability can be a performance and life limiter because PZT is brittle, lacks high strength, and can exhibit fatigue (i.e., slow crack growth) susceptibility. That brittleness and relatively low strength can be overcome though with proper design. This project combines in situ micromechanical testing, microstructural-scale finite element analysis, probabilistic design sensitivity, and structural ceramic probabilistic life prediction methods to systematically characterize and optimally design PZT piezoelectric stack actuators that will enable maximized performance and operational lifetime.

Technology

A piezoelectric stack actuator is fabricated from multilayers of piezoceramic sheets, and those sheets are normally tape cast. Assembly of the complete actuator includes screen printing, lamination, cutting, and sintering operations. Strength- and fatigue-limiting flaws can be introduced at any of those stages. The goals are to either minimize or eliminate flaw introduction or design the piezoelectric stack actuator so that operating conditions do not activate strength- or fatigue-limiting effects from the flaws. Refinements in ceramic processing and the use of structural ceramic design methods are able to satisfy those goals.

Status

The establishment of a piezodilatometer test facilitiy was accomplished this year. The piezodilatomer enables accelerated fatigue and electric breakdown testing for developmental and commercially available piezoceramic materials (Figures 3 and 4).

Figure 1: Piezoelectric actuated fuel injector used in Ford 6.4L Power Stroke diesel engine.

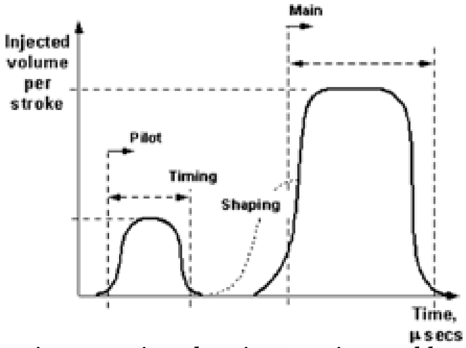

Figure 2: Piezoelectric actuation enables advanced rate shaping and better control of injection timing and fuel quantity.

Benefits

- *Identify stronger and more reliable piezoceramics.*
- *Identify more reliable piezoelectric actuators.*
- *Introduce structural ceramic probabilistic component design methods to improve long-term reliability of piezoelectric actuators.*

Mechanical strength of piezoceramic PZT-5A was measured using ball-on-ring under the applied high electric field. Results showed that the poled PZT-5A exhibited a strength decrease under an inverse coercive electric field. Also, a strength increase was observed when the applied electric field level was greater than the coercive field independent of electric field direction. This observed strength-electric field dependence will be used in future design sensitivity and reliability analysis efforts with the multilayer PZT piezoelectric actuators.

In addition, fatigue responses of PZT-5H and PZT-5A multilayer PZT stacks were studied under unipolar and semi-bipolar cycling electric fields under an applied preload. Significant reductions in mechanical strain and piezoelectric coefficients along with extensive surface charging were observed during the cycling depending on the measuring conditions. These surface events, as well as related breakdown, resulted in the erosion of external electrode and the outcrop of internal electrode, which partially accounted for the observed reductions. The results from this study demonstrate the feasibility of using a semi-bipolar mode to drive a PZT stack under a mechanical preload and illustrate the potential fatigue performance of the stack in service. A 3-year Cummins Inc.–Oak Ridge National Laboratory Cooperative Research and Development Agreement to pursue this line of research was officially approved by the U.S. Department of Energy in September 2008..

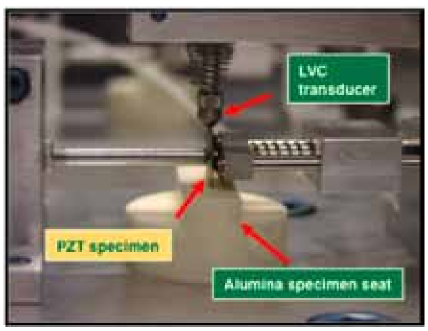

Figure 3. Piezodilatometer enables accelerated electric fatigue and break-down testing of piezoceramics.

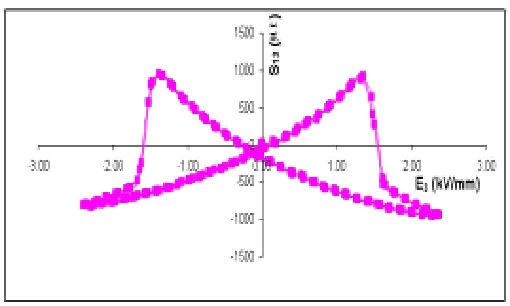

Figure 4:. Mechanical strain verses E field of piezodilatomer was calibrated using a soft PZT piezoceramic.

Contacts

D. Ray Johnson
Field Technical Manager
Oak Ridge National Laboratory
(865) 576-6832
johnsondr@ornl.gov

Jerry L. Gibbs
Technology Development Manager
U.S. Department of Energy
(202) 586-1182
jerry.gibbs@ee.doe.gov

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High Temperature Materials Laboratory

User Projects on Batteries

Background

The Oak Ridge National Laboratory (ORNL) High Temperature Materials Laboratory (HTML), a collaborative materials research facility, works with industry, universities, and other research organizations to develop materials-based, energy-efficient, and environmentally friendly highway transportation technologies. In its support of the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program (VTP) goals, HTML is characterizing new materials for rechargeable batteries with the objective of reaching VTP energy storage goals for electric and hybrid electric vehicles.

User Projects

1. Using HTML's X-14A synchrotron beamline, Brookhaven National Laboratory and HTML researchers conducted X-ray diffraction studies on cathodes for lithium batteries to investigate the changes during charge-discharge cycling in electronic and crystal structures for both uncoated and carbon-coated $LiFe_{1/4}Mn_{1/4}Co_{1/4}Ni_{1/4}PO_4$ cathode materials. These experiments will lead to a deeper understanding of the charge-discharge process in these materials and result in improving the safety characteristics of lithium ion batteries.

2. University of Michigan researchers (Figure 1) initiated an HTML user project to characterize lithium ion battery active materials. They partnered with HTML research staff to determine the microstructure of carbon fibers and various cathode materials using X-ray diffraction and scanning and transmission electron microscopy. The University of Michigan team also complemented its user project by collaborating with ORNL researchers to prepare thin films of $LiMn_2O_4$ by radiofrequency magnetron sputtering deposition. Models based on the results are expected to enable the development of safer, more durable batteries for electric vehicles.

Figure 1: University of Michigan researchers Myonggu Park (left) and HyonCheol Kim prepare to conduct X-ray diffraction tests on lithium ion battery materials.

Benefits

- *Improved safety characteristics of lithium ion batteries for electric and plug-in hybrid electric vehicles.*
- *Enhanced charging characteristics of batteries.*
- *Development of multiphysics models of battery electrodes that account for thermomechanical and electrochemical phenomena.*

Contacts

Edgar Lara-Curzio
Director
High Temperature Materials Laboratory
Oak Ridge National Laboratory
(865) 574-1749
laracurzioe@ornl.gov

James Eberhardt
Technology Development Manager
U.S. Department of Energy
(202) 586-9837
james.eberhardt@ee.doe.gov

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High Temperature Materials Laboratory

User Projects on Thermoelectric Materials

Background

The Oak Ridge National Laboratory High Temperature Materials Laboratory (HTML), a collaborative materials research facility, works with industry, universities, and other research organizations to develop materials-based, energy-efficient, and environmentally friendly highway transportation technologies. HTML supports the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program by assisting facility users in the development of thermoelectric materials with high figure of merit to recover waste heat from internal combustion engines. Only about 30–35% of the fuel's energy currently is used for vehicle propulsion, while about 35–40% is lost in the exhaust gases and another 30–35% is lost to the coolant.

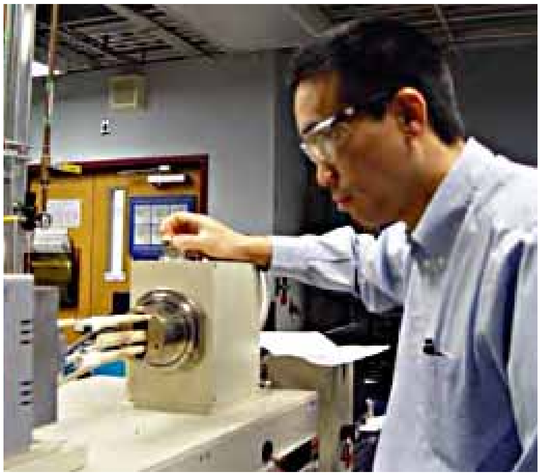

Figure 1: General Motor's Dr. Jihui Yang tests thermoelectric generator materials.

User Projects

1. Researchers from HTML and Marlow Industries characterized thermoelectric alloys referred to as "TAGS-x," which are some of the most promising materials for thermoelectric applications. Understanding the structure-property relationships will enable researchers to optimize the thermoelectric properties of TAGS-x and related thermoelectric materials. Optimized thermoelectric materials are essential to efficient recovery of waste heat from internal combustion engines and industrial furnaces.

2. A General Motors R&D Center researcher (Figure 1) and HTML staff members studied filled skutterudite materials for automotive waste heat recovery applications to improve material transport properties by increasing the power factor while lowering thermal conductivity. The improvement in transport properties could allow thermoelectric generators to operate more efficiently and raise fuel efficiency by 2–3% toward DOE's waste heat recovery program

Benefits

- *Potential for 10% or more improvement in overall engine efficiency as well as significantly increased vehicle fuel economy.*
- *Improved material transport properties from lowered thermal conductivity.*
- *Improved design of reliable waste heat recovery devices.*
- *Design information for developing durable, reliable thermoelectric generators.*

goal of 10%. Based on results showing them to be one of the best n-type bulk thermoelectric materials, General Motors has selected skutterudite materials as the leading material for their thermoelectric generators.

3. Researchers from Michigan State University and HTML assessed the effect of temperature and thermal cycling on the elastic properties of lead-antimony-silver-tellurium (LAST) and LAST-tin. The results of this investigation provided valuable design information for minimizing thermal stresses and enabling development of durable and reliable thermoelectric generators that use waste heat to produce electricity.

Contacts

Edgar Lara-Curzio
Director
High Temperature Materials Laboratory
Oak Ridge National Laboratory
(865) 574-1749
laracurzioe@ornl.gov

James Eberhardt
Technology Development Manager
U.S. Department of Energy
(202) 586-9837
james.eberhardt@ee.doe.gov

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High Temperature Materials Laboratory

User Projects on Automotive Lightweighting Materials

Background

The Oak Ridge National Laboratory (ORNL) High Temperature Materials Laboratory (HTML), a collaborative materials research facility, works with industry, universities, and other research organizations to develop materials-based, energy-efficient, and environmentally friendly highway transportation technologies. HTML supports the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program activity in automotive lightweighting materials through characterization of structural materials for body and chassis applications that significantly reduce the weight of passenger vehicles without compromising vehicle life-cycle cost, performance, safety, or recyclability. Developing such materials requires an understanding of the properties of polymer composites and lightweight metals in structural components.

User Projects

1. Metalsa Inc., a Tier 1 supplier to heavy truck manufacturers in North America, initiated a project with HTML to study fatigue life of the rail side for trucks and to compare processing and properties of high-strength, low alloy steel to the industry standard heat-treated rail side. Based on data analysis of the samples, it is clear there is a complex relationship between the metallurgical, thermal, and mechanical properties generated by the different processes. Studies of the residual stresses from hole-cutting the rail sides to reduce weight revealed the potential for Metalsa to save as much as 200 pounds per truck. This represents an annual savings of up to 30,000,000 pounds of steel, with an accompanying reduction in energy consumption and resources to produce the steel.

2. Using the high-temperature X-ray diffraction (XRD) facility at HTML, researchers from HTML, ORNL, and the University of Tennessee investigated the morphological evolution of carbon fibers (Figure 1) as a function of time, temperature, and chemical structure. Data from this HTML user project will provide the knowledge base for the carbon fiber processing window, aid in exploring alternative low cost carbon precursors such as lignin-based fibers, and enable the commercialization of low cost carbon fibers.

Benefits

- *Models for lightweight structural materials that enable producing lightweight materials with improved properties yet with unchanged vehicle life-cycle cost, performance, safety, or recyclability.*
- *Development of low cost carbon fibers and recovery of carbon fibers from scrapped or recycled composites at a 50% cost savings over producing new carbon fibers.*
- *New component designs that enable technologies to predict the response of materials after long-term loading, under exposure to different environments, and in crash events.*
- *Confirmation of the advantages of electromagnetic pulse welding, an attractive low cost joining technology for automotive applications.*

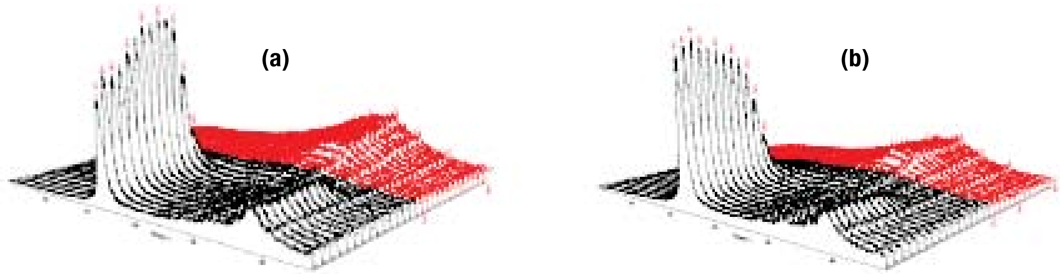

Figure 1: Morphological evolution as observed by online XRD during heat treatment of (a) as-spun polyacrylonitrile (PAN) and (b) radiation modified PAN fibers.

3. Materials Innovation Technologies LLC has developed a process to recover carbon fibers from manufacturing scrap and end-of-life components for less than 50% of the cost of virgin carbon fibers. HTML researchers assisted the company in characterizing these recovered carbon fibers. Initial results show promise, and successful development of this technology could enable the cost-effective use of carbon-fiber-reinforced composite materials on automobiles and transportation vehicles.

4. Mississippi State University (MSU) researchers have developed a predictive model of creep and fatigue behavior of an E-glass–vinyl ester composite, a candidate for lightweighting vehicles. They visited HTML to generate the necessary material creep and fatigue input parameters for modeling composite components. Monotonic tensile testing at ambient conditions and at 90°C was completed, and creep tests were initiated to determine creep deformation and rupture times as a function of applied stress. Future testing to determine rupture parameters at higher temperatures and lower stress levels is planned.

5. An HTML project from the MSU Center for Advanced Vehicular Systems gathered data to support accurate modeling of magnesium's highly anisotropic behavior (Figure 2). It is hoped that modeling with physics-based and experimentally verified behavior will result in the next generation of lightweight components, further enhancing energy efficiency and reducing energy consumption.

6. L&L Products manufactures structures known as "Composite Body Solutions," macrocomposites made of a metal, thermoplastic, or thermoset carrier and heat-activated expanding adhesive. These structures can be used at key locations to reinforce vehicles and improve crashworthiness. Researchers from L&L and HTML performed preliminary bend crush tests to establish baseline data on the suitability of L&L's custom three-point bend test fixture and to verify the reliability of the test configuration for collecting the desired high-rate data. A test matrix with more than 100 specimens will be completed in FY 2009.

7. Ohio State University and HTML researchers performed nanoindentation measurements across electromagnetically welded interfaces in aluminum and copper. The results from this user project in mechanical properties, when contrasted with traditional fusion welding techniques, reveal higher hardness and no brittle intermetallic phases.

8. General Motors and the University of Tennessee studied how hydrogen content affects mechanical properties of castings. Research was conducted at the neutron scattering mapping facility operated by HTML at the

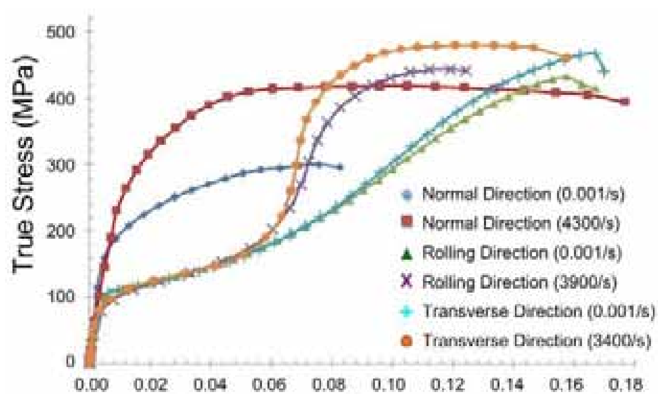

Figure 2: Compression stress-strain response revealing highly anisotropic and strain rate dependent behavior.

ORNL High Flux Isotope Reactor (Figure 3). It is hoped the project will result in tools to map hydrogen content and its effects within a casting, resulting in lighter weight castings and reduced materials and energy use.

Figure 3: LEAP tomographic reconstructions of 5 % Zn isoconcentration surfaces for the ZA73 alloy (Mg–7Zn–3Al) aged at 423 K for 100 hours using the laser mode.

9. John Deere and HTML researchers are verifying Deere's welding simulation models using neutron diffraction to determine the residual stresses. Ultimately, this modeling research will help John Deere produce better, longer-lasting parts, which in turn will conserve energy and increase fuel efficiency because of lighter weight vehicles.

10. Researchers from the Electric Power Research Institute and HTML characterized the through thickness residual stresses in a set of Inconel 182 weld overlay material plates to benchmark traditional nondestructive examination (NDE) techniques that are applicable to stress characterization of weld bead repairs. The plates also will be used to identify promising field-deployable NDE techniques, which is critical to evaluating the effectiveness of mechanical and induction heat stress improvement processes that are applied in the transportation industry.

11. University of Tennessee and HTML researchers determined the feasibility of using scanning acoustic microscopy (SAcM) to examine wood and lyocell fibers and to evaluate the mechanical properties of wood cell walls via nanoindentation techniques. The researchers concluded that SAcM was not the proper tool to characterize these materials but also found that thermomechanical refining steam pressure plays an important role in the physical damage and mechanical properties of refined fiber cell walls. These results will help identify optimized manufacturing processes for biocomposites and may perhaps lead to the use of these materials for lightweight nonstructural components in automotive applications.

Contacts

Edgar Lara-Curzio
Director
High Temperature Materials Laboratory
Oak Ridge National Laboratory
(865) 574-1749
laracurzioe@ornl.gov

James Eberhardt
Technology Development Manager
U.S. Department of Energy
(202) 586-9837
james.eberhardt@ee.doe.gov

A Strong Energy Portfolio for a Strong America

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High Temperature Materials Laboratory

User Projects on Catalysis

Background

The Oak Ridge National Laboratory High Temperature Materials Laboratory (HTML), a collaborative materials research facility, works with industry, universities, and other research organizations to develop materials-based, energy-efficient, and environmentally friendly highway transportation technologies. HTML supports the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program goal of achieving emissions reduction targets through its collaborations with users to characterize catalytic materials used in aftertreatment devices. Fundamental research is focused on understanding the thermodynamics and kinetics of nucleation, growth, and sintering.

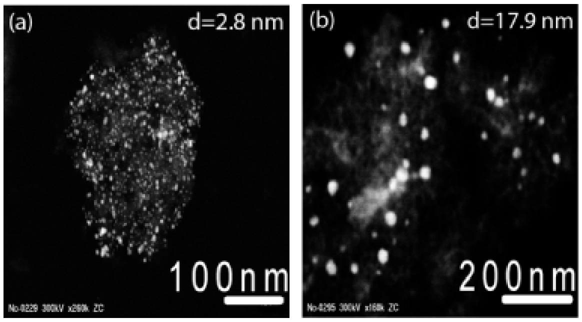

Figure 1: Z-contrast scanning transmission electron microscope images of fresh (a) and aged (b) LNTs show sintering of Pt particles with aging.

User Projects

1. A University of Tennessee graduate student is working with HTML and National Transportation Research Center researchers to study thermal deactivation mechanisms in fully formulated lean NO_X trap (LNT) catalysts when they are aged by lean-rich cycling in simulated diesel exhaust gases at aging temperatures of 700, 800, 900, and 1,000°C. As shown in Figure 1, it was found that platinum (Pt) sintering increases with increasing aging temperature and number of aging cycles but that particle growth is already significant at an aging temperature of only 700°C. Combining these results with other measurements, researchers concluded that the reduction in NO_X conversion after aging at temperatures greater than 900°C appears to be primarily a result of surface area loss, with Pt sintering and loss of active storage sites also contributing.

2. University of Texas-Austin research (Figure 2) at HTML's aberration-corrected electron microscope (ACEM) focused on characterization of bimetallic nanoparticles during heating and gas reactions to develop a fundamental understanding of their catalytic behavior. In situ heating of gold-palladium nanoparticles revealed that adjacent particles sometimes did not sinter

Benefits

- *Development of more effective catalytic materials for use in aftertreatment devices.*
- *Improved fundamental understanding of the thermodynamics and kinetics of nucleation, growth, and sintering.*
- *Enhanced catalysts for lean-burn diesel engines and their greater use in automotive vehicles*

together, but instead one particle gradually decreased in size while the grain in a closely adjacent particle concomitantly enlarged. Additional systematic experiments are planned to better understand catalyst materials intended for fuel cells and other vehicle-related applications.

Figure 2: University of Texas-Austin researcher Dr. Miguel Jose Yacaman analyzes ACEM images.

3. Using atomic-resolution electron microscopy on HTML's ACEM and various other spectroscopic tools such as nuclear magnetic resonance, researchers from the Pacific Northwest National Laboratory and HTML studied the properties and behavior of LNT catalyst systems, particularly the strong interaction between barium oxide and penta-coordinated Al^{3+} sites formed on alumina surfaces. Diesel engine emissions reduction from more effective catalytic systems may ultimately allow the highly fuel-efficient diesel engine to be more fully incorporated into the U.S. fleet of passenger vehicles.

4. University of Michigan and HTML researchers are studying bimetallic catalysts for lean-burn diesel engines to determine the spatial distribution of elements in alumina-supported Pt-palladium (Pd) bimetallic catalysts, resulting in a more complete picture of the role of Pd in the behavior of Pt catalysts. This research could lead to the development of higher durability NO oxidation catalysts for lean-burn diesel engines and identification of the optimal means to produce Pt-Pd bimetallic catalysts.

5. An HTML project from the University of Missouri-St. Louis used a newly developed in situ heating system on ACEM to make real-time observations of the novel structure and behavior of Pd-ZnO nanocatalysts. Results help explain the unique activity/selectivity data previously reported and could accelerate the development of improved catalysts for producing hydrogen in fuel cells and other energy-production applications.

Contacts

Edgar Lara-Curzio
Director
High Temperature Materials Laboratory
Oak Ridge National Laboratory
(865) 574-1749
laracurzioe@ornl.gov

James Eberhardt
Technology Development Manager
U.S. Department of Energy
(202) 586-9837
james.eberhardt@ee.doe.gov

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High Temperature Materials Laboratory

User Projects on Diesel Particulate Filter Materials

Background

The Oak Ridge National Laboratory High Temperature Materials Laboratory (HTML), a collaborative materials research facility, works with industry, universities, and other research organizations to develop materials-based, energy-efficient, and environmentally friendly highway transportation technologies. Researchers at HTML are supporting U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program efforts to address emissions from diesel engines by characterizing diesel particulate filter (DPF) materials. A focus has been on developing a clearer picture of aftertreatment technologies and studying DPF devices in operation under high temperature and high flow-rate conditions.

User Projects

1. GEO_2 Technologies LLC, a Massachusetts start-up firm, worked with HTML researchers to characterize the properties and microstructure of the company's trade-marked fibrous DPF substrates to understand the relationships between the microstructure and the mechanical (e.g., fracture toughness) and thermal (e.g., thermal conductivity) properties of fibrous DPF materials. Figure 1 illustrates the superior properties of the GEO_2 substrates.

2. Colorado School of Mines and HTML researchers used in situ Raman analysis of ß-eucryptite pressure-induced transformation to develop a fundamental understanding of phase transformations in ß-eucryptite, a DPF material that exhibits greater resistance to thermal shock conditions in advanced emissions control technologies.

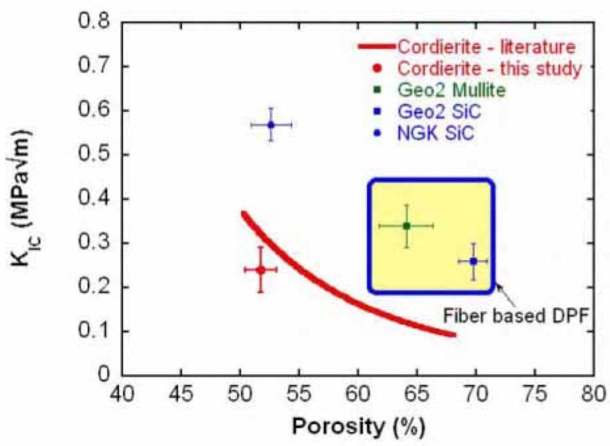

Figure 1: A comparison of the fracture toughness of fibrous (GEO_2) and commercially available porous monolithic ceramic DPF substrates.

Benefits

- *Diesel particulate filters with lower pressure drop for higher engine efficiency.*
- *Potential design and manufacture of tough, durable catalyst supports and DPFs.*
- *Improved heat transfer model and techniques for reducing soot deposition.*

3. University of Utah (Figure 2) and HTML research staff characterized soot deposition behavior from transportation fuels (e.g., JP-8, diesel) and the effect of these deposits on heat transfer. This research was used to determine thermal conductivity values for a heat transfer model. An improved model will lead to techniques for reducing soot deposition from diesel engine exhaust and thereby enhance performance of internal combustion engines.

Figure 2: University of Utah student Ignacio Preciado adjusts settings for a thermal conductivity test.

Contacts

Edgar Lara-Curzio
Director
High Temperature Materials Laboratory
Oak Ridge National Laboratory
(865) 574-1749
laracurzioe@ornl.gov

James Eberhardt
Technology Development Manager
U.S. Department of Energy
(202) 586-9837
james.eberhardt@ee.doe.gov

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High Temperature Materials Laboratory

User Projects on Materials for Thermal Management and Wear

Background

The Oak Ridge National Laboratory High Temperature Materials Laboratory (HTML), a collaborative materials research facility, works with industry, universities, and other research organizations to develop materials-based, energy-efficient, and environmentally friendly highway transportation technologies. Projects in thermal management and issues concerning wear enable HTML to address these challenges and help the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program achieve its objectives related to effectively managing thermal reactions and enhancing vehicle-related technologies by reducing wear.

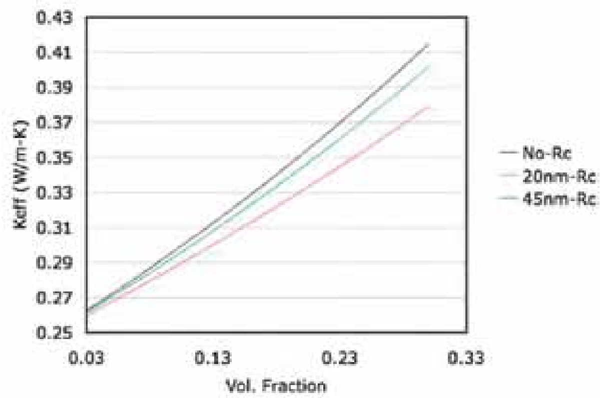

Figure 1: Prediction of effective conductivity for 20 nm and 45 nm silica composite.

User Projects

1. Purdue University and HTML researchers evaluated the thermal boundary resistance of an epoxy-silica particulate composite to determine the effective conductivity of the composite. Particle size was found to affect thermal properties, and results could lead to better thermal management materials for automotive applications. Figure 1 illustrates the relationship between particle size and thermal conductivity.

2. Georgia Institute of Technology and HTML researchers worked together to evaluate the scuffing tendencies of various metal-metal combinations for potential use in current-conducting rails for magnetically accelerated objects. The research data will be useful in developing criteria for selecting scuffing-resistant metallic sliding contacts for public transit systems that use magnets for acceleration.

Benefits

- *Improved thermal management of materials for automobile applications.*
- *Improved models for forging die wear and material selection in the production of lightweight powder metallurgy parts for automobiles.*
- *Criteria to select materials for use by public transit systems that use magnets for acceleration.*
- *Enhanced operating performance and life of TBCs for turbine engines and potentially for diesel engines*

3. HTML staff assisted researchers (Figure 2) from Mississippi State University's (MSU's) Center for Advanced Vehicular Systems to obtain data for a model of the wear characteristics of powder metal forging dies. Their experiments evaluated an alternative method to assess the abrasive wear of hardened steel forging die materials against lightweight alloy powders. Research data will be used by MSU to develop dependable models for calculating die wear rates and die life.
4. State University of New York-Stony Brook and HTML researchers applied advanced characterization techniques to thermal barrier coatings (TBCs) to understand and predict the long-term performance and lifetime of TBCs in engines. Results indicated that using the nondestructive technique of resonant ultrasound spectroscopy for characterizing the elastic modulus anisotropy of TBCs provides industry with a critical tool for assessing and optimizing the operating performance of TBCs.

Figure 2: MSU researchers Wei Li (left) and Prof. Seeong Park prepare to conduct abrasion tests.

Contacts

Edgar Lara-Curzio
Director
High Temperature Materials Laboratory
Oak Ridge National Laboratory
(865) 574-1749
laracurzioe@ornl.gov

James Eberhardt
Technology Development Manager
U.S. Department of Energy
(202) 586-9837
james.eberhardt@ee.doe.gov

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Propulsion Materials

Environmental Effects on Power Electronic Devices

Background

Weight, volume, and cost targets for the power electronics subsystems in electric and hybrid electric vehicles must be achieved before these vehicles gain greater popularity among consumers. Such targets will be satisfied with the availability of more efficient inverters with higher temperature capabilities; smaller, more light weight converters; more effective thermal control and packaging technologies; and advanced motor-inverter concepts.

Most of the technical barriers are directly linked to the limitations of the contemporary materials found in devices that are used in inverters, converters, and motors. For automotive power electronic devices (PEDs), contemporary material limitations include insufficient temperature capability, excessive thermal insulation, and excessive electrical insulation (i.e., they generate excessive heat).

Technology

Higher-temperature-capable PEDs (e.g., insulated gate bipolar transistors or IGBTs) will enable more efficient and powerful inverters for electric and hybrid electric vehicles. But they are presently limited. This project seeks to (1) understand the complex relationship between environment (temperature, humidity, and vibration) and automotive PED performance through materials characterization and modeling and (2) identify alternative material constituents and architectures that will improve their reliability and enable their operation at higher temperatures without compromise to electronic function.

Status

This project is a blend of modeling, experiment, and materials science and engineering. This past year, we achieved the following.

- Characterized the architectures of commercial IGBTs by dissecting them, measuring the constituent dimensions, and identifying all

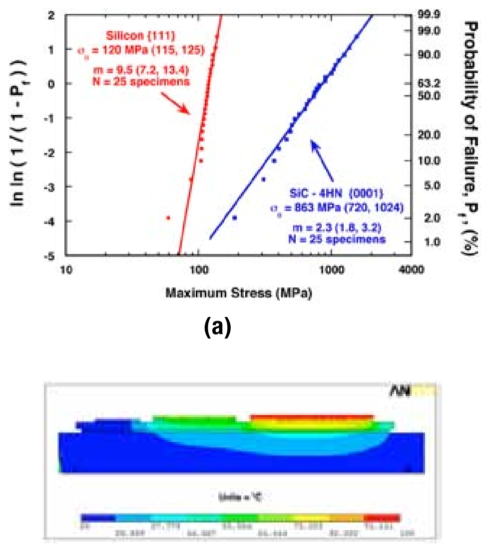

Figure 1: (a) Measured strength differences in Si and SiC chips. (b) Modeled thermal profile of a PED cross section. The PED is an IGBT, its silicon chips generate heat, and active cooling seeks to limit the maximum temperature they experience.

Benefits

- *Higher-temperature-capable power electronic devices (IGBTs).*
- *Improved thermal management.*
- *More reliable devices.*
- *Better device life prediction.*

constituent materials, and developed thermomechanical models to estimate service stress states.

- Measured and contrasted the mechanical strength distributions of commercially available silicon (Si) and silicon carbide (SiC) semiconductor chips.
- Measured and contrasted the mechanical strength distributions of commercially available ceramic substrates.

Such data are needed to model the reliability of PEDs which contain these materials.

We are continuing to pursue the development of a polycrystalline SiC electrical insulating material. It has the potential to match the thermal expansion of Si or SiC semiconductor chips, has high thermal conductivity (needed for better thermal management), and will be relatively low cost.

We are now modeling PEDs using the above results and recommending new architectures with improved thermal management without compromises to electronic function (Figure 2).

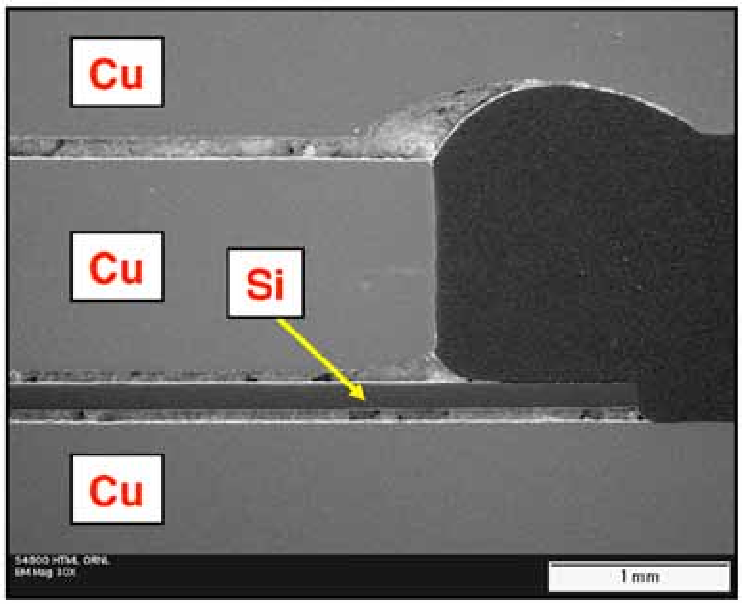

Figure 2: Dual-side cooling of IGBTs is attractive for improved thermal management. Shown here is the architecture of the constituents surrounding a silicon chip and providing dual paths (up and down) for its cooling.

Contacts

D. Ray Johnson
Field Technical Manager
Oak Ridge National Laboratory
(865) 576-6832
johnsondr@ornl.gov

Jerry L. Gibbs
Technology Development Manager
U.S. Department of Energy
(202) 586-1182
jerry.gibbs@ee.doe.gov

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Propulsion Materials

Friction and Wear Reduction in Diesel Engine Valve Trains

Background

Depending on engine design and operating conditions, between 5 and 20% of the energy losses from friction in internal combustion engines are attributable to rubbing between valve train components. Furthermore, improvements in the wear-resistance of valve train materials can reduce diesel engine emissions by ensuring proper sealing of the combustion chamber. The objective of this effort is to develop a more comprehensive understanding of the synergism between mechanical damage and oxidation at high temperatures and to use that knowledge to develop a multidisciplinary model for valve-seat wear. The goal is to enable engine designers to select the best-performing materials for exhaust valves in energy-efficient diesel engines. The approach is to develop a high temperature, laboratory-scale test method and use it to measure repetitive-impact resistance of high-performance diesel engine valve and valve seat materials based on iron, nickel, and cobalt (Figure 1). That data will provide a physical basis for the development of a valve material wear model.

Figure 1: A high temperature, repetitive impact testing apparatus was designed and built for this project. It can accommodate simple coupons or actual exhaust valves.

Technology

The selection of suitable diesel engine exhaust valve alloys depends on the design of the engine and its operating conditions. Likewise, the durability of a given alloy depends on a combination of its mechanical properties and its oxidation behavior, which is affected by the state of surface damage. For example, tests of abraded heat-resistant alloys at elevated temperatures showed how oxidation was affected by the presence of mechanical damage (Figure 2).

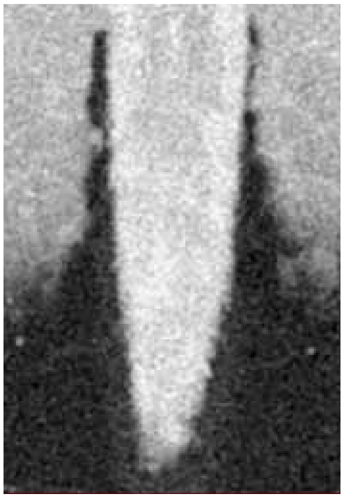

Figure 2: Elemental map of a scratch exposed to 850˚C shows that abrasion damage (center, brighter area) is oxygen rich.

Benefits

- *Develop new laboratory test methods to characterize the conjoint effects of wear and oxidation.*
- *Understand the evolution of surface damage on valve and seat surfaces as a function of time and temperature.*
- *Combine prior models of impact wear with new experimental results to develop an improved, multi-disciplinary model for exhaust valve surface recession.*

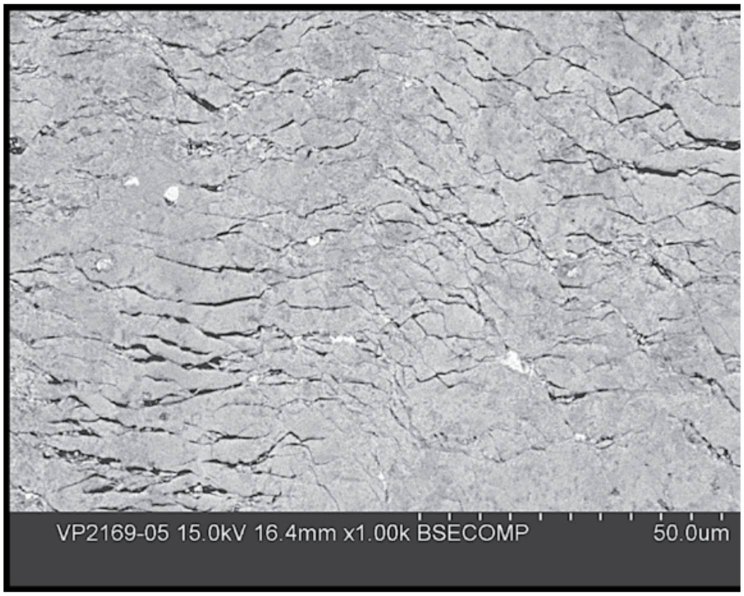

Figure 3: Back-scattered electron image of a densified, heterogeneous deposit of oxides of iron and chromium formed on a nickel alloy block after 20,000 impacts against a cobalt alloy pin at 750˚C in the HTRI apparatus (Figure 1).

Status

The static oxidation rates of iron-, nickel-, and cobalt-based alloys at exhaust valve temperatures have been studied. Studies of abrasion damage, like that in Figure 2, verified that oxides that formed on damaged portions of surfaces differed from those that formed on non-damaged areas. High temperature, repetitive-impact (HTRI) tests revealed the formation of densified, plastically sheared glazes (tribo-layers) on contact surfaces (Figure 3). These layers contained compressed mixtures of oxidation products and metallic particles. First results of this work were published in an archival journal (*Tribology Letters*) in 2008. Additional results have been accepted for presentation at two international conferences on wear in FY 2009. In addition, these results have been shared with two U.S. diesel engine manufacturers.

During FY 2008, and continuing into FY 2009, HTRI tests are being conducted at temperatures in the range of exhaust valve use (750–850°C). Alloys of varying compositions, including a commercial diesel engine exhaust valve alloy, were studied to identify the key material responses to be incorporated into a multidisciplinary valve material wear model, the final deliverable of this project. The components of the wear model include plastic deformation, surface oxidation, tribo-layer formation, and counterface wear.

Contacts

D. Ray Johnson
Field Technical Manager
Oak Ridge National Laboratory
(865) 576-6832
johnsondr@ornl.gov

Jerry L. Gibbs
Technology Development Manager
U.S. Department of Energy
(202) 586-1182
jerry.gibbs@ee.doe.gov

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Propulsion Materials

Materials for High Pressure Fuel Injection Systems

Background

The efficiency of diesel engines can be increased and their emissions reduced by raising the pressure in the fuel injection system. Over the past 10 years, engine designers have increased this pressure significantly. High pressure pulses place additional demands on both the alloys and the manufacturing tolerances of injector tips (Figure 1). To address the selection and characterization of materials that will withstand such environments, a Cooperative Research and Development Agreement was established between Oak Ridge National Laboratory (ORNL) and Caterpillar Inc. The objectives of this work are to characterize manufacturing-induced residual stresses, fatigue response, microstructures, and fine geometric details of spray holes in fuel injector tips. Special methods to measure hole geometry, hole wall surface roughness, and residual stresses in the material adjacent to holes are being developed. In FY 2009, methods to fatigue test the material will be developed to investigate the effect of spray holes on the ability of metallic alloys to repetitively withstand high pressures. In the final year of this project (FY 2010), the effects of the hole-making method on the durability of the fuel injector tips will also be determined.

Figure 2: A high precision coordinate measuring machine provided dimensional data that were used to position injector tips for X-ray and neutron residual stress analyses.

Technology

A variety of specialized techniques are being used to measure spray holes, the residual stresses in nozzles, and the fatigue response of candidate materials (Figure 2). Optical and electron microscopy techniques are used to characterize the surface roughness inside minute spray holes. Several advanced X-ray and neutron diffraction residual stress methods are being compared to determine their suitability for nozzle tip sizes and geometries.

Figure 1: Commercial diesel engine fuel injector nozzles.

Benefits

- *Develop new methods for characterizing fine spray holes in fuel injector tips.*
- *Investigate the strengths and limitations of X-ray and neutron residual stress measurement techniques applied to small volumes surrounding holes.*
- *Develop and apply new methods to evaluate the fatigue resistance of metal alloys for high pressure fuel injectors.*
- *Provide properties data for fuel injector nozzle materials selection.*

The ORNL-Caterpillar team is using a two-pronged approach to develop appropriate fatigue and fracture testing methods. Together, they will quantify the durability of current and future developmental alloys under repetitive stressing, especially in the vicinity of holes that are equal to or smaller in diameter than a typical human hair.

Status

Using production parts provided by Caterpillar, we have demonstrated the ability to image and measure the roughness of holes in fuel injector nozzles using two measurement techniques: (a) a back-scattered electron imaging method that uses quadrupole detectors with three-dimensional (3D) reconstructive imaging software (Figure 3) and (b) optical profiling of hole cross sections using an integrated vertical scanning system.

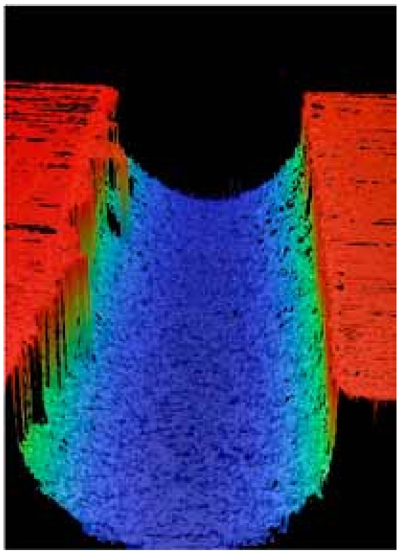

Figure 3: A 3D reconstruction of the bore of a spray hole. Hole diameter is about 200 µm.

Initial studies to evaluate the suitability of various residual stress measurement options have been conducted in ORNL's X-ray diffraction laboratory, at the ORNL High Flux Isotope Reactor, and at Brookhaven National Laboratory's National Synchrotron Light Source. Results are under evaluation.

Plans are underway to obtain promising new fatigue-resistant alloys from a U.S.-based specialty-metal producer and to compare their fatigue resistance to that of the current nozzle alloy.

This 3-year project began in July of 2008. Plans for FY 2009 include the development of specialized fatigue- and fracture-testing protocols for metal coupons that contain tiny holes.

Additional plans include further residual stress studies, and the metallurgical characterization of current and candidate nozzle alloys. Working with diesel fuel systems designers will ensure relevance of this work to the challenges presented by highpressure fuel injectors

Contacts

D. Ray Johnson
Field Technical Manager
Oak Ridge National Laboratory
(865) 576-6832
johnsondr@ornl.gov

Jerry L. Gibbs
Technology Development Manager
U.S. Department of Energy
(202) 586-1182
jerry.gibbs@ee.doe.gov

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Propulsion Materials

Thermoelectric Mechanical Reliability

Background

Successful implementation of thermoelectric (TE) devices will only be enabled if the device is designed to overcome the thermomechanical limitations (i.e., brittleness) inherent in TE materials. A TE material with a combination of low thermal conductivity, high coefficient of thermal expansion, and poor strength can readily fail in the presence of a (needed) thermal gradient, thereby preventing the exploitation of the desired TE function. This seemingly insurmountable problem can be overcome through the combined use of established probabilistic design methods developed for brittle structural components, development and use of databases with good thermoelastic and thermomechanical property data on candidate TE materials for the TE devices, and iteratively applied design sensitivity analysis.

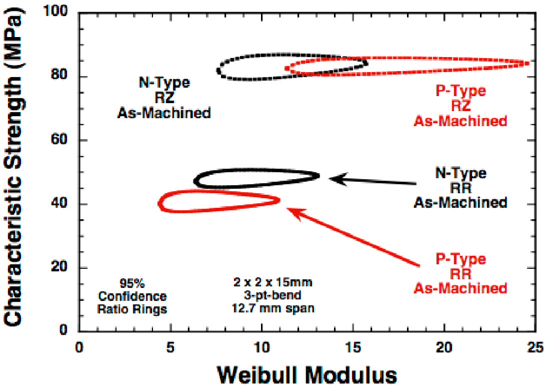
Technology

There is strong interest in the use of TE devices for potential waste heat harvesting in the transportation and industrial sectors. TE devices have been around for decades now; however, systems incorporating them tend to have relatively low efficiencies and temperature capability. Developmental TE materials with high temperature capabilities offer the potential for improved efficiencies, but their adaptation for use in devices for transportation and industrial applications has been hindered by continuing concerns over the potential for poor high temperature performance (mechanical properties). Thermomechanical modeling of TE devices provides guidance on what strengths and fatigue resistances are needed from TE materials for long-term successful operation at high temperatures.

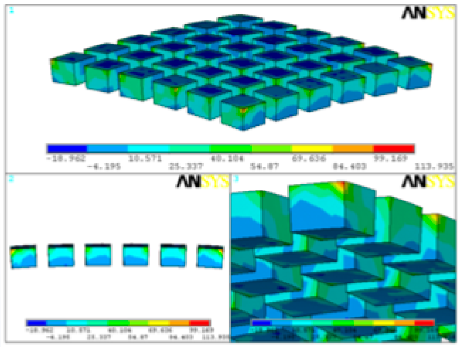
Status

This project comprises several quite distinct, but interrelated tasks. Progress on each over the past year is described below.

A database with relevant strength data on materials of interest didn't exist, so one of our initial tasks was the creation of one. We



(a)



(b)

Figure 1: (a) Measured strength distributions of TE materials. (b) Stresses in TE material legs in a 6x6 arrayed TE device.

Benefits

- *More efficient waste heat harvesting at higher temperatures.*
- *More reliable TE materials.*
- *More reliable TE devices.*

established a statistically significant strength database for a reference TE material, usable for future comparisons with new TE materials with high temperature capabilities.

To create the database, we studied fracture behavior in a reference TE material; examined strength as a function of n- and p-type materials, orientation, and temperature; and measured thermal conductivity, coefficient of thermal expansion, elastic modulus, and Poisson's ratio (Figures 1 and 2). All these data are needed for reliability analysis and design sensitivity analysis of TE devices.

A Cooperative Research and Development Agreement with a TE material and device manufacturer (Marlow Industries) was developed. We continued collaborations with an automotive end user of TE devices (General Motors).

Testing and evaluation of high-temperature-capable TE materials is occurring in FY 2009. A thermo-mechanical test system is being developed in FY 2009 to enable strength measurement of TE specimens while a thermal gradient is concurrently imposed through the specimen thickness.

(a) **(b)**

Figure 2: Uniaxial flexure (a) and biaxial flexure (b) testing of TE specimens provide needed strength data for TE device design.

Contacts

D. Ray Johnson
Field Technical Manager
Oak Ridge National Laboratory
(865) 576-6832
johnsondr@ornl.gov

Jerry L. Gibbs
Technology Development Manager
U.S. Department of Energy
(202) 586-1182
jerry.gibbs@ee.doe.gov

Propulsion Materials

Ultrahigh Resolution Electron Microscopy for Catalyst Characterization

Background

Ultrahigh resolution electron microscopy using the Oak Ridge National Laboratory's (ORNL's) aberration-corrected electron microscope (ACEM) has recently been advanced by the introduction of a unique new capability for in situ heating to allow, for example, the behavior of catalytic species to be studied as a function of specimen temperature. This development uses a microelectromechanical systems- (MEMS-) based technology introduced by Protochips Inc. (Raleigh, North Carolina), with whom we are collaborating by leveraging funding through a Work for Others-Small Business Innovation Research project. The goal of all catalyst research is to understand the processes at the atomic level by which catalytic materials evolve and degrade under conditions of use, so the new heating capability is a step towards that end. Progress has been made in developing the procedures for using in situ heating with the novel performance of the MEMS devices (called "Aduro" by Protochips; Latin for "I light on fire").

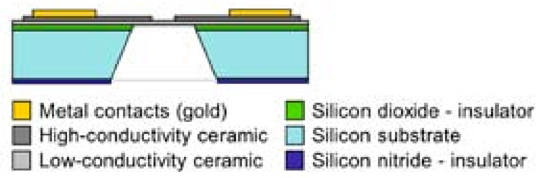


Figure 1: Schematic of baseline Aduro device.

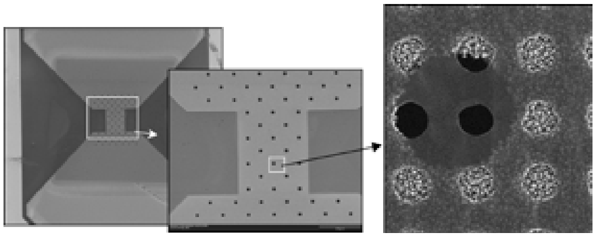


Figure 2: Cross section of Aduro heater chip. The low-conductivity ceramic heats to >1,000°C in 1 msec.

Technology

The Aduro device comprises a silicon chip with a low-conductivity ceramic membrane extending over a small (0.5 mm^2.) hole etched in the silicon (Figure 1). This membrane is patterned with 3-micron holes, over which a holey carbon film with 1-micron holes is deposited (Figure 2). The carbon film supports catalyst powder samples for study; when the ceramic is heated directly by passing a current through it. The low mass of the membrane allows it to reach 1,000°C in 1 msec and to cool just as quickly. It is highly stable because of the symmetry of the chip, and allows the full resolution of our aberration-corrected JEOL 2200FS electron microscope to be routinely achieved, even at elevated temperatures. Figure 3 shows the prototype specimen holder, with a new chip design to allow X-ray analysis with the chip at elevated temperatures in the microscope. The remarkable heating performance of the Aduro device also allows new modes of operation, which we are exploring. This includes the capability to heat a sample with the holder in the microscope's airlock chamber, at up to atmospheric pressure, in a chosen gas. This capability permits studies of catalysts in many instances under conditions nearer to "real world" conditions, adding an important dimension to our studies.

Benefits

- *Sub-ångstrom resolution microscopy provides unique information leading to fundamental understanding of how catalysts behave at the atomic level.*
- *Future work encompassing in situ gas reaction techniques via an environmental cell, developed using the Aduro techonology, to allow the kinetics and mechanisms of catalyst performance to be studied.*
- *Attraction of top catalyst researchers in the country eager to collaborate with the U.S. Department of Energy.*

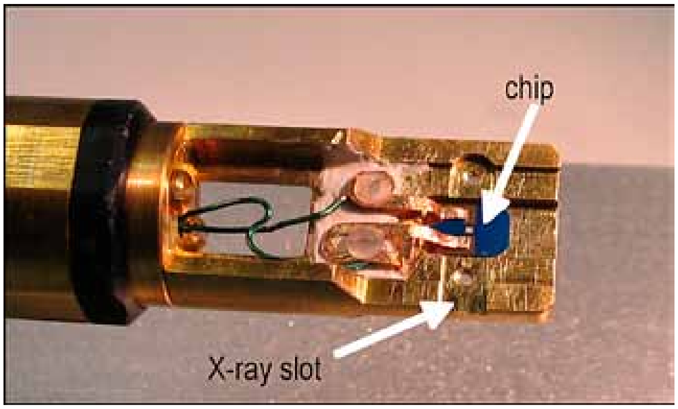


Figure 3: View of prototype heater holder showing new-style chip in place with slot cut out to allow X-rays to reach the new energy-dispersive X-ray spectroscopy (EDS) detector system on ACEM.

Status

An example of a heating experiment is shown in Figure 4, in which bimetallic gold-palladium (Au-Pd) particles are imaged at 350°, 500°, and 700°C. The Au-Pd particles originally display a core-shell structure, with a core rich in Pd (dark contast), an inner shell rich in Au (brighter contrast), and an outer shell of nearly pure Pd (darker contrast). Slow changes were noted with time at 350°C, but after a period at 500°C the composition homogenized and particles began to change shape. At 700°C, growth of one particle (A) at the expense of another (B) was seen, suggesting an Ostwald ripening mechanism. The appearance of other particles (as at the arrows), however, indicated a coalescence mechanism involving dispersed atomic species was also active.

Studies such as these offer a powerful new potential for gaining information on the behavior of catalytic materials at the atomic level, where the important mechanisms controlling performance are operative. These studies are of interest to a number of collaborators from industry, academia, and other national laboratories (e.g. Pacific Northwest National Laboratory), and we are also supporting catalyst research in the High Temperature Materials Laboratory user program, ongoing Cooperative Research and Development Agreement activities with Cummins Inc., and nanoscience programs within the U.S. Department of Energy's Office of Basic Energy Sciences, all of which provide support that allows us to leverage funding to further advance the programmatic research interests of all parties in this exciting new area of materials characterization.

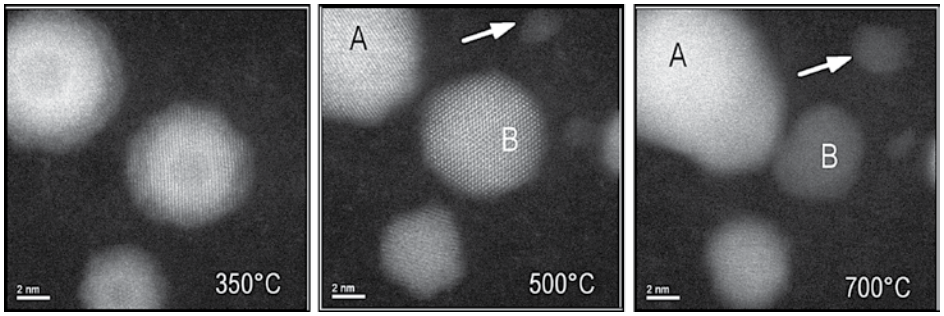


Figure 4. View of prototype heater holder, showing new-style chip in place, with slot cut out to allow X-rays to reach new EDS detector system on ACEM.

Contacts

D. Ray Johnson
Field Technical Manager
Oak Ridge National Laboratory
(865) 576-6832
johnsondr@ornl.gov

Jerry L. Gibbs
Technology Development Manager
U.S. Department of Energy
(202) 586-1182
jerry.gibbs@ee.doe.gov

Vehicle Systems

Engine and Aftertreatment Models for Integrated Systems Simulation of Hybrid and Plug-In Hybrid Electric Vehicles

Background

Improving the fuel efficiency and fuel flexibility of hybrid electric vehicles (HEVs) and plug-in HEVs (PHEVs) is critical to achieving widespread use of advanced hybrid technologies for reducing consumption of imported petroleum. Due to the complexity of these technologies, assessing the performance of HEVs and PHEVs requires an integrated systems approach to evaluate the many possible combinations of engines, fuels, energy storage systems, exhaust aftertreatment devices, etc. Thus development of an accurate, flexible set of vehicle level simulation tools has become a high priority for the Vehicle Systems activity in the Department of Energy's Office of Vehicle Technologies. Oak Ridge National Laboratory (ORNL) is contributing to this effort by providing experimental data and component models for advanced engines, emissions controls, and other key system components that can be used to address important questions about advanced powertrain technologies. The goal is to derive simulated results that accurately reflect the impact of the specific technology options on both petroleum consumption and the environment.

Technology

Currently, internal combustion engines are essential components of all car and truck drivetrains, including HEVs and PHEVs. Achieving fuel economy goals is a delicate balancing act between engine efficiency and controlling harmful emissions such as nitrogen oxides (NO_X), carbon monoxide (CO), and total hydrocarbons (THC).

The ORNL modeling team is developing computer models for simulating engines, emissions controls, and exhaust heat recovery components tailored specifically to address key questions about HEV, PHEV, and other advanced engine technologies. As much as possible, these models are physically based to maximize accuracy while capturing the fully integrated performance of drivetrains operating in standard transient drive cycles.

Status

In 2009, the ORNL Vehicle Systems modeling team made numerous systems-level simulations of HEVs and PHEVs to study the impact of lean-burn exhaust aftertreatment and advanced low-temperature combustion modes on fuel efficiency and emissions. These simulations were the first ever made by any

Benefits

- *Rapid, more accurate identification of new technological options for maximizing HEV and PHEV fuel efficiency.*
- *Improved understanding of aftertreatment needs to support use of advanced combustion engines in hybrid vehicles.*
- *More effective targeting of research and development resources at national and industrial laboratories to accelerate the elimination of barriers to broader use of HEVs and PHEVs.*

Contacts

David E. Smith
Program Manager
Advanced Vehicle Systems
Oak Ridge National Laboratory
(865) 946-1324
smithde@ornl.gov

Lee Slezak
Technology Development Manager
U.S. Department of Energy
(202) 586-2335
lee.slezak@ee.doe.gov

national laboratory to reveal the impacts of these technologies on HEV fuel efficiency and emissions under realistic drive cycle conditions. One key contribution from ORNL in this area has been the development of algorithms for accurately simulating the transient temperature and emissions profiles produced by engines operating under highly transient drive cycle conditions where aftertreatment catalysts are subjected to repeated engine starts and stops. An example of our success in simulating cold start engine transients is illustrated in Figure 1, which compares results from simulations using our Powertrain System Analysis Toolkit (PSAT) with experimental data.

Under repeated engine start-up and shutdown, the performance of both lean-burn exhaust aftertreatment devices and conventional three-way catalysts (TWCs) can be significantly degraded. This degradation can, in turn, result in failure to meet federal emissions regulations or increases in fuel consumption to maintain emissions compliance. Using the transient engine simulation capability, ORNL has also been able to quantify the expected impact of replacing conventional gasoline engines with diesel engines in HEVs and PHEVs. As shown in Figure 2, the fuel efficiency penalty associated with maintaining NO_X control for a diesel PHEV significantly reduces the potential fuel economy advantage of the diesel engine over a gasoline engine.

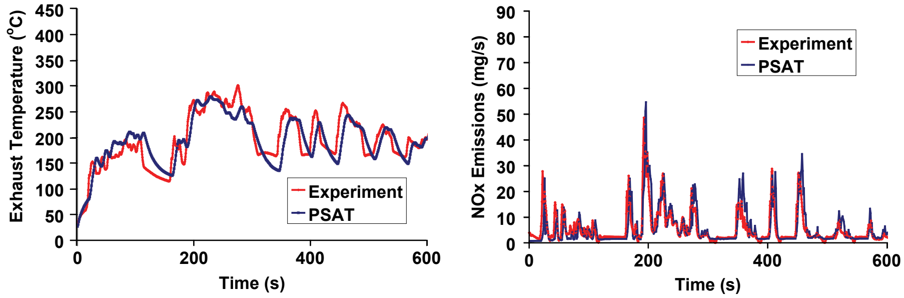


Figure 1: Comparison of measured and predicted engine exhaust temperature and NO_X emission transients for a Mercedes A-170 diesel vehicle after a cold start and operating over a standard Urban Dynamic Driving Schedule (UDDS). The type of engine in this vehicle is similar to those which might be used for diesel-powered HEVs and PHEVs. Hybrid operating strategies typically involve numerous engine starts and stops, which greatly affect the transient exhaust properties. In this case the predicted cycle-average fuel economy of 40.4 mpg compared very favorably with the measured value of 40.3 mpg. Predicted cumulative emissions of CO, THC, NO_X, and particulates all fell within 1% of the measured values.

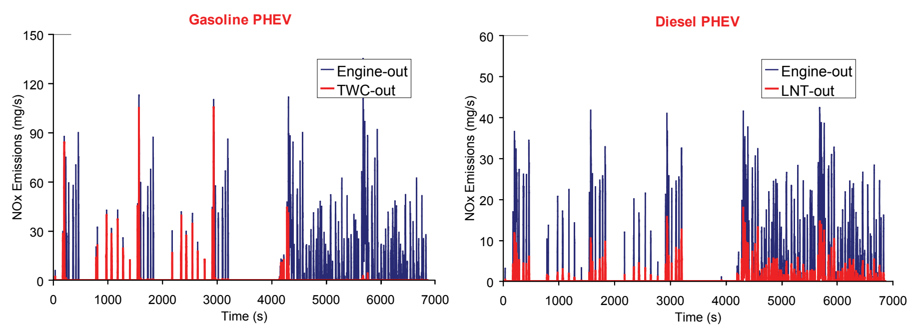


Figure 2: Comparison of simulated NO_X emissions from Prius-type gasoline and diesel PHEVs operating over five consecutive UDDS cycles. Even though the overall fuel economy of the diesel PHEV is about 3% better than the gasoline PHEV (which includes accounting for the energy density differences between gasoline and diesel fuel), about half of the diesel's potential efficiency advantage is lost in maintaining NO_X emissions control [lean NO_X trap (LNT)]. The gasoline PHEV is able to maintain NO_X control with a TWC that does not require excess fuel to function.

A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.