


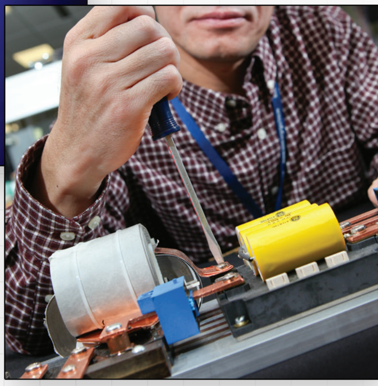

Sustainable Transportation Program

Annual Report
Fiscal Year 2009

Supporting
Vehicle Technologies Program
Office of Energy Efficiency and Renewable Energy
U.S. Department of Energy

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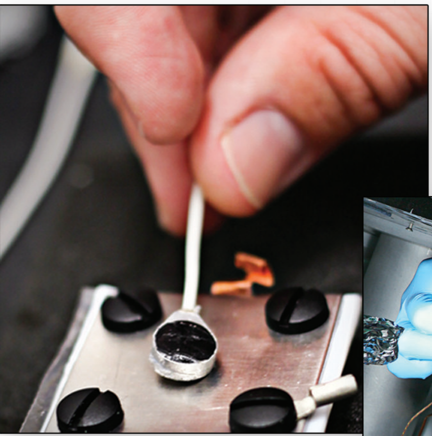
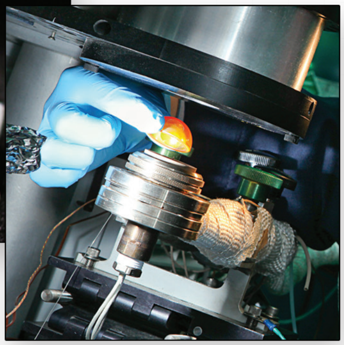

Oak Ridge National Laboratory

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Contents

Guide to Acronyms Used

3G	third generation
ac	alternating current
ACC	Automotive Composites Consortium
ACEM	aberration-corrected electron microscope
ACERT	advanced combustion emissions reduction technology
AE	acoustic emission
Al	aluminum
Al2O3	aluminum oxide/alumina
AN	acrylonitrile
APEEM	Advanced Power Electronics and Electric Machines
APF	active power filter
Au	gold
AVS	Advanced Vehicle Systems
BNL	Brookhaven National Laboratory
BTE	brake thermal efficiency
C-	carbon-coated (e.g., cathode materials: C-LiFe0.6Mn0.4PO4)
CF-A	aerospace grade carbon fiber
CF-C	commodity grade commercial carbon fiber
CF-T	textile grade carbon fiber (made from textile-based precursors)
CFTC	Carbon Fiber Technology Center
CO	carbon monoxide
CR	compression ratio
CRADA	Cooperative Research and Development Agreement
CRC	Coordinating Research Council
CSI	current source inverter
dc	direct current
DCGenT	Duty Cycle Generation Tool
DOC	diesel oxidation catalyst
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
DPF	diesel particulate filter
E85	85% ethanol : 15% gasoline blend
E-cell	environmental cell
EERE	Office of Energy Efficiency and Renewable Energy
EGR	exhaust gas recirculation

EIVC	early intake valve closing
EOL	end-of-life
EPA	U. S. Environmental Protection Agency
EPFL	École Polytechnique Fédérale de Lausanne
EV	electric vehicle
FACE	Fuels for Advanced Combustion Engines
FCV	fuel cell vehicle
FEERC	Fuels, Engines, and Emissions Research Center
FeOX	iron oxide
FFV	flexible-fuel vehicle
FIB	focused ion beam
FY	fiscal year
GaN	gallium nitride
GC	gas chromatography
Gen 1	first generation
Gen 2	second generation
GHG	greenhouse gas
GM	General Motors
H2	hydrogen
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
ICME	Integrated Computational Materials Engineering
IGBT	insulated gate bipolar transistor
IMEP	indicated mean effective pressure
IR	infrared
ISFC	indicated specific fuel consumption
JFET	junction field effect transistor
KAT	Knoxville Area Transit
LAST	lead-antimony-silver-tellurium
LCCF	low cost carbon fiber
Li	lithium
Li1–XFePO4	lithium iron phosphate
LIF	laser-induced fluorescence

LIVC	late intake valve closing
LM	Lightweighting Materials
LNT	lean NOX trap
MCMB	mesocarbon microbead
MEMS	microelectromechanical systems
MESG	Motorola Energy Systems Group
Mg	magnesium
MOU	Memorandum of Understanding
MPa	megapascal
MSTD	Materials Science and Technology Division
MSU	Michigan State University
MTDC	Medium Truck Duty Cycle
NDE	nondestructive evaluation
NH3	ammonia
NO	nitric oxide
NO_x	oxides of nitrogen/nitrogen oxide
NREL	National Renewable Energy Laboratory
NRSF2	Second Generation Neutron Residual Stress Mapping Facility
NSF	National Science Foundation
NSLS	National Synchrotron Light Source
NTRC	National Transportation Research Center
OBD	onboard diagnostics
OBP	Office of Biomass Program
ORC	organic Rankine cycle
ORNL	Oak Ridge National Laboratory
OSU	Ohio State University
P4	programmable powdered preform process
PA66	polyamide (nylon) 6,6
PAN	polyacrylonitrile
PbS-PbTe	lead-sulfide–lead-telluride
PCCI	premixed charge compression ignition
Pd	palladium
PE	power electronic
PHEV	plug-in hybrid electric vehicle
PM	particulate matter
PNNL	Pacific Northwest National Laboratory
PSAT	Powertrain System Analysis Toolkit
PSF	performance shaping factors

Pt	platinum
PVdF	polyvinylidene fluoride
PWM	pulse-width modulation
PZT	lead zirconate titanate
R&D	research and development
Re	rhenium
RFS	renewable fuel standard
RG	regular gasoline
SCR	selective catalytic reduction
SEI	solid-electrolyte interphase
SEM	scanning electron microscope
SiC	silicon carbide
SIMS	secondary ion mass spectrometry
SPICE	Simulation Program with Integrated Circuit Emphasis
SRIM	structural reaction injection molding
SwRI	Southwest Research Institute
TiAl	titanium aluminide
TMAC	test machine for automotive crashworthiness
TWC	three-way catalyst
UL	Underwriters' Laboratory
ULSD	ultralow-sulfur diesel
VCR	variable compression ratio
VSI	voltage source inverter
VTP	Vehicle Technologies Program
WBG	wide bandgap
WEG	water-ethylene glycol
WFO	Work for Others
WGSR	water-gas shift reaction
XRD	x-ray diffraction
Zn	zinc

Introduction

The Sustainable Transportation Program (STP) at Oak Ridge National Laboratory (ORNL) encompasses research and development (R&D) activities in support of the Vehicle Technologies Program (VTP), Biomass Program, and Fuel Cell Technologies Program within the U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE); as well as complementary R&D and analyses for the U.S. Department of Transportation and its modal agencies. This report documents ORNL's FY 2009 R&D in support of the VTP mission, which constitutes the largest segment of the Sustainable Transportation Program as shown in Figure 1. The VTP mission is "to develop more energy-efficient and environmentally friendly highway transportation technologies (for both cars and trucks) that will enable America to use significantly less petroleum and reduce greenhouse gas (GHG) emissions while meeting or exceeding drivers' performance expectations and environmental requirements."[1] The VTP mission supports national goals relating to energy security and GHG reductions.

Table 1 illustrates the flow down 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 2009 R&D support of the VTP performance goals is described in more detail beginning on page 8.

Much of the ORNL STP R&D is performed in partnership with industry, primarily under two umbrella collaborative arrangements between DOE and industry. The FreedomCAR and Fuel Partnership comprises DOE, the U.S. Council for Automotive Research,[2] and five energy companies. The FreedomCAR and Fuel Partnership focuses on high-risk, precompetitive research "needed to develop the component and infrastructure technologies necessary to

Table 1. Flow Down of National Goals to VTP Performance Measures[1].

Goals	Energy Security and Greenhouse Gas Reductions				
Stategies	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/ renewable 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/ renewable fuel blends	Reduce high-energy battery cost
	Capture and use waste heat		Reduce cost of power electronics and motors		Field demonstration of plug-in hybrid vehicles

1 Office of Chief Financial Officer. February 2010. FY 2011 Congressional Budget Request. DOE/CF-0046 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.

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 power-train manufacturers, DOE, U.S. Department of Defense (DOD), U.S. Department of Transportation (DOT), and U.S. Environmental Protection Agency (EPA). The partnership's objective is to "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

Direct Funding

The Sustainable Transportation Program received about $48 M in new budget authority from VTP in FY 2009 (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 $44.3M 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 about $10.9M to external subcontracts with industry, universities, and consultants.

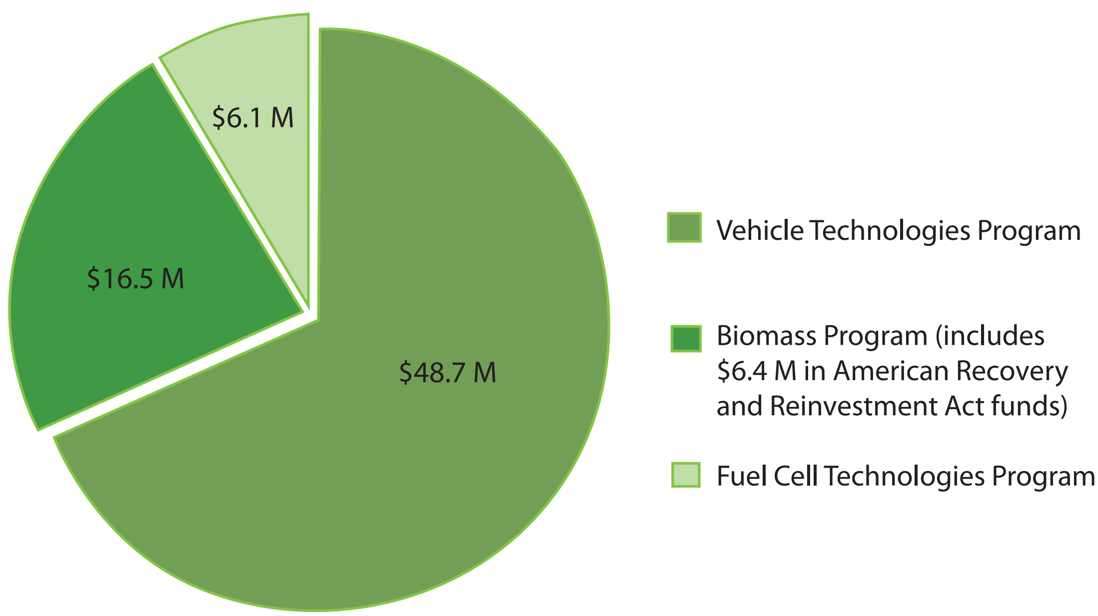

Figure 1. FY 2009 New Budget Authority by Activity

3 FreedomCAR and Fuel Partnership. March 2006. Partnership Plan. Available at http://www1.eere.energy.gov/vehiclesandfuels.

4 21st 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 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.

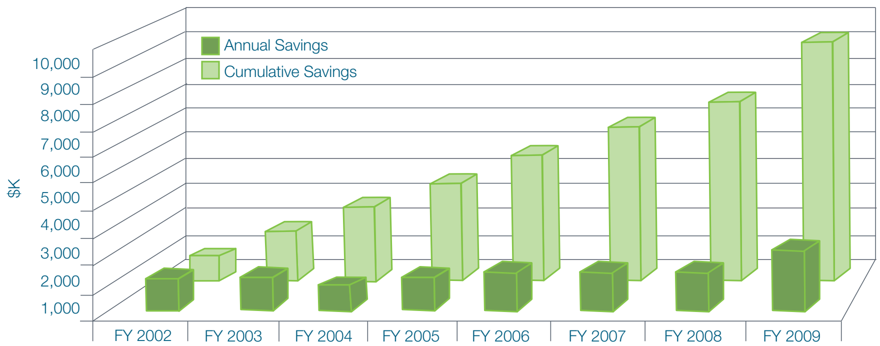

Figure 2. Cumulative overhead savings of nearly $9,000K have been applied to VTP-sponsored R&D at NTRC.

Sponsored Research — Work for Others

Sustainable 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 2009 WFO is shown in Figure 3.

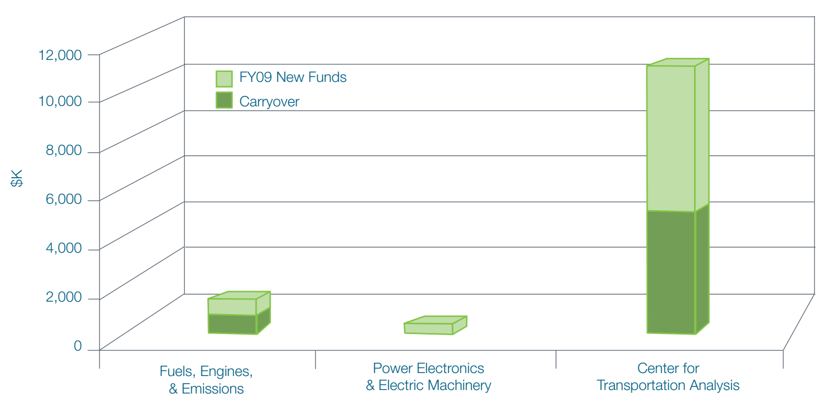

Figure 3. FY 2009 funding for research sponsored by industry, academia, and other federal agencies.

5 Activities primarily conducted at the NTRC are advanced power electronics, education, safety codes and standards, technology validation, legislative and rulemaking, vehicle technologies deployment, combustion and emission control R&D, solid state energy conversion, advanced petroleum based fuels, non-petroleum fuels and lubricants, and vehicle and systems simulation and testing.

Program Metrics

Patents

Sustainable Transportation Program research staff members filed 17 invention disclosures and had 5 patent applications published in FY 2009. Seven patents based on previous filings were awarded and issued during the period (Table 2).

Table 2. Invention Disclosures, Patent Applications, and Patents Awarded in FY 2009

Inventors	Invention Disclosures, Patent Applications, and Patents
J. Hsu	Patent 7,518,278—High Strength Undiffused Brushless Machine and Method Patent 7,514,833—Axial Gap Permanent-Magnet Machine with Reluctance Poles and PM Element Covers Invention Disclosure 2227—Two-Parallel-Flux-U-Motors Patent 7,560,847—Two-Stage Eutectic Metal Brushes Patent 7,550,892—High Slot Utilization Systems for Electric Machines
R. Wagner, C. Daw, J. Green, and K. Edwards	Patent 7,431,011—Method and Device for Diagnosing and Controlling Combustion Instabilities in Internal Combustion Engines Operating in or Transitioning to Homogeneous Charge Combustion Ignition Mode
R. DeVault	Patent Application 12/137,744—Self-Learning Control System for Plug-In Hybrid Vehicles
J. Parks II and W. Partridge Jr.	Patent Application 12/491,781—Optical Backscatter Probe for Sensing Particulate in a Combustion Gas Stream
C. Maxey, S. Lewis, J. Parks II, and W. Partridge Jr.	Patent Application 12/326,233—Optically Stimulated Differential Impedance Spectroscopy
R. Graves, B. West, S. Huff, and J. Parks II	Patent 7,469,693—Advanced Engine Management of Individual Cylinders for Control of Exhaust Species
F. Paulauskas, T. White, and D. Sherman	Patent 7,534,854—Apparatus and Method for Oxidation and Stabilization of Polymeric Materials
A. Naskar, F. Paulauskas, C. Janke, and C. Eberle	Invention Disclosure 1973—Novel Compositions for PAN Based Carbon Fiber Precursors
P. Menchhofer, F. Baker, and F. Montgomery	Invention Disclosure 2060—Carbon Nanotubes Grown on Bulk Materials and Methods for Fabrication
F. Baker	Invention Disclosure 2187—Production of Composite Cellulose/Carbon Fiber Filters for HVAC Systems
C. Eberle, C. Janke, V. Kunc, A. Naskar, F. Paulauskas, M. Abdallah, and S. Ozcan	Invention Disclosure 2212—Carbon Fiber Composites with Enhanced Compression Strength
C. Eberle, C. Janke, A. Naskar, F. Paulauskas, and C. Warren	Invention Disclosure 2239—Polyolefin Based Flame Retardant Material
F. Paulauskas and A. Naskar	Invention Disclosure 2241—Extremely Flame Retardant Material from PAN Fibers via Advanced Oxidation
F. Baker, C. Eberle, J. Mielenz, A. Naskar, R. Norris, and J. Pickel	Invention Disclosure 2293—Genetically Modified Lignin-Derived Bio-Thermoplastics for Polymer Matrix Composites
J.-Y. Wang	Invention Disclosure 1958—Apparatus for Prestress-Straining Rod-Type Specimens in Tension for In Situ Passive Fracture Testing Invention Disclosure 1992—Apparatuses for Prestressing Rod-Type Specimens in Torsion for In Situ Passive Fracture Toughness Testing in an Extremely High-Pressure Environment of Hydrogen

Inventors	Invention Disclosures, Patent Applications, and Patents
J.-Y. Wang	Patent Application DOE S-115,037—Apparatus for In Situ Materials Fatigue Testing in Pressurized Hydrogen Environment at Ambient or Moderate Temperatures Under Closed-Loop Controlled, Fully-Reversed Cyclic Loading Being Actuated by the Active Hydrogen Gas in the Chamber
J. Qu and S. Dai	Invention Disclosure 200902257—Hybrid Highly Ordered Nanostructured Materials for Energy Harvesting and Storage
C. Eberle	Invention Disclosure 2168—Aerodynamic Control of Wind Turbine Blades
C. Eberle, A. Naskar, F. Paulauskas, and J. Rivard	Invention Disclosure 2322—Precursor Materials and Fiber Formation for Ultra High Strength Carbon Fibers
C. Eberle, G. Mackiewicz-Ludkta, G. Ludkta, A. Naskar, F. Paulauskas, and J. Rivard	Invention Disclosure 2323—Conversion of Ultra High Performance Carbon Fibers
C. Narula and C. Daniel	Invention Disclosure 2234—Methods of Making Solid Lithium Ion Conducting Electrolytes
C. Daniel, N. Dudney, K. Rhodes, and S. Kalnaus	Invention Disclosure 201002367—Copper Coated Mylar Window for In-Site XRD of Lithium Battery Materials
R. Wiles, A. Wereszczak, C. Ayers, and K. Lowe	Patent Application 12/400,081—Direct Cooled Power Electronics Substrate
C. Narula, R. Bhave, and B. Bischoff	Invention Disclosure 2313—Inorganic Separators

Awards and Professional Recognition

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

Table 3. Significant Honors, Awards, and Professional Recognitions During 2009

Name	Award or Recognition
W. Partridge Jr., J. S. Choi, J. Storey, and S. Lewis	Federal Laboratory Consortium Award (FLC) for Excellence in Technology Transfer for the commercialization of the Smaci-MS.
B. West	SAE Lloyd L. Withrow Distinguished Speaker Award
W. Partridge Jr.	ORNL Distinguished Engineer Award
R. Graves	Selection to the National Academy of Sciences Committee on Medium Heavy Truck Fuel Economy
R. Boeman, R. Graves, and L. Marlino	Judge for the PACE Awards
W. Partridge Jr.	Keynote Speaker, North American Catalysis Society Meeting
C. D. Warren	2008 Outstanding Leadership Team Award presented by the Society of Plastics Engineers Automotive Division for working to advance plastics in automotives
F. Baker	Fellow of the American Carbon Society
F. Baker	Graffin Lecturer for the American Carbon Society
E. Lara-Curzio	Fellow of the American Ceramic Society
E. Lara-Curzio	2009 Arthur Federick Greaves-Walker Award from the American Ceramic Society and the National Institute of Ceramic Engineers

Name	Award or Recognition
E. Lara-Curzio	Counselor, Engineering Ceramics Division of the American Ceramic Society
J-A. Wang and E. Lara-Curzio	2009 R&D 100 Award recipient for the invention of the MELCOT: Methodology for Estimating the Life of Power Line Conductor-Connector Systems Operating at High Temperatures
J. Qu	John Bollinger Outstanding Young Manufacturing Engineer from the Society of Manufacturing Engineers.
H.-T. Lin	Lee Hsun Lecture Award, Chinese Academy of Science
S. Sokhansanj	Leadership In Agricultural Engineering related to Bioenergy from the Association of Agricultural Engineers
D. Greene	Energy Efficiency Hall of Fame by the Alliance to Save Energy
D. Greene	Science Communicator of the Year Award by UT-Battelle
K. Rhodes	2nd place - Excellence in Student Research by ASM Materials for Megawatts
G.-J. Su, L. Tang, and Z. Wu	2009 Best Paper Award at the IEEE Vehicle Power and Propulsion Conference for their paper entitled “Extended Constant-Torque and Constant-Power Speed Range Control of Permanent Magnet Machine Using Current Source Inverter.”
M. Shen, F. Z. Peng, and T.L.M.	2009 IEEE Power Electronics Society Transaction Prize Paper Award for authorship of “Multilevel DC-DC Power Conversion System with Multiple DC Sources.”
C. Daniel	2009 ORNL Science and Technology Early Career Award for Engineering Accomplishments for Catalyzing Research in Energy Storage at ORNL through Technical Insights, Strategic Vision, and Team Building and for Laying the Groundwork for Substantial Funding Increase by Articulating a Specialized and Unique Research and Development Program
A. Wereszczak	Chair, Engineering Ceramics Division of the American Ceramic Society
A. Wereszczak	Richard M. Fulrath Award from the American Ceramic Society’
P. Maziasz and D. R. Johnson	Federal Laboratory Consortium Award (FLC) for Excellence in Technology Transfer for the commercialization of CF8C-Plus Stainless Steel

Publications and Presentations

ORNL R&D staff produced more than 439 papers and presentations on VTP-sponsored R&D during FY 2009, a 131% increase over FY 2008. Figure 4 provides a breakdown by type of publication or presentation for VTP subprograms.

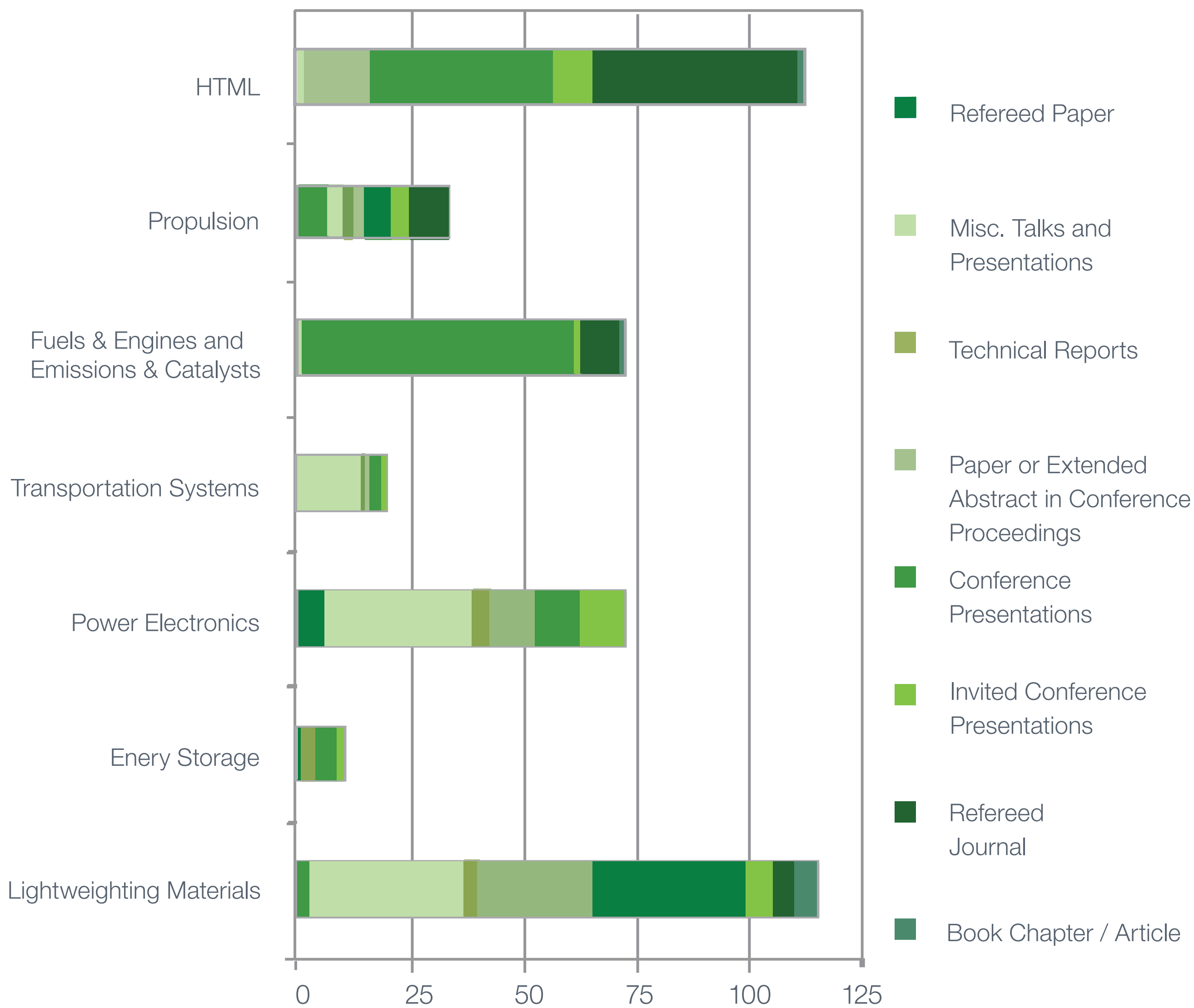

Figure 4. FY 2009 Publications and Presentations.

Program Summaries

Advanced Power Electronics and Electric Machines

The Power Electronics and Electrical Power Systems Research Center conducts high-risk, long-term research; evaluates hardware; and provides technical support to the DOE VTP Advanced Power Electronics and Electric Machines 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, thereby meeting VTP goals. These activities 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).

Key Technical Accomplishments

Direct water-cooled power electronics substrate

- Simulated various designs using thermal and mechanical finite element analysis.
- Fabricated direct bonded copper substrates (copper clad, plated, and dies attached with ribbon bonds).
- Fabricated test fixture and completed flow tests on prototypes using water-ethylene glycol at various temperatures, including 105°C.
- Validated models based on comparisons between experimental results and modeling results.

New class of switched reluctance motors

- Assessed feasibility of various design techniques and selected a preferred methodology.
- Developed and simulated hardware and software solutions for reducing torque ripple and acoustic noise.
- Demonstrated that for low and moderate torque levels, near zero torque ripple could be achieved.
- Demonstrated the potential for increased power density via continuous conduction control.
- Developed two universal dynamic simulators (crucial for structural and acoustic noise modeling).
  - Parametric simulator: efficient means to optimize control and design parameters.
  - Finite element analysis simulator: highly accurate, but more suited for known control and design conditions.

Novel flux coupling machine without permanent magnets

- Completed the development of analytical tools used for the design of the novel flux coupling machine without permanent magnets.
- Performed electromagnetic simulations for motor performance and mechanical finite element analysis for rotational stress loading for design optimization.

Wide bandgap materials

- Acquired, tested, and characterized silicon carbide (SiC) junction field effect transistors (JFETs), metal-oxide semiconductor field effect transistors, and diodes.
- Completed evaluation of a 10 kW SiC JFET-based inverter.
- Completed the feasibility study of an air-cooled 55 kW inverter design.

Active filter approach to the reduction of the dc link capacitor

- Built a simulation model of a traction drive system to establish the performance requirements for an active power filter (APF).

- Analyzed the parameter dependence of the APF and the underlying barriers of this method.
- Demonstrated the tradeoff in losses against the reduction in dc bus capacitance through the use of an APF.

High temperature, high voltage fully integrated gate driver circuit

- Designed and taped out the third generation (3G) gate driver circuit, which has current drive strength of more than 5 A at room temperature.
- Optimized design by making some of the critical functional blocks in the 3G gate driver circuit temperature insensitive.
- Incorporated multiple voltage regulator circuits in the gate driver chip.
- Integrated short-circuit protection, undervoltage lockout, and thermal shutdown circuitries with the core gate driver circuit.

Current source inverter for HEVs and FCVs

- Derived analytical equations for computing the average losses of insulated gate bipolar transistors (IGBTs) and diodes in the current source inverter (CSI) topology.
- Completed a custom IGBT module design for the CSI switch leg using Infineon IGBT and Semikron diode chips rated with maximum junction temperature of 175°C.
- Completed a design for a 55 kW CSI for operation with a 105°C coolant using the custom IGBT modules. The total capacitance is 390 µF. Estimated IGBT and diode junction temperatures are 148.2 and 134.1°C, respectively, which are well within the safe operating region.
- Designed and fabricated digital signal processors and gate drive boards for operation in the 105°C coolant environment using components rated in the automotive temperate range of –40 to 125°C.

Using the traction drive power electronics system to provide plug-in capability for PHEVs

- Designed, fabricated, and successfully tested a HEV power electronics system prototype consisting of a 55 kW motor inverter and a 30 kW generator inverter for operation as a battery charger and mobile power generator (Figure 5).
  - Attained a maximum charging efficiency greater than 95% with a 120 V input and greater than 98% with a 240 V input.
  - Attained a grid current harmonic distortion factor of less than 9% at 120 V input and less than 7% at 240 V input at rated power during charging operation.
  - Attained a maximum efficiency of 80% with a 120 V output in engine-powered generation mode.
  - Attained a maximum efficiency of 97% at 240 V output and 94% at 120 V output in battery-powered generation mode.

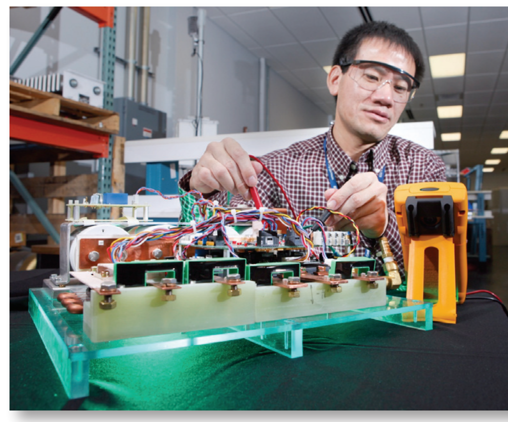

Figure 5. Gui-Jia Su testing an HEV traction drive inverter system that can provide bidirectional plug-in battery charging capability.

Segmented drive system with a small dc bus capacitor

- Validated the segmented drive concept through a simulation study.
  - Achieved more than 65% reduction in capacitor ripple current compared with the standard inverter configuration.
  - Achieved 80% reduction in battery ripple current.
  - Achieved 70% reduction in dc bus ripple voltage.
  - Achieved 50% reduction in motor ripple current.
  - Completed a conceptual design for a 55 kW prototype.

Benchmarking competitive technologies

- Conducted end-of-life (EOL) assessments to find and explore any detrimental impacts sustained over the life of a 2004 Toyota Prius.
- Compared observations from EOL assessments to those made during original benchmarking of the 2004 Prius.
- Determined that subcomponents of the 2004 Toyota Prius sustained no substantially negative impacts.
- Conducted preliminary design/packaging studies of the 2010 Prius power control unit and electrically controlled variable transmission, and noted significant differences with respect to the 2004 Toyota Prius.

Materials and Processing for Energy Storage Devices and Systems

The ORNL Materials Science and Technology Division (MSTD) conducts fundamental and applied materials research for basic energy sciences programs and a variety of energy technologies, including energy efficiency, renewable energy, transportation, conservation, fossil energy, fusion energy, nuclear power, and space exploration. In support of the EERE VTP, MSTD conducts applied research and development on materials processing for energy storage devices in partnership with major battery developers and chemical suppliers such as A123 Systems Inc., Johnson Controls, Dow Kokam, Porous Power Technologies, Planar Energy Devices, other organizations such as the Michigan Economic Development Corporation. The research focuses on high yield, low cost production of energy storage devices, a substantial increase in quality control procedures, and high-risk, long-term research and development on intercalation and degradation mechanisms of batteries.

Lithium ion batteries are currently the leading contenders to power electric vehicles (EVs). However, safer, more efficient, batteries with a longer life are needed. Battery life is limited by the process of degradation of electrode materials with repeated charging and discharging. During battery operation, lithium ions are shuttled between cathode and anode when the battery is being charged and discharged. Degradation mechanisms are related to the development of internal stresses in electrode particles due to repeated lithium insertion and removal, development of solid-electrolyte interphase (SEI) layers, and other microscopic developments in the cells. Stresses can result in cracks in and fracture of particles. SEI layers reduce the amount of lithium in cells. An understanding of these mechanisms in different electrode compounds will lead to the understanding of lifetime limitations and guidance for microstructural design of advanced electrodes (Figure 6).

Figure 6. Inspection of electrode material in glove box.

Key Technical Accomplishments

Materials processing for energy storage devices

- Increased visibility in industrial sector.
- Developed new industrial partnerships with battery developers and chemical suppliers.
- Implemented new coating line for experimental work.

Modeling battery degradation mechanisms

- Successfully started new collaboration with University of Michigan to study the mechanical side of battery degradation mechanisms.
- Micromachined electrodes fabricated for individual charge-discharge behavior investigations and development of intercalation models and stress and strain relationships.
- Initiated in situ characterization of micromachined electrodes (Figure 7).

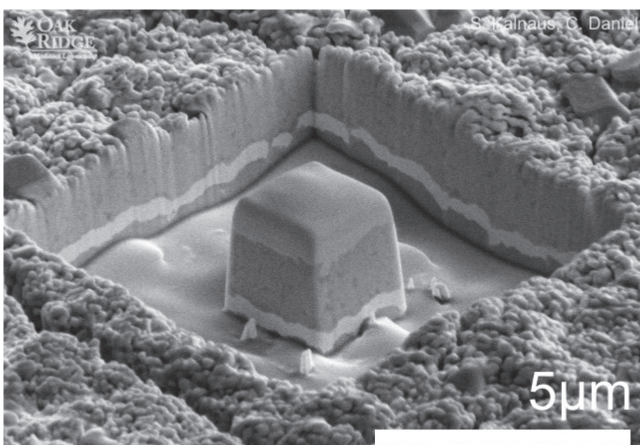

Figure 7. Micromachined electrode for electrochemical cycling.

Acoustic emissions for studying mechanical degradation of electrodes during cycling

- Completed development of acoustic emission spectroscopy to analyze degradation of electrodes in situ (Figure 8).
- Started x-ray and neutron diffraction studies on electrode materials.
- Started in situ optical microscopy development for electrode materials.
- Obtained critical size limitations for silicon electrode particles.

Figure 8. Mounting of battery cell for in situ acoustic emission spectroscopy and x-ray diffraction.

In situ microscopy

- Completed liquid transmission electron microscopy holder development for liquid cells.
- Started electrochemical cell development

Long living polymer electrolytes

- Completed surface hardening of polymer electrolytes to theoretical limit of dendrite penetration.
- Started conductivity analysis and further battery integration.

Fuels Technology and Advanced Combustion Engines

The ORNL Fuels, Engines, and Emissions Research Center (FEERC), located at NTRC, conducted R&D for multiple VTP subprograms in 2009, including Advanced Combustion Engines, Fuel Technologies, Vehicle Systems, Propulsion Materials, Clean Cities, 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, seven private sector firms plus other federal agencies sponsored R&D at FEERC in FY 2009.

FEERC staff members are highly engaged in supporting FreedomCAR and 21st Century Truck Partnership programmatic activities such as the Advanced Combustion and Emission Control technical team, the Diesel Cross-Cut Team, and the 21st Century Truck "Lab Council." ORNL, as part of a coordinating subcommittee of industry, government, and academic representatives, provides leadership of the Cross-Cut Lean Exhaust Emissions Reduction Simulations activity, an R&D focus project of the Diesel Cross-Cut Team. In fuels utilization, FEERC staff members have worked with industry, the National Renewable Energy Laboratory (NREL), and EPA to carry out tests of intermediate ethanol blends on legacy vehicles, which is a strategic component of satisfying the biofuels utilization target of the Energy Independence and Security Act. The Intermediate Ethanol Blends Test Program is cosponsored by VTP and the Office of Biomass Programs (OBP). FEERC staff members also participate in Coordinating Research Council (CRC) working groups.

Key Technical Accomplishments

Compound-cycle light duty diesel yields new efficiency level (Joule milestone achieved)

ORNL researchers developed and demonstrated an organic Rankine cycle (ORC) to convert exhaust heat to electrical power on a light duty diesel engine (Figure 9). The ORC generated more than 2.9 kW of net electrical power in recent experiments. In combination with a conservative but achievable brake thermal efficiency (BTE) of 42.3% for the engine (this same engine reached 43% in FY 2008), this yields a total BTE of 44.1%. Simulations indicate the potential of generating enough power from the ORC for a combined 45% BTE, which is the 2010 FreedomCAR light duty engine efficiency target. The technical path has been grounded in an improved understanding of thermodynamic loss mechanisms and has exploited improvements in combustion, thermal energy recovery, fuels, and lubricants.

Figure 9. Organic Rankine bottoming cycle major components.

Systems approach makes use of advanced combustion to lower fuel penalties for active emissions control

During FY 2009, two experimental engine studies were completed to quantify the potential fuel efficiency benefits of low temperature combustion modes integrated with aftertreatment systems: the benefits of low oxides of nitrogen (NO_X) emissions from premixed charge compression ignition (PCCI) on lowering the fuel penalty from lean NO_X trap (LNT) regeneration were defined, and lower fuel penalties for desooting of the diesel particulate filter (DPF) were demonstrated due to lower particulate emissions from PCCI. Advanced combustion operation in combination with a diesel oxidation catalyst (DOC), DPF, and LNT was used to demonstrate improvements in the engine-system efficiency of a light duty diesel engine for speed/load conditions consistent with light duty drive cycles.

New diagnostic method for fuel dilution in oil licensed to private sector

An invention, known as "Laser-Induced Fluorescence Fiber Optic Probe Measurement of Oil Dilution by Fuel," was licensed to Da Vinci Emissions Services. The technology uses fluorescence spectroscopy to determine the amount of fuel dilution in engine oil, which can occur as fuel-efficient engines are operated in advanced combustion modes to meet increasingly lower emissions regulations (Figure 10). The oil-dilution diagnostic grew out of a CRADA partnership between ORNL and Cummins Inc. With this license agreement, engine and automotive companies will have a private sector entity to go to for this instrument, expanding the benefits from the CRADA to the world at large.

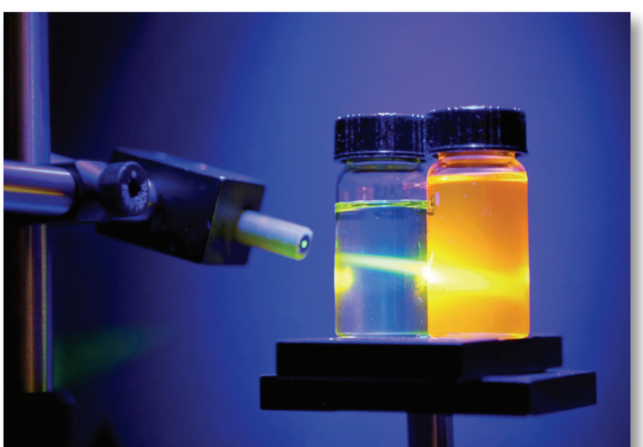

Figure 10. Fuel-in-oil measurement principle is shown here. Laser induces fluorescence response in fuel that is doped with a dye.

New methods characterize ammonia use in hybrid LNT+SCR emission control system

Integration of LNT with selective catalytic reduction (SCR) technology is one of the most advanced high-potential NO_X control systems. ORNL characterized the complex ammonia (NH3) formation and use processes in an LNT+SCR emission control system on a light duty diesel engine using a unique ultraviolet adsorption spectroscopy technique to measure NH3, NOx, and hydrocarbons directly in exhaust (Figure 11). Ammonia storage and subsequent use during low temperature idle periods may have potential for fuel and/or emission control cost savings. An original equipment manufacturer has expressed interest in collaborative work.

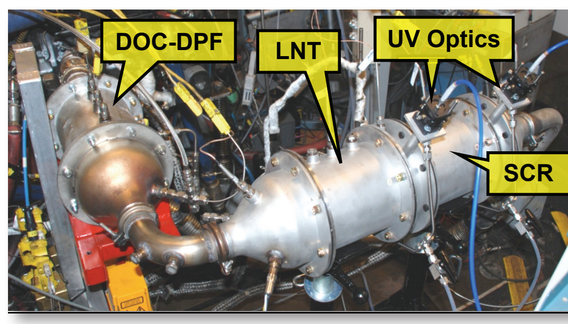

Figure 11. Combined SCR/LNT DPF emission control system integrated with a light duty diesel engine.

Intermediate Ethanol Blends Test Program

ORNL is collaborating with NREL on this DOE VTP-OBP program. Progress in the past year includes the following:

- A report detailing the results of vehicle and small engine studies on midlevel ethanol blend effects was prepared and published in October 2008, released publicly, and announced by Secretary Bodman in conjunction with rollout of the National Biofuels Action Plan. An updated report, jointly published by ORNL and NREL, was issued by NREL in February 2009.

- A vehicle aging project at Southwest Research Institute (SwRI), conducted with CRC, was officially kicked off in October 2008 to age matched vehicle sets on midlevel ethanol blends (contract was placed in FY 2008). In less than 1 year, more than 20 vehicles have been purchased, emissions tested, and instrumented, and nearly 1 million test miles have been accrued on mileage accumulation dynamometers (Figure 12). More than 40,000 gallons of test fuel have been purchased. A second parallel contract to expand and accelerate the effort was placed with Transportation Research Center in March 2009, and 12 vehicles have been purchased, instrumented, and emissions tested.

Figure 12. Mileage accumulation vehicle dynamometers at SwRI used to age cars on intermediate ethanol blends.

Fuel property effects on engine efficiency and emissions performance

- The first publicly-available data from the use of the FACE (Fuels for Advanced Combustion Engines) diesel fuels in engine studies were presented. The effect of fuel properties on homogeneous charge compression ignition (HCCI) and PCCI were explored in a single-cylinder engine and a multicylinder light duty diesel engine, respectively. The single-cylinder experiments showed the importance of both cetane number and fuel volatility on engine efficiency for pure HCCI operation. The second study using a production-like light duty diesel engine operating in PCCI modes found significant particulate emissions advantages for specific fuel properties with no substantial impact on engine thermal efficiency. These accomplishments satisfied a midyear Joule milestone.

- ORNL has worked with Pacific Northwest National Laboratory, National Centre for Upgrading Technology (Canada), and Chevron 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. These analyses are being publicly released through CRC to foster interest in the use of the fuels by combustion researchers.

New data, first-of-kind results, innovations regarding biodiesel use

- Completed and published results from a study of the effects of biodiesel use on diesel exhaust gas recirculation (EGR) cooler fouling processes. The results showed that under steady-flow conditions use of biodiesel does not produce EGR cooler performance degradation that is worse than that when ultralow-sulfur diesel (ULSD) is used.
  - This study produced direct, in situ measurements of the thermal conductivity and other fouling layer properties that are critical to successfully modeling the fouling process.
  - These measurements are believed to be unique, first-of-their kind results.
  - This effort has spawned other funded research and expanded collaboration in this technical area.

- Published data on PCCI-like high efficiency clean combustion (HECC) with biodiesel blends.

- Studies of particulate oxidation kinetics have helped explain why particulates produced when using some biodiesel blends exhibit lower ignition temperatures and faster oxidation rates than particulates produced when using ULSD.

- This behavior was linked to both the combustion behavior of fuel molecules as it relates to soot morphology and the characteristics of fuel hydrocarbons that are a part of the soluble organic fraction.
- This project also produced first-of-their kind neutron tomographic images of full-size particulate filters loaded with particulate (Figures 13 a,b). This technique produces detailed cross-sectional images and opens a new pathway to studies of fuel and aftertreatment system compatibility.

Figure 13 a.

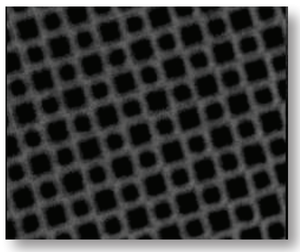

Figure 13 b.

Figure 13 a. Neutron tomographic image of DPF showing soot loading in (rounded) channels
b. a close-up

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

- ORNL continued to work with Underwriters' Laboratory (UL) in 2009 following rapid response to a need for data in support of UL recertification of E85 fuel dispensers in 2008. Researchers at ORNL continued to operate two coupon exposure vessels for dynamic materials compatibility experiments targeted towards increased ethanol use. These devices are unique in that they provide the ability to investigate materials compatibility with ethanol blends at standardized elevated temperatures (60°C) with moving fluid.

- ORNL continued work with Delphi Automotive Systems Corporation (Delphi) under a CRADA for maximizing ethanol engine efficiency.
  - Documented effect of compression ratio.
  - Replaced variable compression ratio (VCR) engine with fully variable valve timing engine.
  - Delphi-prepared research engine was operational and delivery to ORNL before the end of FY 2009 was expected.

Advanced lubricants research

- A new CRADA with General Motors was initiated to investigate the potential benefits of ionic liquid lubricants. These lubricants exhibit reduced friction and wear and do not contain known catalyst poisons.

- FEERC partnered with the ORNL High Temperature Materials Laboratory and the University of Tennessee to establish a new research platform at FEERC for investigating efficiency gains through advanced lubricants.

Health impacts—real-world emissions studies

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. Known as mobile source air toxics, they are EPA-defined emission constituents that include particulate matter (PM) and volatile and semivolatile organics. In collaboration with the University of Maryland, FEERC compared PM from advanced HECC combustion modes with conventional combustion particulate on a light duty diesel engine platform at ORNL. A novel technique called the aerosol particle mass analyzer allowed measurement of particle density and PM morphology was determined with transmission electron microscope analysis. It was determined that HECC gives smaller primary particle diameters, but the aggregate morphology is the same as conventional particulate density. PM morphology was determined with transmission electron microscope analysis. It was determined that HECC gives smaller primary particle diameters, but the aggregate morphology is the same as conventional particulate.

Improvements in Facilities and Capabilities

Upgrade of FEERC Vehicle Research Laboratory completed

The upgrade included purchase and installation of a new single roll, 48-inch Burke Porter alternating current motor-in-the-middle-style chassis dynamometer (Figure 14). Aside from simply replacing a well-used 1970s-era twin roll unit, this installation incorporated several laboratory improvements, including the following:

Figure 14. Upgraded vehicle dynamometer in FEERC was commissioned in March 2009.

- Larger test vehicle weight range and improved dynamic load control.
- Mezzanine installation to accommodate the required dynamometer control and drive unit and to improve the laboratory's space limitations.
- Installation of new data acquisition system with integrated vehicle controller area network (or vehicle electronic control unit data link) access.
- Design and installation of a critical flow venturi full flow dilution tunnel with the capability of four discrete flow rates.
- Redesign of emissions sampling system to provide multiple discrete critical flow sample rates and improve ethanol measurement capabilities.

Single cylinder variable valve engine operational

The research platform (Figure 15) is currently being used for ethanol optimization work in a CRADA project with an industrial partner. This engine experiment represents an important new capability at ORNL: freeing researchers of the constraints of conventional cam-based valve trains, for easier study of HCCI combustion and other alternate thermodynamic cycles. Currently, the engine platform is scheduled to be used for a number of activities in FY 2010: HCCI fuel effects, in-cylinder charge motion effects, spark-assisted HCCI, effects of FACE gasolines, and a Laboratory Directed Research and Development study investigating a promising six-stroke engine cycle.

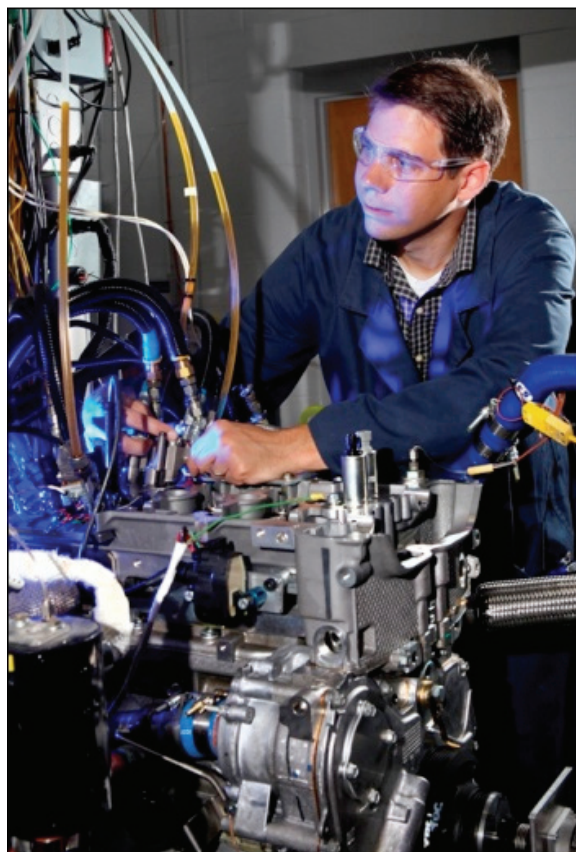

Figure 15. Dr. Jim Szybist prepares variable valve timing single cylinder engine for experiments.

Additional engine cell construction completed and operational

A new engine cell with 600 hp direct current and 230 hp alternating current double-ended motoring dynamometers (industry-donated or purchased with non-VTP funds) is now operational (construction began in FY 2008). Three industry partners are supplying engines and/or controls to accommodate multiple WFO and ethanol engine CRADA projects in this engine cell. ORNL has provided about $1,100k of internal funding to support the development of this capability (Figure 16).

Figure 16. Advanced combustion emissions reduction technology engine.

Capillary electrophoresis separation capability added to mass spectrometer

A capillary electrophoresis instrument has been coupled to a Bruker mass spectrometer. The new capability allows a broader range of new exhaust materials from novel fuels to be successfully separated and characterized. Capillary electrophoresis mass spectrometry fills a significant gap with more conventional instruments, especially for exhaust components such as the only slightly water soluble organic acid soot precursors that are difficult to solubilize and resolve via other separations platforms.

Automated catalyst bench flow reactor

FEERC completed installation of a fully automated bench core reactor (Figure 17) that can be operated unattended, around-the-clock, which is essential for the full execution of the catalyst aging protocol recently established with an industrial partner.

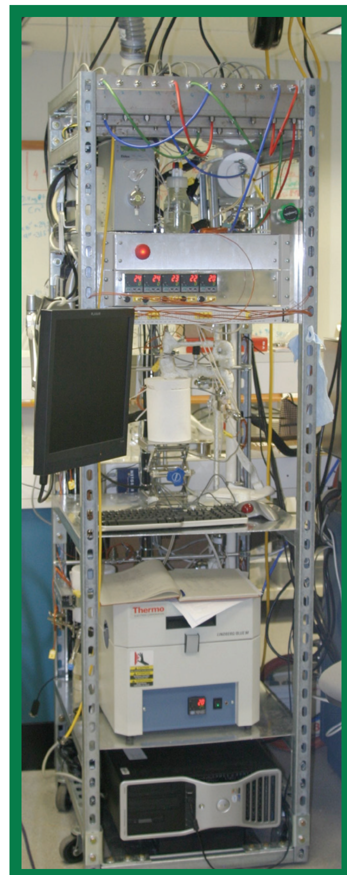

Figure 17. Fully automated bench core reactor.

High Temperature Materials Laboratory User Program

The mission of the High Temperature Materials Laboratory (HTML) User Program is to support the goals of the DOE VTP by enabling the development of materials-based, energy-efficient, and environmentally friendly highway transportation technologies that will help reduce oil consumption in the United States. The HTML User Program specializes in materials characterization and conducts collaborative materials research with industry, universities, and other national laboratories.

The HTML User Program received 43 new proposals in FY 2009: 20 from industry, 19 from universities, and 4 from national laboratories. These new projects and projects from previous years that were continued in 2009 address key technical and cost barriers and the overarching VTP energy, economic, and environment objectives. Relevant areas include lightweight alloys, high-strength steels, fiber-reinforced composites, batteries, thermoelectric materials, and catalysts.

During 2009, HTML User Projects with Brookhaven National Laboratory, the Massachusetts Institute of Technology, Motorola Energy Systems, the Ohio State University, and ORNL focused on characterizing new materials for rechargeable batteries with the objective of reaching VTP energy storage goals for EVs and hybrid EVs. Some of these projects also focused on developing a better understanding of the mechanisms that are responsible for the stability and durability of batteries.

Projects with Innegrity, the Automotive Composites Consortium (ACC), Plasan Carbon Composites, Michigan State University, Cosma, Mississippi State University, Pratt & Whitney, the University of Tennessee, Caterpillar, Deere & Company, and ORNL evaluated and characterized graphite fibers; fiber-reinforced composites; aluminum (Al) and magnesium (Mg) alloys; and titanium aluminides, which are being considered for lightweighting vehicular applications. User projects also focused on investigating residual stresses in castings using neutron diffraction methods in order to reduce the weight of components and improve manufacturing methods.

General Motors and Michigan State University continued utilizing the program to characterize thermoelectric materials with improved figure of merit values. These materials will enable the design of reliable and durable thermoelectric generators to recover waste heat from internal combustion engines. Enhanced capabilities from upgrades and new instrumentation have helped establish world-class capabilities for the characterization of thermoelectric materials and for the determination of thermophysical properties at HTML.

During 2009, new projects were initiated to characterize catalytic materials used in aftertreatment devices and for biofuels and hydrogen production. The objective of these projects is to develop a fundamental understanding of behavior of these materials through unique imaging and analytical capabilities available through the HTML User Program.

Lightweighting Materials Program

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 and heavy vehicle body and chassis weight without compromising other attributes such as safety, performance, recyclability, and cost.

The specific goals of the LM program are to develop material and manufacturing technologies that, if implemented in high volume, could cost-effectively reduce the weight of passenger vehicle body and chassis systems by 50% with safety, performance, and recyclability comparable to current production vehicles.

The program is pursuing five primary areas of research: cost reduction, manufacturability, design data and test methodologies, joining, and recycling and repair. The current long-range plan for activities in these areas is found at www.eere.energy.gov. Because the single greatest barrier to the use of LM is cost, priority is given to activities aimed at reducing costs through development of new materials, forming technologies, and manufacturing processes. Priority LM include advanced high-strength steels, Al, Mg, titanium (Ti), and composites including metal-matrix materials and glass-, natural-, and carbon-fiber-reinforced thermosets and thermoplastics.

Key Technical Accomplishments

Advances in melt spinning

A route that is significantly faster than the previously reported stabilization route for polyolefins has been developed at ORNL. Polyolefins are an attractive alternative carbon precursor because of their low cost, high carbon yield, and melt spinnability. Initial conversion conditions were explored during FY 2009. The precursor fibers were melt spun from neat and modified resin using standard melt spinning equipment at a U.S.-based melt spinning equipment manufacturer's facility. Melt spun precursor fibers with varied diameters (8–15 m) and orientation parameters were produced. Those include unoriented yarn, partially oriented yarn, and highly oriented yarn. The sulfonation protocol and conversion technology are now being developed at ORNL for production of carbon fiber from low cost, melt processable polyolefin precursor (Figure 18).Conditions were established for continuous melt spinning of multifilament fiber from a biorefinery lignin (organosolv-pulped), as received, without purification,   a plasticizer. Using this lignin material, sustained continuous melt spinning of multifilaments of the target diameter (10 μm) was repeatedly demonstrated at speeds up to 1,500 m/min, the maximum limit of the winder on the melt spinning equipment (i.e., 2.5 times the baseline speed assumed in the Kline economic model) (Figure 19). Elimination of the need for lignin purification and the ability to melt spin at much higher speeds than the baseline assumption are of significant economic benefit with respect to the production of carbon fiber from lignin materials. In very marked contrast to commercially available lignin from the kraft pulping of wood (for paper production), the organosolv pulping process produces a lignin material that readily meets the stringent purity requirements for melt spinning and carbon fiber production.

Residual levels of detrimental elements such as Na, K, Ca, and S are exceptionally low (e.g., Na < 20 ppm) and even lower ash content levels have been achieved [e.g., 0.001 wt % (preliminary ash specification is 0.1 wt %)]. The purity of the organosolv lignin, Alcell, is exemplified by the data shown in Table 4, as is the progress made in isolating much cleaner lignin from the kraft pulping process.

Figure 18. Polyolefin precursor fiber spool.

Figure 19. Melt-spun lignin precursor fibers.

Table 4. Compare data for ligninsamples "HWL" and "SWL-K2"

Lignin Material[a]	Constituent					
	C (%)	S (%)	Na (ppm)	K (ppm)	Ca (ppm)	Ash (%)
HWL	59	2.45	19,000	1,770	650	2.800
HWL - Aq	65	1.48	73	70	225	0.030
HWL - Org	65	1.40	1,160	104	76	0.010
SWL - K2	67	1.18	2,390	100	78	0.200
Alcell	66	0.05	17	44	163	0.001

[a]Acronyms and abbreviations: HWL = kraft hardwood lignin as received from commercial supplier; HWL Aq = same kraft hardwood lignin purified by ORNL (aqueous procedure); HWL-Org = same kraft hardwood lignin purified by supplier (organic procedure); SWL K2 = kraft softwood lignin as received from Kruger Wayagamack; Alcell = organosolv lignin as received from Lignol Innovations.

Advances in joining technology

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. Heat generated during the resistance spot welding process can be used to monitor weld quality. Working with the U.S. Council for Automotive Research and using preliminary results supported by results from HTML User Projects, ORNL has successfully developed an online inspection technique using infrared (IR) thermography (Figure 20). A well

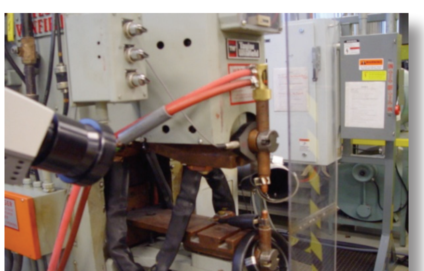

Figure 20. Infrared imaging of resistance spot welds.

designed test matrix was prepared at ORNL and spot weld coupons were made at ArcelorMittal. Postmortem IR inspections using several heating and cooling techniques were carried out to assess weld quality.

This concept feasibility project has shown the promising potential of the IR inspection technique. Future work has been planned using image processing and new software algorithms to improve the inspection speed.

A preliminary round of testing with four different stir tool designs on uncoated DP 780 showed that lap-shear strengths increased with welding time for all four (Figure 21). The strengths

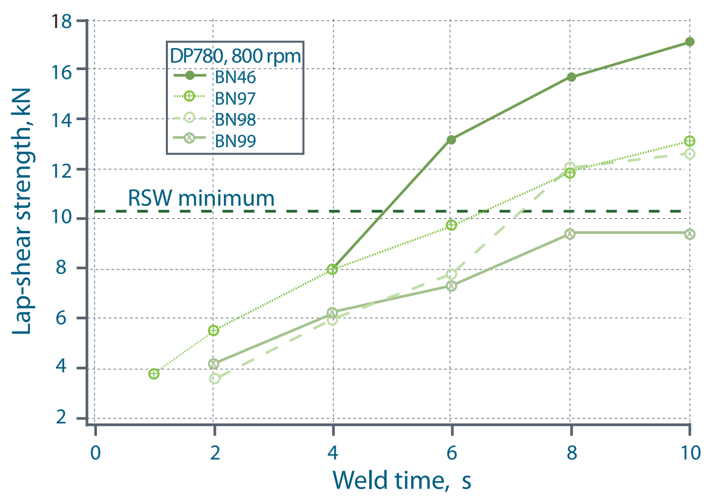

Figure 21. Variation of lap-shear tensile strength with weld time.

of spot welds made with pin tools of three different designs were similar at each welding time, indicating that pin surface features did not significantly influence the results. A less conventionally shaped stir tool, identified as BN46, resulted in consistently higher joint strengths. The initial testing confirmed that for either type of stir the lap-shear strengths of certain welding conditions exceeded the minimum value of 10.3 kN specified in the industry standard, AWS D8.1.

Additional spot welds were made with a fixed total welding time of 4 s. The results show that for otherwise identical welding conditions, increasing tool rotation speed from 800 to 1,600 rpm increased strength values. Using a two-segment welding procedure rather than a one-segment procedure had a similar effect. Average lap-shear strengths exceeding 10.3 kN were obtained with both types of stir tools on both the uncoated and the galvannealed DP 780. The ability of the BN46 stir tool to produce higher lap-shear strengths was further supported. Analysis of machine output data showed that with a two-segment procedure the stir tools were fully engaged with the sheet for longer times. This promoted heating of the weld regions while maintaining them under steady pressures. The likelihood of diffusion and mechanical interlocking making contributions to lap-shear strength was suggested by metallographic examination of the joints.

The ability to metallurgically bond Mg alloys to steels will be an important element of increasing the amount of Mg that is used in the construction of both passenger and commercial vehicles to lower their weights. One way that metallurgical bonding can be achieved is with conventional fusion welding processes. However, chemical reactions occur when Mg and steels are melted together during fusion welding that produce rapid formation of brittle phases that compromise mechanical properties. Because melting is avoided in solid-state welding processes like friction stir welding and ultrasonic welding, they should not be subject to the limitations inherent in fusion welding processes. Perfecting the application of friction stir welding and ultrasonic welding for Mg-steel joints will support development of low cost, multi-material, magnesium-intensive, lightweight, body-in-white structures and closure panels.

Specimens of the Mg alloy AZ31B-H24 that were 1.6 mm thick were ultrasonic spot welded to 0.8 mm thick galvanized mild steel. Two different welding tips were used with face dimensions of either 5 mm × 7 mm or 7 mm × 7 mm. The rapid rise of strength with welding time followed by a much lower rise or plateau suggests that thermally activated processes enable the bonding, and this possibility is a focus of continuing analysis. Above a welding time of 0.4 s, the joint strengths range from 3–4.5 kN, which is in the range of the strengths of resistance spot welds in AZ31B sheet metal (Figure 22). This is a remarkable achievement for welding Mg to steel, which, conventional wisdom considered impossible.

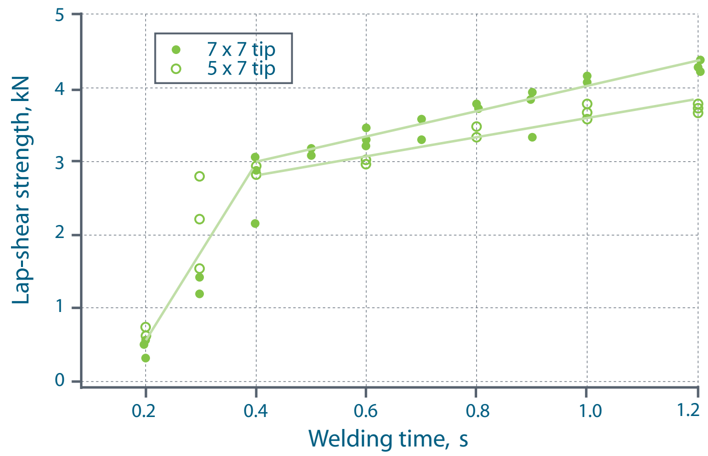

Figure 22. Variation in lap-shear tensile strength with time and welding tip dimensions for Mg alloy AZ31B-H24 welded to galvanized mild steel.

Integrated Computational Materials Engineering

A primary requirement of the DOE Integrated Computational Materials Engineering (ICME) isotopic diffusion project is the capability to quickly and accurately measure isotopic ratios in Mg samples using secondary ion mass spectrometry (SIMS). The SIMS instrument at the University of Central Florida (Cameca IMS3f) has been calibrated for depth profiling (using profilometry) and isotope ratio measurements at various depths using Mg and Mg-base alloys. Thin films of pure Al with thicknesses in the range of a few hundred nm were successfully deposited using physical vapor deposition on several disc specimens of pure Mg. These coated specimens were annealed at 300°C for 2 hours and quenched. Depth profile measurements of Al in pure Mg were carried out, and the Al impurity diffusion coefficient in Mg was determined. An experimental procedure (deposition, diffusion anneal, and SIMS) has been established that provides accurate and repeatable measurements of impurity diffusion coefficients (and thus tracer when available) for very dilute substitutional solid solutions.

Based on six measurements using three different experimental runs, the impurity diffusion coefficient of Al in Mg was determined as DAl = 1.74 (±0.4) × 10-13 cm2/s. The precision within an experimental run (e.g., one sample but three different regions) was determined to be ±0.2 × 10-13 cm2/s. Preliminary results are shown in Figure 23.

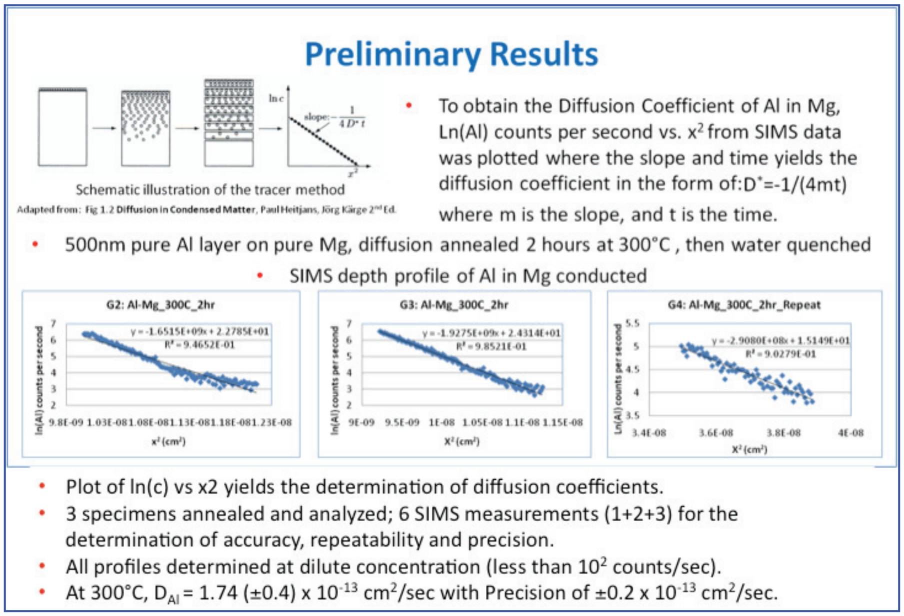

Figure 23. Preliminary impurity diffusion coefficient of Al in Mg results.

Advances in polymer matrix composite technology

As part of a continuing program with ACC, we successfully demonstrated off-robot and on-robot chopper deposition rates up to 18.7 kg/min using Twintex (comingled fiberglass-polypropylene fiber) with an upgraded Wolfangel chopper versus limits of approximately 4.5 kg/min with the baseline Applicator chopper. The chopper was extensively characterized, first on a test stand and then on the robot, using rapid start and stop programs. As expected, each progression required upgrading fiber handling capabilities (Figure 24) and full programming controls to mitigate fiber entangling, fiber breaking, and chopper jams. The upgraded chopper is fully capable of sustained operations at greater than 18 kg/min and starting and stopping consistent with robot capabilities. The current hardware allows relatively continuous operations at these speeds, although additional minor fiber handling hardware modifications and programming tweaking would be required for continuous production operations.

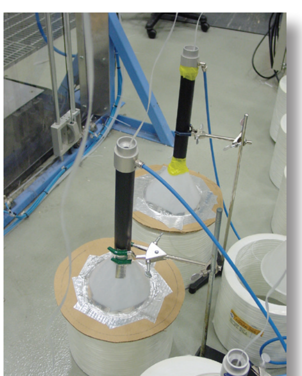

Figure 24. Air tensioning hardware for high speed chopper operations.

ORNL is developing testing and modeling methodologies that will enable prediction of the effects of mechanical loadings and environmental exposures on the durability of an automotive composite-to-metal (multi-material) joint. The focus application is the joining of a polymer matrix composite underbody to the rest of the vehicle structure. Durability testing was initiated this year using composite-to-steel weld bonded specimens tested via cyclic tensile fatigue (Figure 25 a,b) and with specimens manufactured using the same fabric sheet molding compound material that has been selected for ACC's composite underbody. In addition to providing input for the multi-material joint model development and validation efforts, this data will provide important joint durability information on design hardware to the automotive community.

Figure 25 a. Weld bonded composite-to-metal joint specimen.

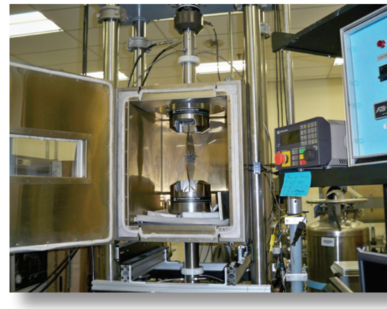

Figure 25 b. Weld bonded specimen tested in cyclic tensile fatigue.

Improvements in Facilities and Capabilities

ORNL's precursor and fiber evaluation capability enables the evaluation of small quantities of precursor. It can be used to heat treat a single filament. Tows as small as 10 filaments can be converted under controlled tension, with exact required filament count for tensioning dependent on precursor characteristics. This equipment enables evaluation of the convertibility of test tube quantities of precursor fibers and very thorough parametric exploration of their conversion space during development of conversion protocols.

In FY 2009, the precursor fiber evaluation capability was enhanced significantly. The upper temperature limit was raised from 1,700°C to 2,500°C by the acquisition of a new ultrahigh-temperature tube furnace (Figure 26), which is being installed at this writing. The upper temperature is sufficiently beyond that required for carbonization of low cost precursors to remove any furnace limits on low cost carbon fiber conversion evaluations. Because the 1,700°C carbonization furnace was quite old, showing considerable wear, and contained hazardous materials that would prevent its repair in the event of failure, it was replaced by a new 1,750°C tube furnace with readily replaceable ceramic retort. It has delivered significantly improved temperature stability and control.

A box oven with custom rollers and tow pass-through was designed and built to mimic full-scale industrial oxidation ovens (Figure 27). This oven features five tow passes through the heated zone and can be coupled with tensioning-stretching equipment to precisely evaluate the effects of tension, stretching, and temperature during air oxidation.

Figure 26. New 2,500°C furnace.

Figure 27. Laboratory box oven for tow oxidation.

Improved tensioning and transport equipment were added to the laboratory-scale pilot line to enable processing multiple tows with each tow independently tensioned. This is a very important feature for maintaining good mechanical properties in all multiple tows. Precise tow stretching equipment was acquired to enable controlled tow stretching in any of the precursor evaluation system's heat treatment steps. New pieces of equipment are shown in Figure 28.

Figure 28. a. New tensioning equipment: low force tension controller.

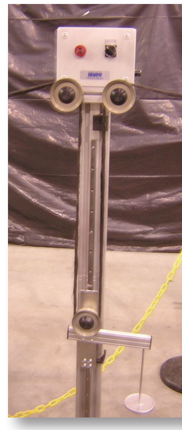

Figure 28. b. Dancing tension controller.

Propulsion Materials

The Propulsion Materials program is a partner and supporter of the VTP Hybrid and Vehicle Systems, Energy Storage, Power Electronics and Electrical Machines, 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 to meet Vehicle Technologies Program goals

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 55% thermal efficiency heavy duty diesel engines.
- Materials for waste heat recovery via thermoelectric modules, with the potential for a 10% increase in fuel efficiency.
- Materials technologies for efficient and effective reduction of tailpipe emissions, including diesel particulate filters, catalyst characterization and testing, and EGR coolers.
- Materials technologies for EVs and HEVs, including advanced power electronics materials and electric motors.
- Materials for alternate-fuels vehicles, including materials compatibility and corrosion.

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 VTP propulsion technologies. Each project consists of several related R&D agreements.

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

Key Technical Accomplishments

- Patent application for a "direct cooled power electronics substrate" published (12/400,081).
- Laboratory methodology developed to evaluate degradation of power electronics materials by evaporative liquids.
- Computational thermodynamics models were used to identify low cost compositions for high temperature valve alloys, and tensile properties of selected alloys were evaluated, yielding encouraging results.
- Caterpillar Inc. and ORNL have addressed the wear and failure modes of current on-highway heavy duty diesel exhaust valves and seats and then evaluated changes in seat-insert processing and advanced exhaust-valve alloys that will enable higher temperature capability and better performance and durability.
- A model for the effects of abrasive wear, deformation, and high temperature frictional contact on exhaust valves and seats was developed.
- An advisory board of industry specialists from nine diesel engine companies has been assembled and a midyear effort initiated to evaluate EGR cooler fouling and provide characterization data to enable models which may lead to improved coolers.
- A new CRADA for the reliability characterization of candidate high pressure piezoelectric multilayer actuators used in fuel injectors has been initiated between ORNL and Cummins Inc.
- A new CRADA was initiated between ORNL and Caterpillar Inc. to improve diesel engine performance, efficiency, and emissions through the application of materials-enabled technologies.
  - Caterpillar provided ORNL with two 600 hp motoring dynamometers and a C15 ACERT engine.
  - The test cell, control room, cooling water, ventilation, and bedplates and other infrastructure were all completed and installed in FY 2009.
  - Caterpillar, working with ORNL, will develop and provide 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.
- The durability of DPFs is being evaluated by ORNL research staff and Cummins Inc. via application of probabilistic design tools, non-destructive evaluation, and refinement and use

of lifetime-prediction models. Mechanical and thermal shock characterization test procedures developed previously were used to measure properties in cordierite, aluminum titanate, and mullite DPF materials.

- Design strategies for thermoelectric materials are being developed based on first principles calculations of electronic, vibrational, and transport properties to identify potentially low cost, high performance thermoelectric materials suitable for application in vehicles.

- New insights into thermoelectric materials performance have emerged from density functional calculations in conjunction with transport theory.

- These results suggest new opportunities for developing high performance, lower cost thermoelectrics for vehicular waste heat recovery.

Advanced Vehicle Systems

The Advanced Vehicle Systems (AVS) research program is part of the ORNL Energy and Transportation Science Division, Energy and Engineering Sciences Directorate. Its mission is “to provide key expertise for testing, evaluation, simulation, and integration of advanced vehicle technologies that will facilitate better understanding of the benefits of these technologies to the transportation sector.” In accomplishing this mission, AVS strives to maintain a cohesive and integrated research program that draws upon advanced engine technologies; advanced power electronics and electric machines; and laboratory-to-roadside testing, evaluation, modeling, and analysis to meet the research needs of the DOE VTP and to support public decision making regarding the benefits of adopting advanced energy efficient transportation technologies.

Focus

The AVS R&D program draws upon and integrates the following ORNL core transportation research strengths.

- Advanced Engine Technologies—advanced combustion modes, fuels, thermal energy recovery, emissions aftertreatment, etc.

- Advanced Power Electronics and Electric Machines—motor drives, components, power electronics devices, advanced converter topologies, etc.

- Vehicle Testing and Evaluation—chassis and component dynamometers, integrated powertrain stands, test track evaluations, field operational testing, etc.

- Modeling, Simulation, and Analysis—data collected from vehicle testing and evaluation are used to develop and utilize sophisticated models and simulations and, through appropriate analyses, develop an understanding of the performance and benefits of advanced transportation technologies.

The ORNL AVS research program strengthens its knowledge base through close collaborations with industry, academia, and other government entities (e.g., other national laboratories). Industry involvement is key to the development, transfer, and commercialization of successful technologies. Collaboration with experts from academia and other national laboratories is important to make efficient use of all available resources and to provide improved cost-benefit to DOE.

Key Technical Accomplishments

Development of models for advanced engines and emission control components

ORNL has developed a methodology for modifying steady-state engine maps to account for cold- and warm-start transients that has been successfully demonstrated for multiple light duty engines, including both gasoline and diesel engines, similar to those expected to be used in advanced hybrid vehicles. An idealized full-range HECC exhaust map for a 1.7 L Mercedes diesel engine was developed and used to estimate the potential impact of full HECC operation on hybrid vehicle fuel economy and emissions. A preliminary three-way catalyst component model has been improved and validated with experimental data from multiple sources. A catalyzed DPF component aftertreatment model was developed from the noncatalyzed DPF model developed previously, validated with data from the literature, and implemented in Powertrain System Analysis Toolkit (PSAT) simulations of hybrid vehicles. A DOC component aftertreatment model was developed and validated to a limited extent to account for carbon monoxide, nitric oxide, and hydrocarbon oxidation. A coolant thermal storage component model (for waste heat recovery and more rapid aftertreatment catalyst light-off) has been developed and implemented in PHEV systems simulations. PHEV simulations comparing diesel and gasoline-power vehicles equipped with appropriate NOx control aftertreatments indicate that diesel vehicles will have modest efficiency advantages, but these are reduced from what is ultimately possible due to emissions control fuel penalties.

Heavy and Medium Truck Duty Cycle Program

This program involves efforts focused on the collection, analysis, and management of data and information related to heavy and medium truck real-world operation. The collected data support the development and evaluation of Argonne National Laboratory's Heavy Truck PSAT module and provide real-world-based duty cycle data and information for the assessment of the energy efficiency benefits of new and emerging technologies. In addition to supporting the development and evaluation of truck energy efficiency models, the data and information from this program will be useful to

- provide input to DOE regarding heavy truck energy efficiency technology investment decisions;
- generate customized, real-world-based data for the heavy truck energy efficiency research community; and
- conduct real-world-based energy efficiency studies related to factors shaping heavy truck performance.

Data and information have been collected on long-haul Class-8 trucks (700,000 miles of real-world operating data over 12 months), and data and information collection for two Class-7 vocations (combination tractor-trailers and transit busses) is nearly complete. Two additional Class-7 vocations (wrecker and utility trucks) will be initiated later in FY 2010. The data collected under these efforts involve a large number of information channels/performance measures (about 60 for the Class-8 trucks and 80 for the Class-7) related to the truck's operational situation including information related to weight, grade, weather, time-of-day, and location (rural, interstate, metropolitan, etc.). Such performance shaping factors (PSFs) are important for understanding the significance of standard duty cycle data that are basically composed of velocity and time. This program has also developed specialized analysis tools that will allow the user to

- select PSFs that are of particular importance
- statistically combine the duty cycles of multiple operational segments into one duty cycle that reflects the acceleration and speed profiles of the contributing segments.

One of the goals of this program is to collect data from volunteer fleets that allow instrumentation developed by ORNL to be installed on their vehicles for a 12-month period. Currently ORNL has six data collection platforms valued at about $35,000 each that provide the data collection capability for these efforts. To date, the program has engaged in Memorandums of Understanding (MOUs) with three commercially operating fleets (an additional two will be signed in FY 2010). In addition, for the data collection associated with the Class-7 combination vehicles, DOT's Federal Motor Carrier Safety Administration (FMCSA) has been a partner and is collecting data on brake and tire performance. The program was able to leverage DOT's experience in collecting instrumented vehicle data wirelessly. A similar partnership is being sought with EPA.

The program has also conducted specialized studies that address energy efficiency interests. These studies have been done for the Class-8 data through a partnership with Michelin. Michelin's interest involved an assessment of the fuel efficiencies of their single wide-based tires in comparison to their standard dual tires. Michelin donated new tires for six tractor-trailers for this study. The real-world data showed an average fuel savings of about 6% with the single wide-based tires, and for a fully loaded 80,000 lb tractor-trailer, the single wide-based tires were more than 10% better in fuel economy than the dual tires. Other studies related to fuel economy and vehicle speed were also conducted and a preliminary study on fuel consumption and driver aggressiveness has been initiated. Similar studies are planned for the Class-7 data.

Lastly, unless characteristic duty cycles exist for various truck vocations, estimation of the energy efficiency benefits of new technologies will be difficult to make. Even within a particular vocation, duty cycles tend to vary due to terrain, regional weather, and operating protocols. Knowledge of the expected variation of a vocational duty cycle would help to bound the energy efficiency benefits of new technologies. However, the collection of sufficient data to define such variation requires a significant amount of effort, number of analyses, and amount of resources. A new facet of this program called the Large Scale Duty Cycle effort is seeking to define a method to inexpensively collect duty cycle data (velocity, time, grade, location, and if possible other parameters) from a large number of vehicles. While such data will not have the depth of the data collected in the Heavy and Medium Truck Duty Cycle (HTDC and MTDC) efforts, they are expected to be able to define the expected variance in the duty cycles associated with a particular vocation thus allowing the fuel economy benefits of advanced efficiency technologies to be assessed among different vocations.

Key Technical Accomplishments

- Implementation of MOUs with the Knoxville Area Transit (KAT) and H.T. Hackney (Hackney) Corp. for their voluntary participation in the MTDC effort.
- Partnership with DOT's FMCSA to collect brake and tire performance data.
- Instrumentation of three KAT vehicles and three Hackney vehicles and initiation of data collection.
- Initiation of wireless data collection from all instrumented vehicles replacing manual data downloading.
- Publication of the HTDC final report and distribution of the report (digitally) to more than 150 interested parties.
- Completion of two specialized studies on fuel efficiency and weight/tires and fuel efficiency and speed/tires and initiation of a preliminary fuel efficiency and driver aggression study.
- Preparation of a paper for presentation at the Transportation Research Board's Annual Meeting in January 2010.

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

Active Filter Approach to Reduce the dc Link Capacitor

Background

In an electric traction system composed of a battery, a three-phase inverter, and an electric motor, the harmonic current of the direct current (dc) bus introduced by the switching behavior of the inverter is significant. Excessive harmonic current can cause thermal stress on the dc bus capacitor and generate electromagnetic interference which can interfere with communication and control systems.

The dc bus capacitor is used to filter the dc bus current harmonics and to reduce the dc voltage ripple. It occupies 35–40% of the whole traction inverter volume and weight and can account for up to 23% of the inverter cost. Electric vehicle and hybrid electric vehicle manufacturers are seeking savings in the cost, weight, and volume of these capacitors. An active power filter (APF) could be one way to achieve these savings. Oak Ridge National Laboratory (ORNL) research described here addresses these issues by presenting a method to replace the bulky capacitor with an active filter in a 55 kW traction drive system and analyzing the problems with and barriers to application of this method.

Technology

The purpose of the APF is to supply the ripple current and load demands thereby letting the battery supply only the dc component, thus eliminating the current harmonics on the dc link. A simulation model was developed using MATLAB Simulink with the PLECS toolbox to assess the ability of the APF to reduce the ripple currents. To produce the ripple current, an H-bridge current-source APF topology composed of an inductor and a single full bridge inverter was developed. The selection of a current source inverter for the study necessitated the use of reverse blocking insulated gate bipolar transistors (IGBTs), which currently have limited commercial availability. Conventional IGBTs were used in the model, with series diodes to accomplish the reverse blocking. A small capacitor was still necessary for some smoothing, but it was less than one-fourth the size of the original dc bus capacitor. A control algorithm was developed to achieve active filtering at reduced cost and size and increased filtering efficiency (Figure 1).

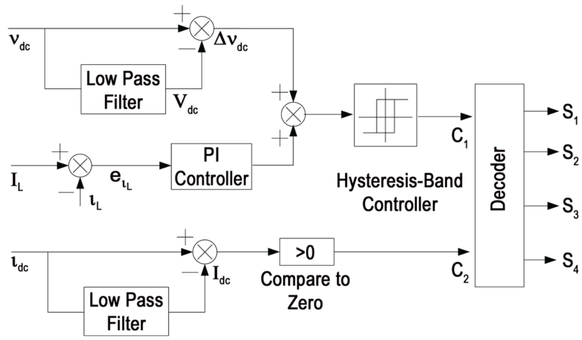

Figure 1: APF control circuit.

Benefits

- *The weight and volume of the traction inverter will be reduced while the reliability and lifetime of the inverter will be increased.*
- *Reduction in the capacitance required will help enable higher temperature operation.*

Status

ORNL simulation studies demonstrated that by using the selected APF control method the dc bus capacitor could be dramatically minimized—from 2,200 μF to 500 μF (Figure 2). However, because of the high operation frequency and the large inductor current, the size and weight of the APF, and the loss associated with the additional semiconductor switches, the APF method is still far from being practical in a traction drive inverter. Therefore, a decision was made to discontinue the research. Extensive knowledge was gained through this project and it may be revived in the future when new devices with lower losses become available.

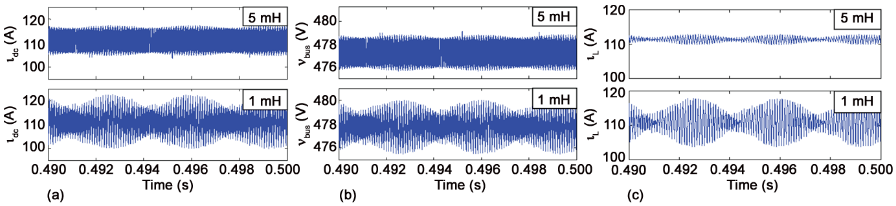

Figure 2: Effects of filter inductance: (a) = input current, (b) = dc bus voltage, and (c) = APF inductor current.

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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 and hybrid electric vehicles (HEVs) use inverters that operate off a voltage source because the most readily available and most efficient energy storage devices (batteries) are inherently voltage sources. The voltage source inverter (VSI), however, possesses several drawbacks that make it difficult to meet the FreedomCAR Partnership goals in terms of volume, lifetime, and cost. 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 in a VSI. In addition, steep rising and falling edges of the output voltage in the form of pulse trains generate high electromagnetic interference, 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.

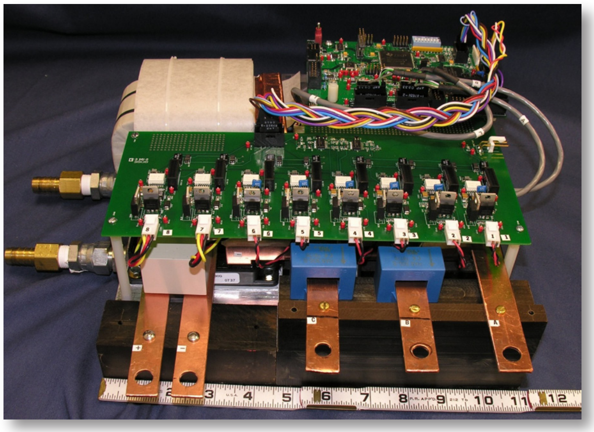

Figure 1: A 55 kW CSI prototype.

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 bus capacitance required and uses only three small alternating current (ac) filter capacitors; 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 it (1) doesn’t need antiparallel diodes in the switches, (2) can tolerate phase-leg shoot-through, (3) provides sinusoid-shaped voltage output to the motor, and (4) can boost the output voltage to a higher level than the source voltage to enable the motor to operate at higher speeds. These advantages translate

Benefits

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

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 requirement in plug-in HEVs (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, further, could enable air-cooled power inverters in the future when silicon-carbide-based switches become commercially viable.

The proposed CSI includes a novel interfacing circuit to transform the voltage source of a battery or ultracapacitor bank into a current source to the inverter bridge that will provide 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 (Figure 1). The total capacitance was reduced to 195˚F. 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 involve teaming with Michigan State University (MSU) to merge the CSI technology with previous ORNL-MSU work with Z-source inverters to design and build an inverter with all the benefits of the CSI technology along with the added capability of universal charging for PHEVs.

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Advanced Power Electronics and Electric Machines

Direct Cooled Power Electronics Substrate

Background

Established power electronics packaging and cooling methods in hybrid electric vehicles involve heat transfer from the silicon dies through multiple solder layers, a direct bonded copper substrate, a baseplate, and a thermal interface material into a heat exchanger. The heat exchanger circulates water-ethylene glycol (WEG) coolant at roughly 70˚C to remove the heat. Progress in meeting FreedomCAR cost targets can be made by eliminating this auxiliary cooling loop, which is estimated to add $175 to the system cost. The existing 105˚C engine coolant exiting the radiator could be used for cooling the power electronics, but this would involve challenges in designing a reliable system that could keep commercially available silicon power devices within their safe operating range.

Technology

Researchers at Oak Ridge National Laboratory have developed a power electronics substrate that is directly cooled with 105˚C WEG coolant that eliminates the baseplate, thermal interface material, and cold plate and enables a novel three-dimensional inverter design. Using this concept, the coolant flows directly through the ceramic substrate delivering cooling more directly to the semiconductor dies, which are sintered or soldered to copper plating on top of the ceramic. The new design and resulting reduction of the thermal stack is expected to achieve an inverter power density of 13.4 kW/L and significantly reduce system costs.

Status

Multiple designs have been evaluated and extensive finite element analyses performed to validate the concept. Prototype substrates have been fabricated, copper clad, and plated, and the dies have been attached with ribbon bonds. A single leg prototype of the direct cooled substrate was built and tested, which has validated the modeling efforts. Extensive long-term corrosion tests are ongoing to assess any detrimental effects to ceramic materials from WEG.

A conceptual design and ceramic materials providing maximum heat transfer have been selected (Figure 1).

Benefits

- *Achieves packaging concept with reduced thermal resistance.*
- *Enables use of 105˚C coolant for silicon-based electronics.*
- *Achieves inverter power density of 13.4 kW/L.*

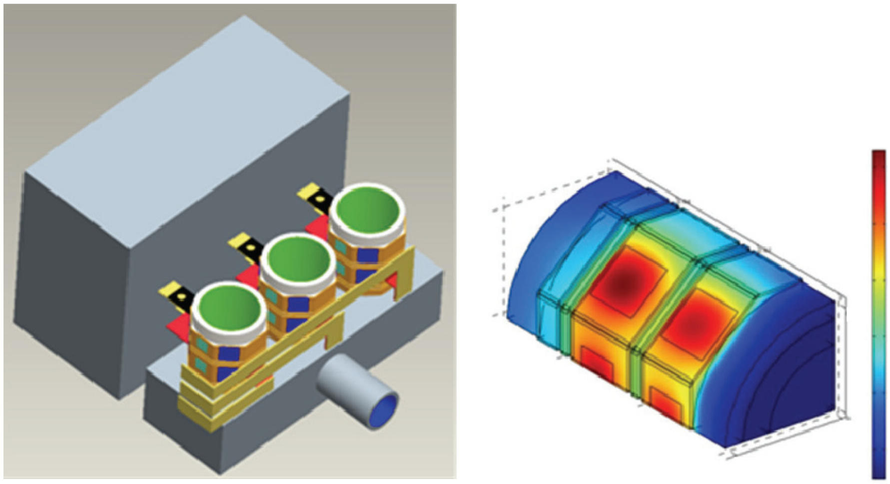

Figure 1: Two conceptualizations of the inverter showing two-chip-deep annulus design.

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Advanced Power Electronics and Electric Machines

Segmented Drive System with a Small dc Bus Capacitor

Background

The standard voltage source inverter- (VSI-) based traction drive is widely used in current hybrid electric vehicles (HEVs). The VSI is mainly composed of six power semiconductor switches, diodes, and a large bus capacitor (typically insulated gate bipolar transistors and a film capacitor) and switches the battery voltage according to a pulse-width modulation (PWM) scheme to regulate the motor current and voltage. In performing the switching operations, the switches generate a large ripple current in the dc link, necessitating the use of a dc bus filter capacitor so that a relatively constant current flows into the battery. The capacitor ripple current can reach levels as high as 200 Arms. A bulky and costly dc bus capacitor of about 2,000˚F is required to absorb this ripple current and prevent it from damaging and shortening the battery's life. The dc bus capacitor presents significant barriers to meeting the FreedomCAR targets for cost, volume, and weight for inverters. Currently, the dc bus capacitor contributes up to 23% of the cost and weight of an inverter and up to 30% of an inverter's volume.

The large ripple currents become even more problematic for the film capacitors (the capacitor technology of choice for EVs/HEVs) in high temperature environments as their ripple current handling capability decreases rapidly with rising temperatures. There is thus an urgent need to reduce the ripple currents altogether or to divert them from the bus capacitor.

Technology

Oak Ridge National Laboratory (ORNL) is currently performing research on a segmented drive system topology to respond to these issues. The segmented topology does not need additional switches or passive components but enables the use of optimized PWM schemes to significantly reduce the dc link ripple current generated by switching of the inverter output currents. Unique aspects of this technology include the fact that while it significantly reduces the capacitor ripple current, it does not

- need additional silicon or passive (L or C) components,
- need additional sensors, or
- add control complexity.

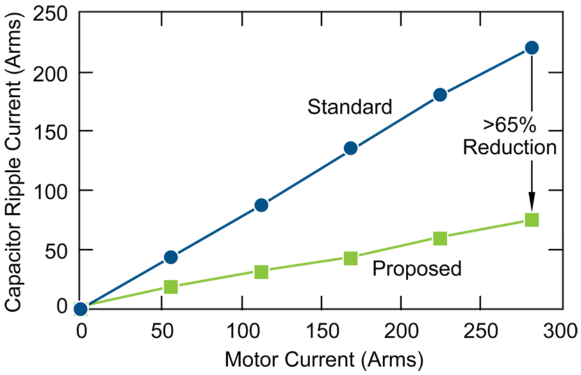

Figure 1: Illustration of dc bus capacitor ripple current reduction with segmented drive system.

Benefits

- *Reduces cost and volume by 15% compared to standard VSI.*
- *Reduces dc link bus capacitor size and cost by more than 60% (caps about 25% of cost and 33% of volume of VSI).*
- *Reduces battery losses and improves battery operating conditions by reducing battery ripple current.*
- *Significantly reduces motor torque ripples (up to 50%).*
- *Reduces switching losses by 50%.*
- *Increases inverter reliability.*
- *Enables high temperature operation.*

Status

To date, ORNL has completed simulation studies of a 55 kW traction drive inverter using the segmented drive topology, and the results show the following:

- Achieved more than 65% reduction in dc bus capacitor ripple current intensity (Figure 1).
- Achieved 80% reduction in battery ripple current.
- Achieved 70% reduction in dc bus ripple voltage.
- Achieved 50% reduction in motor ripple currents (Figure 2).

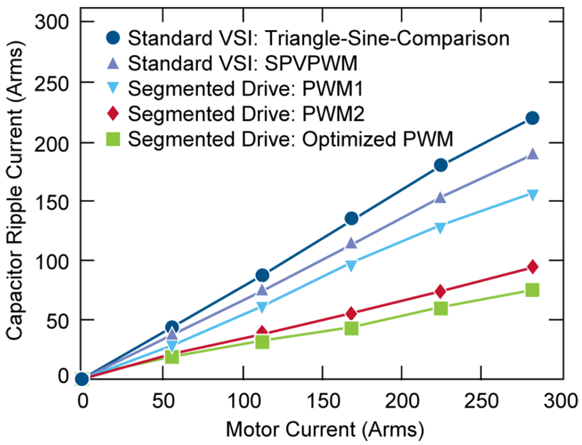

Figure 2: Comparison of capacitor ripple current vs motor current.

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Advanced Power Electronics and Electric Machines

Wide Bandgap Materials

Background

There is an increasing need for higher temperature operation of power electronics in automotive applications. The ability for components to operate reliably at elevated temperatures can result in cost and weight savings through reduced heat sinks and the elimination of secondary cooling loops. Additionally, devices capable of increased frequency operation can result in decreased requirements for passive components, leading to further reductions in cost, weight, and volume. Wide bandgap (WBG) devices, specifically silicon carbide (SiC) and gallium nitride (GaN) semiconductors, are emerging technologies that enable both increased temperature and increased frequency operation as well as efficiency and reliability improvements.

Technology

Oak Ridge National Laboratory (ORNL) has established an automated Wide Bandgap Characterization Test Station which accurately performs static and dynamic characterization analyses of new devices over expanded temperature ranges (Figure 1). Using the parameters obtained through testing, models of these components can be created which can then be used in simulations to assess the benefits of their operation in power electronics applications. A comprehensive database of these tests and device parameters is maintained at the Power Electronics and Electric Power Systems Research Center at ORNL.

Figure 1: Wide Bandgap Characterization Test Station.

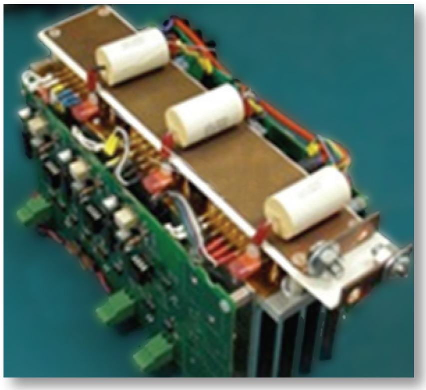

Figure 2: Prototype SiC junction field effect transistor (JFET) inverter.

Benefits

- *Evaluation of device performance provides insight into the development of maturing high temperature device technologies.*
- *Potential for smaller automotive power converters that can operate at higher temperatures and efficiencies.*
- *Reduction in the capacitance required will enable higher temperature operation.*

Status

Numerous WBG devices and modules have been tested to date. This year, state-of-the-art SiC and GaN devices and modules were analyzed as well as an all SiC 10 kW inverter (Figures 2 and 3). Simulations show that the use of these devices can result in 30% or more reduction in losses in the power electronics systems of a hybrid electric vehicle.

The feasibility study of an air-cooled inverter was also completed. Simulations show that the 55 kW inverter design, with a device temperature of Tj=200˚C, can achieve a power density of 12 kW/L.

Future activities will be to expand the testing capabilities through the development of fast gate drive circuits and a new current source for double pulse testing. Additionally, Simulation Program with Integrated Circuit Emphasis (SPICE), a circuit simulation software model development will be initiated to aid in ORNL packaging work over the next few years.

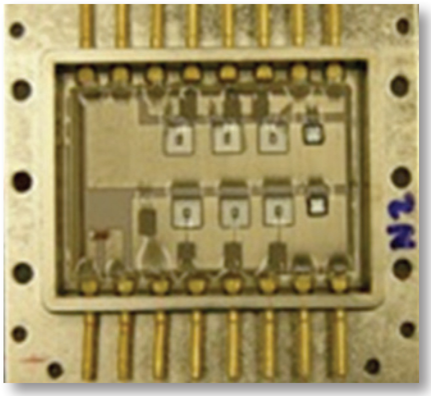

Figure 3: SiC JFET phase leg module.

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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 vehicles.

Oak Ridge National Laboratory estimates that the Fuel Economy Information Program reduced U.S. petroleum consumption by more than half a billion gallons in 2009 (Figure 1).

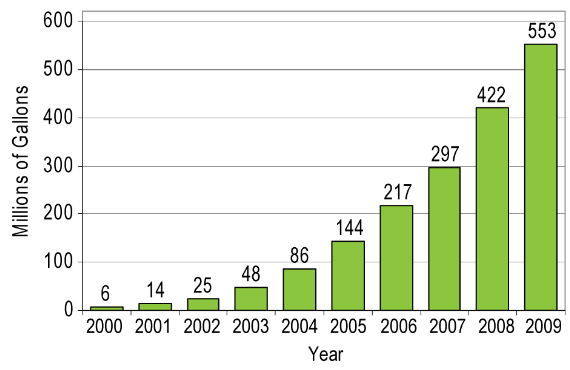

Figure 1: Estimated fuel savings by year from the Fuel Economy Information Program.

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 tens of millions of consumers each year (more than 39 million user sessions in 2009).*
- *Estimated to have reduced U.S. petroleum consumption by more than 500 million gallons in 2009.*
- *In 2008, more than 1,200 television, Internet, radio, and print sources shared site information, providing reliable fuel economy information to their audiences. Media outlets include CNN, CBS News, and USA Today.*
- *In 2009, served as the principle information site for consumers participating in the "Cash-for-Clunkers" program.*

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 has just completed 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. In 2009 (Oct. 2008–Nov. 2009), the site hosted more than 39 million user sessions (Figure 2). The site is a nationally established resource for fuel economy information. In 2008, more than 1,200 television, Internet, radio, and print articles featured the site or information from the site.

Fueleconomy.gov played a critical role in the 2009 "Cash-for-Clunkers" program. Presented as part of the cars.gov Web site, fueleconomy.gov hosted all the consumers seeking to determine whether their trade-ins and intended purchases qualified for the program and also supplied the data for validating transactions submitted by car dealers.

In 2009, ahorremosgasolina.org, a Spanish language version of fueleconomy.gov, was launched. With this new Web site, Spanish speakers can more easily make fuel economy comparisons and access energy efficient driving tips.

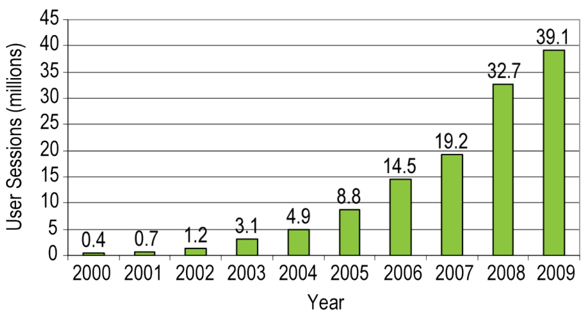

Figure 2: Fueleconomy.gov user sessions by year, showing dramatic increases in use since its launch in 1999.

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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.

Energy Storage Technologies

Coupled Kinetic, Thermal, and Mechanical Modeling of Focused Ion Beam Micromachined Electrodes

Background

Development and design of electric vehicles (EVs), hybrid, plug-in hybrid, and all electric, is one of the primary research directions for reduction of vehicle emissions and reduction of U.S. dependence on foreign oil. Lithium- (Li-) ion-based electrochemical energy storage technology is the primary candidate for the electrification of vehicle drivetrains. Ongoing collaborative research between companies and research institutions provides evidence of the high potential for use of Li-ion batteries in EVs. However, despite the attractive features of Li-ion battery systems and a wide range of applications in smaller scale devices such as consumer electronics, the service life of Li-ion battery systems is still limited due to degradation of electrode materials with repeated charging and discharging cycles.

Technology

It is commonly accepted that Li-ion battery life is limited due to continuous capacity loss. During battery operation, Li ions are shuttled between cathode and anode when the battery is being charged and discharged. One of the degradation mechanisms is related to the development of internal stresses in electrode particles due to repeated Li insertion and removal. The stresses ultimately result in cracks in and fracture of particles. To explore the mechanical side of battery degradation mechanisms, Oak Ridge National Laboratory has partnered with the University of Michigan on a project using the equipment and intellectual capabilities of both institutions, as well as those of the Shared Research Equipment Collaborative Research Center of the U.S. Department of Energy Office of Science, Basic Energy Science Program. The project targets the fundamental understanding, description through mathematical modeling, and controlled experimental validation of internal stress generation in and morphology change of electrode particles in Li-ion batteries.

Status

Experiments are being performed on model systems represented by microscopic specimens of electrode material. The modeling work is being done on preselected geometries of specimens to

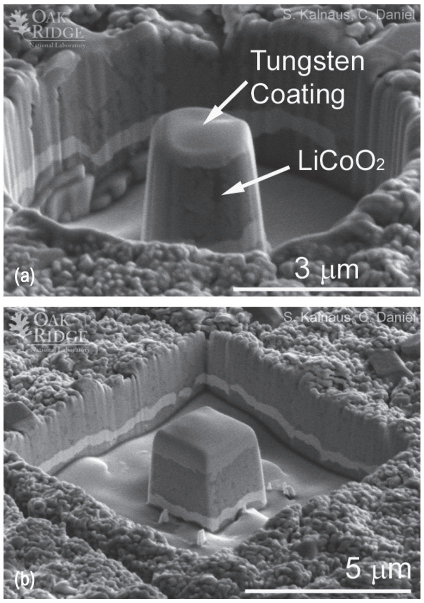

Figure 1: FIB machined specimens with: (a) circle and (b) square as a base shape.

Benefits

- *Fundamental understanding of electrode failure mechanisms.*
- *Model development for accurate life prediction.*
- *Guidance for future development of novel electrode materials and structures with longer life and higher performance.*

validate the constitutive approach. Different cathode materials are being investigated, including $LiCoO_2$, $LiMn_2O_4$, and $Li_4Ti_5O_{12}$. At the preliminary stage, sample electrode specimens were micromachined from the layer of $LiCoO_2$ deposited by physical vapor deposition on the gold current collector. Fabrication of samples was performed using a Hitachi NB5000 dual beam focused ion beam– (FIB–) scanning electron microscope (SEM). Two of the samples are shown in the SEM pictures in Figure 1.

Preliminary computational results were obtained based on a cylindrical homogenous $LiMn_2O_4$ particle. Intercalation-induced stresses during a discharge process (current density i = 2 A/m^2) were simulated using a stress-diffusion coupling model. Three cases were considered to quantify the stress level (Figure 2): (a) a single particle, (b) two agglomerated particles, and (c) two particles combined by a polyvinylidene fluoride (PVdF) binder.

Figure 2 shows the von Mises stress distribution at the end of the discharge process, where the Li concentration reaches the stoichiometric maximum. In a single particle [case (a)], the stress is larger along the upper edge, where the gradient of lattice spacing is more severe. In case (b), there is a stress concentration at the connection between two particles. However in case (c), there is no stress gradient around that connection due to the presence of Li-free binder, and the stress level and distribution are similar to the case of a single particle.

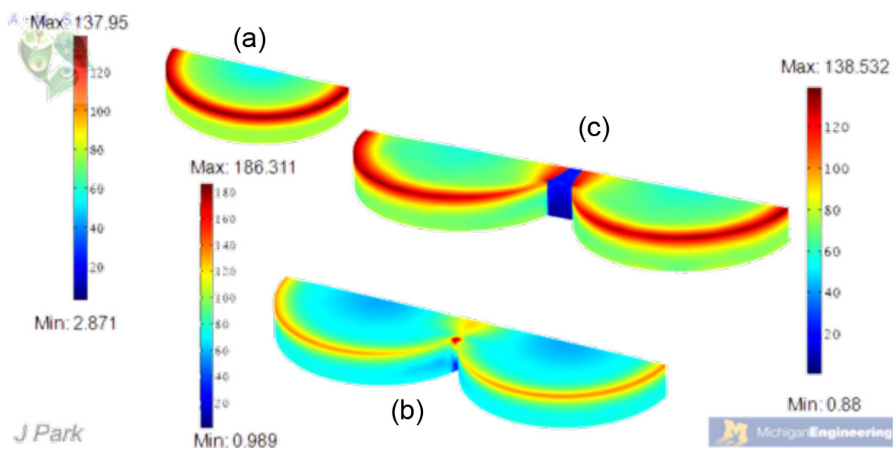

Figure 2: Von Mises stress distribution (in megapascals) in cathode particles at the end of discharge: (a) = the single particle case, (b) = two agglomerated particles, and (c) = two particles combined by a PVdF binder.

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Energy Storage Technologies

Use of Acoustic Emissions for Understanding Degradation in Anode Materials for Lithium Ion Batteries

Background

Volume changes during cycling are typical of intercalation compounds in batteries. Related stress and strain can cause mechanical degradation. The role of mechanical degradation in capacity fade is under debate. A fundamental understanding of the accumulation of point defects, crack initiation, crack growth, and particle fracture and sliding is needed to understand their roles in capacity fade. An understanding of those mechanisms in different intercalation compounds can be used to develop "fatigue-like" models to create better lifetime predictions and guidance for microstructure design of advanced electrodes.

Technology

Acoustic emission (AE) spectroscopy is used to detect, sort, and classify mechanical events such as crack initiation, crack growth, particle or coating fracturing, and particle loosening and sliding during cycling. We plan to use additional characterization methods such as x-ray diffraction, Raman spectroscopy, and various microscopy techniques in situ to link acoustic signatures to "real" events. This will allow for a deeper fundamental understanding of those mechanisms and their contributions to capacity fade. In a later stage of the project, "fatigue-like" models will be developed that can predict cycle life and guide advanced microstructure development for improved mechanical performance (Figure 1).

Status

Initially, carbon electrodes were studied. Future studies will include a variety of other electrode materials. Several classes of events were identified from the AE data. Type 1 emissions may result from crack initiation or propagation in the solid-electrolyte interphase (SEI) layer that develops on and around individual mesocarbon microbead (MCMB) particles. Other authors have associated emissions similar to Type 2 with gas formation. Because CO_2 is a by-product of SEI formation, the formation of CO_2 bubbles is a likely cause of this emission type. A Type 3 emission is characteristically very similar to a Type 2, but with a less-defined waveform and frequency peak

Figure 1: An x-ray diffractometer is used to evaluate how battery materials change during charges and discharges.

Benefits

- *Establish methodology for detection and monitoring of mechanical degradation in lithium ion batteries.*
- *Develop understanding of the relationship between mechanical degradation and capacity fade.*
- *Develop guidance for future battery materials and structure developments.*

average and duration. The cause of this event type is unclear, but it may result from either shifting of the MCMB particles past one another as they expand and contract or tearing of the composite film.

Events were manually sorted into class types and were put in a scatter plot to establish grouping trends. The values of an event's duration, amplitude, and frequency centroid parameters proved particularly important in discriminating between different event types. Amplitude was very useful in filtering electromagnetic interference events that showed very regular emission amplitudes. The duration, amplitude, and frequency centroid proved to be statistically different between Type 1, 2, and 3 emissions based on Student's t-tests with 95% confidence. Figure 2 shows a scatter plot matrix of these three parameters.

A scanning electron microscope (SEM) image of the cycled electrode showed the presence of a fractured SEI layer (see Figure 3). The formation of these cracks is the most likely source of Type 1 events. SEM images of the electrodes in cross section showed a 28% increase in thickness, from 25 to 32 μm, as a result of cycling. This may indicate a loosening of the composite film as cycling proceeds, which may allow for an increased amount of particle shifting and hence the observed increase in Type 3 emissions as cycling proceeds.

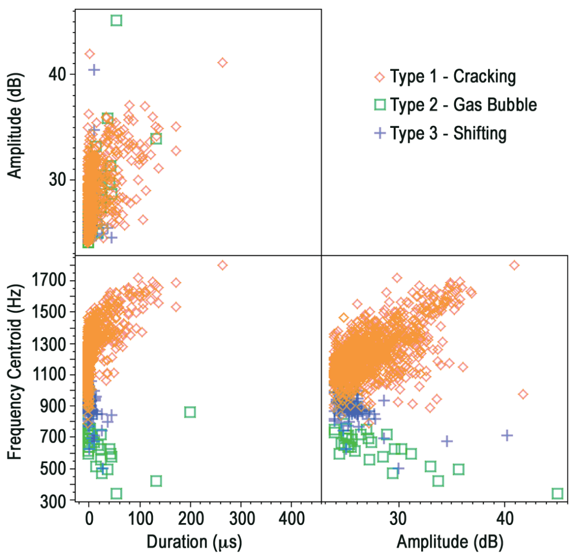

Figure 2: Scatter plot of duration, amplitude, and frequency centroid showing grouping of emissions useful for identifying event types.

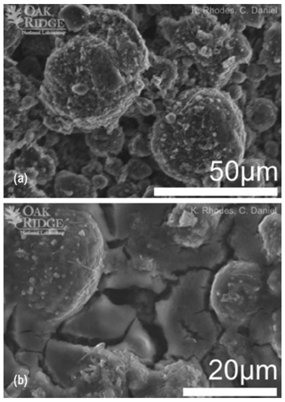

Figure 3: Scanning electron micrograph of (a) a fresh MCMB electrode and (b) the electrode after cycling, showing a fractured SEI layer.

Parts of this research were performed at the High Temperature Materials Laboratory, a National User Facility sponsored by the U.S. Department of Energy, located at ORNL.

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Fuels, Engines, and Emissions

Achieving & Demonstrating the FreedomCAR Efficiency Milestones for Advanced Combustion Engines

Background

The U.S. Department of Energy (DOE) FreedomCAR roadmap has established efficiency and emissions goals for the next several years, one of which is achieving a 45% peak brake thermal efficiency (BTE) 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.

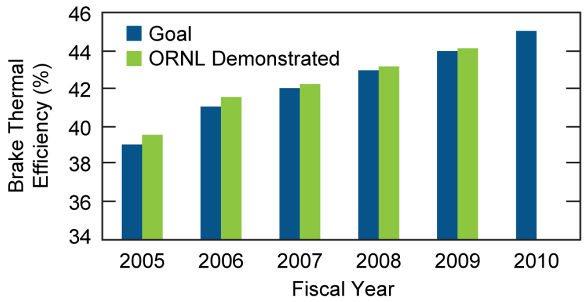

Figure 1: On path to demonstrating FY 2010 FreedomCAR engine and efficiency milestones including 45% peak brake thermal efficiency.

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 advances in engine efficiency. A fundamental thermodynamics perspective, simulations, and laboratory experiments are being used to provide guidance on developing and evaluating a path for meeting 2010 and intermediate milestones and to provide longer term insights into the potential of future high efficiency engine systems.

A peak BTE of 44.1% has been demonstrated on a light duty diesel engine through a combination of engine shaft power and electrical power generated from the exhaust heat of the engine with an organic Rankine cycle. This is an interim milestone on the path to the 2010 FreedomCAR goal of 45% peak BTE and Tier 2 Bin 5 emissions (see Figure 1). Advanced engine technologies identified and investigated in FY 2009 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.

The organic Rankine system produced 2.9 kW of net power from the exhaust heat. Simulations indicate the potential to generate 3.8 kW of net power at the peak efficiency engine condition, which would correspond to a combined engine-system BTE of more than 45% BTE. A picture of the system is shown in Figure 2. The potential

Benefits

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

impact of recovering this discarded thermal energy on fuel economy improvements over a light duty vehicle drive cycle is also being investigated with composite modal experiments and vehicle simulations. These approximations indicate potential fuel savings on the order of 8% with conservative thermal energy recovery estimates.

This activity makes use of research results from internal Oak Ridge National Laboratory (ORNL) activities, other national laboratories, universities, and industry. Internal ORNL activities include those focused on advanced combustion processes, aftertreatment, fuels, and unconventional approaches to improve combustion efficiency. The progress and results of these activities 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 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 processes and appropriate aftertreatment systems. Demonstration and verification will be accomplished with on-engine experiments and vehicle system modeling.

Figure 2: Organic Rankine cycle which is being used to convert exhaust heat to electrical power on a 1.9 L General Motors diesel engine.

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Fuels, Engines, and Emissions

FreedomCAR and Fuel Partnership Highlight: Study of Water-Gas Shift Kinetics in LNT Leads to Method for Monitoring Aging Process

Background

Diesel engines are known to be more efficient than typical gasoline or spark ignition engines—at a price: higher nitrogen oxide (NO_X) and particulate emissions. One way of dealing with the NO_X emissions is lean NO_X trap (LNT) technology, a catalytic process for removing NO_X from exhaust streams. During operation, however, the catalysts also absorb sulfur from the exhaust streams, referred to as sulfur poisoning, which inhibits catalyst performance and hence the ability to remove NO_X.

Monitoring of LNT sulfur poisoning and aging is extremely important. Without the ability to directly monitor the catalyst state, LNTs must be overdesigned (i.e., using larger sizes and excess precious metal loadings—increasing cost and weight) to ensure adequate NO_X control performance during transient driving conditions and over the catalyst lifetime. Similarly, more frequent regeneration and onboard high-temperature catalyst desulfations are required, which increase LNT fuel penalty and tend to exacerbate aging and loss of catalyst function.

Technology

Under Cooperative Research and Development Agreements with Cummins Inc. and the U.S. Department of Energy Cross-Cut Lean Exhaust Emissions Reduction Simulations activity, Oak Ridge and Pacific Northwest National Laboratories (ORNL and PNNL) have been studying the detailed physicochemical mechanisms of LNT sulfur poisoning, sulfur removal, and precious metal sintering under laboratory reactor and engine test-stand conditions. These studies have included highly specialized measurements using techniques such as spatially resolved capillary inlet mass spectrometry (SpaciMS), for which a team from Cummins and ORNL won an R&D 100 award in 2008, and diffuse reflectance infrared Fourier transform spectrometry (Figure 1).

As a result, ORNL and PNNL have provided important new information about the role of the water-gas shift reaction (WGSR) during NO_X reduction (the rich phase) in LNTs.

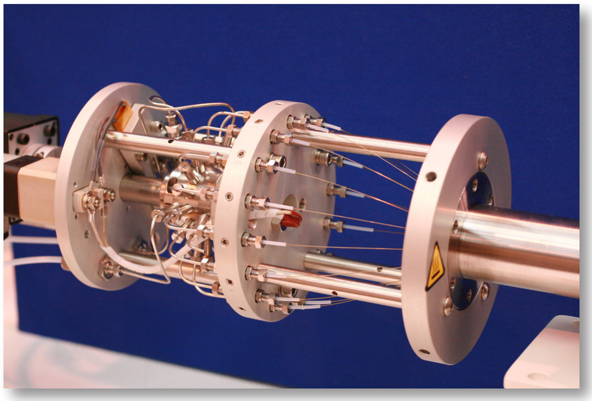

Figure 1: Spatially resolved capillary inlet mass spectrometer (SpaciMS).

Benefits

- *Active tracking of LNT catalyst state is enabled by a combined understanding of how WGSR varies with sulfation and aging and how WGSR-generated H_2 biases oxygen (lambda) sensor readings.*
- *Monitoring oxygen sensor shifts enables continuous tracking of LNT catalyst state over time and thus optimization of the engine and device operating strategies to maximize fuel efficiency, durability, and emissions control performance during highly transient driving conditions.*
- *Use of existing exhaust gas oxygen sensors for improved monitoring of LNT catalyst state won't add to vehicle cost or weight.*
- *Improved control will mean less need for overdesigning LNT hardware and control strategies and thus cost and weight savings.*

In WGSR, exhaust carbon monoxide is transformed into carbon dioxide and hydrogen (H_2). ORNL and PNNL have provided fundamental information on the correlations between WGSR and other catalyst chemical functions and how these activities vary with catalyst sulfation and aging state (Figure 2). This type of fundamental information is required to implement advanced-efficiency control systems.

Status

The fundamental insights provided by the ORNL-PNNL research supported Cummins's development and implementation of a new concept for LNT onboard diagnostics (OBD) that allows the state of LNT aging to be directly monitored using existing exhaust gas oxygen sensors. One version of this novel active OBD method has been used by Cummins as the basis of patent application 20080168824.

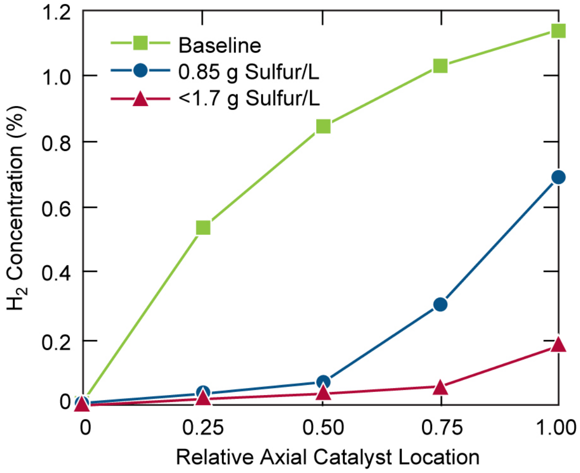

Figure 2: Effect of sulfur concentration on WGSR and H_2 generation along the length of the catalyst. As sulfur exposure increases, less H_2 is produced via WGSR with the effect being most dramatic in the front half of the catalyst.

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Fuels, Engines, and Emissions

Intermediate Ethanol Blends Test Program

Background

The Energy Independence and Security Act of 2007 calls on the nation to significantly increase its use of renewable fuels to meet its transportation energy needs. The law expands the renewable fuel standard (RFS) to require use of 36 billion gallons of renewable fuel by 2022. Given that ethanol is the most widely used renewable fuel in the U.S. market, ethanol will likely make up a significant portion of the 36-billion-gallon requirement.

Most of the ethanol used in the United States is blended with gasoline to create E10—gasoline with up to 10% ethanol. The remaining ethanol is sold in the form of E85—a gasoline blend with as much as 85% ethanol that can only be used in flexible-fuel vehicles (FFVs). Consumption of E85 is currently limited by both the size of the FFV fleet and the number of E85 fueling stations.

Because our annual gasoline consumption is currently about 140 billion gallons, the maximum amount of ethanol as E10 that could be absorbed by the market is only about 14 billion gallons. Given projected growth in ethanol production and the new RFS, most analysts agree that the E10 market will be saturated in the next few years, possibly as soon as 2010. This situation has been termed, the "blend wall" (Figure 1). Although the U.S. Department of Energy (DOE) remains committed to expanding the E85 infrastructure, that market represented less than 1% of the ethanol consumed in 2007 and will not be able to absorb projected volumes of ethanol in the near term. Given this reality, DOE and others are assessing the viability of using intermediate ethanol blends (E15 or E20) as a way to accommodate growing volumes of ethanol (Figures 2 and 3). Before intermediate blends can be introduced into the nation's fueling infrastructure, their effects on the emissions and performance of vehicles and nonroad engines, which were designed to run on gasoline with 0–10% ethanol, must be determined. In fact, provisions of the Clean Air Act prohibit the introduction into commerce of fuel that could cause vehicles or engines to fail to meet emission standards over their useful lives. Data on intermediate ethanol blends are, therefore, critical to this issue.

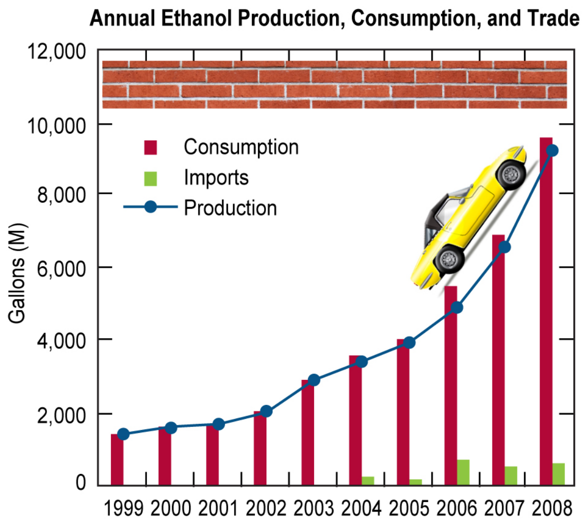

Figure 1: Illustration of the "blend wall" where maximum use of ethanol as E10 hits limit.

Figure 2: Many vehicle dynamometer laboratories, such as this one at ORNL, are involved in the intermediate blends test program.

Program Description

In 2007, DOE initiated the Intermediate Ethanol Blends Test Program to evaluate the potential impacts of intermediate ethanol blends on legacy vehicles and other engines. The program has been co-led and funded by the DOE Office of Energy Efficiency and Renewable Energy (EERE) Biomass Program and the EERE Vehicle Technologies Program with technical support from Oak Ridge National Laboratory (ORNL) and the National Renewable Energy Laboratory. Before designing the test program, DOE tasked ORNL to conduct a literature search on the subject, which indicated that insufficient data exist to predict the impacts of these fuels on U.S. vehicles and engines. The DOE team collaborated with industry, the Environmental Protection Agency, and other experts regarding the development and implementation of the test program. A number of automotive and nonroad engine manufacturers provided significant input into the test protocols. This collaboration has typically been coordinated through industry organizations such as the U.S. Council for Automotive Research, the American Petroleum Institute, the Coordinating Research Council (CRC), the Outdoor Power Equipment Institute, the Alliance of Automobile Manufacturers, and the Association of International Automobile Manufacturers.

The intermediate blends program encompasses roughly 12 different, coordinated activities for vehicles and nonroad engines including the following focus areas:

- emission control durability,*
- regulated and unregulated tailpipe emissions,*
- fuel economy,*
- materials compatibility,*
- driveability (or operability in the case of nonroad engines), and
- evaporative emissions.

*Areas of focus for ORNL

Status

As of October 2009, the intermediate blends test program involves 65 cars, and between DOE and CRC, reports have been published with data for about 30 vehicles and 28 engines. Some of the key findings are summarized below.

Vehicles

Emissions/Catalyst Temperature

- Regulated tailpipe emissions with E15 and E20 were similar to levels with E0 when averaged across multiple newer "clean" vehicles in the pilot study.
- Changes in catalyst temperatures were observed and may affect durability—results not yet clear.

Driveability (via informal observations)

- No driveability issues found with either E15 or E20.
- No malfunction indicator lights or fuel filter plugging.

Fuel Economy

- Volumetric fuel economy decreased for E10, E15, and E20.
- Closely tracked fuel energy content.

Emissions system durability is under investigation in an 82 vehicle study at three sites.

Small Nonroad Engines

Emissions/Temperature. With increasing ethanol content—

- regulated emissions—combined hydrocarbons (HC) and oxides of nitrogen (NOx) largely unchanged due to counteracting HC decrease and NOx increase and
- engine and exhaust temperatures increased.

Durability

- commercial engines—no particular sensitivity observed.
- smaller, residential engines—results not clear.

One potential safety issue was observed: unintended clutch engagement on line trimmer due to increased idle speed with ethanol blends (correctable in this case with carburetor adjustment).

Figure 3: Mileage accumulation dynamometers at Southwest Research Institute used for the emission control durability part of the program. Two other subcontractors are also assisting with the vehicle aging project.

Publications Resulting from the Program

- R. Bechtold, et al., *Technical Issues Associated with the Use of Intermediate Ethanol Blends (>E10) in the U.S. Legacy Fleet*, ORNL/TM-2007/37, August 2007.
- Keith Knoll, et al., *Effects of Intermediate Ethanol Blends on Legacy Vehicles and Small Non-Road Engines,* Report 1—Updated, NREL/TP-540-43543 and ORNL/TM-2008/117. Jointly published by the National Renewable Energy Laboratory and Oak Ridge National Laboratory, February 2009. Available online at http://feerc.ornl.gov/pdfs/pub_int_blends_rpt1_updated.pdf.
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Fuels, Engines, and Emissions

Optimizing Spark Ignition Engines for Ethanol

Background

Research performed by Oak Ridge National Laboratory and Delphi Automotive Systems Corporation shows progress toward reducing the indicated specific fuel consumption (ISFC) difference between regular gasoline (RG) and E85 (85% ethanol : 15% gasoline blend). Using a research engine with a hydraulic valve actuation system that allows for complete control of intake/exhaust valve duration and timing, the approach takes advantage of unique fuel properties of ethanol to help reduce the mile-per-gallon penalty caused by the lower energy content of ethanol. Blended ethanol functions to increase the knock resistance of gasoline, or octane number, allowing higher engine compression ratio (CR), a primary parameter affecting efficiency (Figure 1).

Technology

CR was changed in this study with custom designed pistons. To maintain compatibility with gasoline at high CR, the engine is operated with an early or late intake valve closing (EIVC or LIVC) strategy. These strategies serve to reduce the effective CR, which prevents knock but also reduces the effective displacement of the engine, resulting in reduced power.

Status

Example results (Figure 2) show that E85 produces about 10% more power and is 2–3% more efficient than RG at comparable engine conditions and a CR of 9.2 (i.e., constant engine speed, wide-open throttle, and not knock limited). At a higher CR, efficiency and power for E85 continue to increase because spark timing is not knock limited. For RG, spark advance is knock limited, so an EIVC or LIVC control strategy is used to derate the engine and prevent knocking. These strategies maintain or increase the efficiency for RG as CR increases, but the increase is modest compared to E85. The net effect is that the fuel consumption gap between E85 and gasoline is decreased by about 20%, and does not come at an efficiency penalty for RG. Also significant is a decrease in engine power for RG, represented here as indicated mean effective pressure (IMEP). At the highest CR, the maximum power for E85 is 34% higher than that for RG.

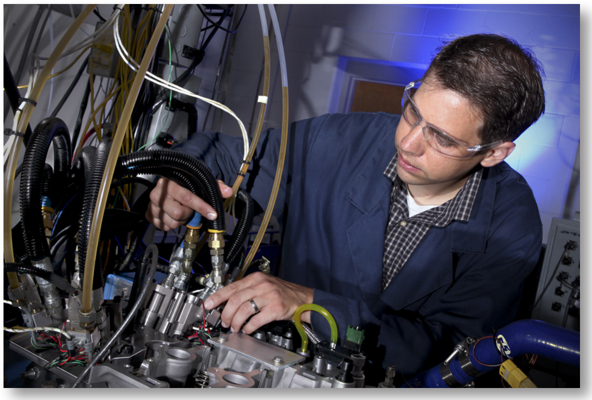

Figure 1: Researchers use a variable valve-train engine to evaluate different types of fuels, including ethanol blends, and their effects on a combustion engine.

Benefits

- *E85 operates more efficiently than RG at all operating conditions, although the difference is more significant at high CR.*
- *The fuel consumption gap between RG and E85 is reduced by about 20% at the highest CR.*
- *This research shows that an engine optimized for E85 can produce both a higher thermal efficiency and a higher power output with E85 than with gasoline.*

In another aspect of this program, a multicylinder engine with a flexible cam-based valve train has been configured. Multiple cam profiles and a high degree of cam phasing authority allow EIVC and LIVC operation for reducing the effective CR for knock-prone fuels at high loads and for operating unthrottled over a large portion of the engine map with all fuels. Cam profiles and operating strategies have been developed for the full engine map using GT-POWER (engine simulation tool from Gamma Technologies Inc.). The engine has been built, and engine baselining is currently underway.

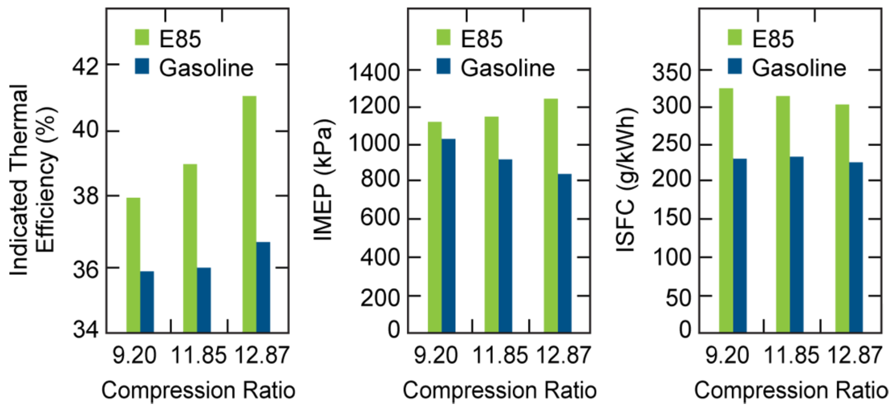

Figure 2: Comparison of E85 and regular gasoline at three compression ratios. Operating condition: 1,500 RPM, maximum power.

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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.

Fuels, Engines, and Emissions

Real-Time On-Engine Measurement of Oil Dilution by Fuel

Background

Diesel engine technology has advanced significantly over the last decade. Modern diesels use advanced injector technology to enable multiple injections of fuel per combustion cycle. Precise control of injection timing allows optimization of efficiency and emissions. Although diesel engines continue to operate cleaner, emission control devices in the exhaust are required to meet emission regulations for new diesel vehicles. Several of the emission control devices require active management, which means the engine is operated at specific conditions to control exhaust conditions for operation of the emission devices. Two example emission control devices requiring active management are the lean NO_x trap (LNT) catalyst and the diesel particulate filter (DPF). The LNT requires periodic net-fuel-rich operation to reduce NO_x emissions from the exhaust, and the DPF requires periodic heating of the filter to burn off collected particulate (soot) which was trapped during normal operation. In both cases, common engine control strategies entail injecting extra fuel into the engine cylinders at precise timing to control the chemistry and temperature in the exhaust system. However, extra fuel injection into the cylinder can lead to other issues such as torque control, noise and vibration control, and oil dilution. A Cooperative Research and Development Agreement (CRADA) between Oak Ridge National Laboratory (ORNL) and Cummins Inc. has addressed the potential problem of oil dilution that can occur when advanced in-cylinder fuel injection techniques are used on a diesel engine.

The conventional method for quantifying oil dilution is based on gas chromatography (GC) and involves extractive sampling and offline analysis. Using this methodology, a development engineer would design and run an engine test matrix and collect oil samples and send them out for analysis. The results from each measurement operation point would be received days later and correlated with the real-time performance data collected during the matrix run, and a new matrix would be designed. Thus, oil dilution analysis represents a significant delay in engine control development. Diagnostics that provide real-time on-engine assessment of oil dilution would significantly streamline the engine control development process. The CRADA has developed such a diagnostic and evaluated it on a running engine and in parallel with conventional GC methods.

Technology

Laser-induced fluorescence (LIF) spectroscopy is used to rapidly measure the fuel dilution of oil in situ (Figure 1). A fluorescent dye, commercially available and suitable for use in diesel fuel and oil systems, is added to the engine fuel. The LIF spectra are monitored to detect the growth of the dye signal relative to the background oil fluorescence; fuel mass concentration is quantified based on a known sample set. The diagnostic is based on

Figure 1: Fuel-in-oil technology provides for real-time, rapid feedback, on-engine assessment of oil contamination by fuel.

Benefits

- *Real-time tuning of the engine system.*
- *Optimization of performance criteria including power, exhaust composition, and durability.*
- *Significantly shorter engine-development time than conventional approaches.*

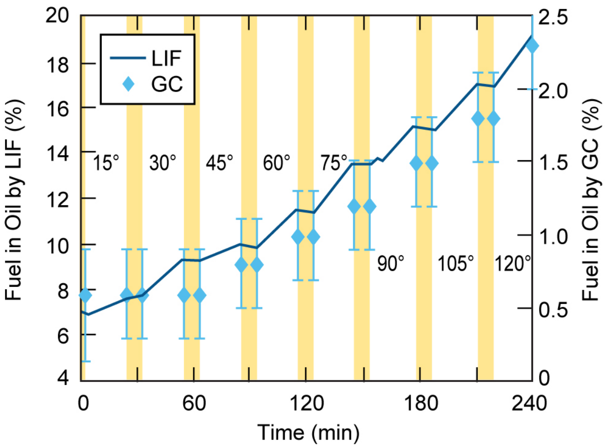

Figure 2: Comparison of LIF- and GC-based fuel-in-oil measurements. The shaded regions represent lean only operation. Lean-rich cycling caused fuel dilution to occur during periods between the shaded regions.

fiber optic probes for excitation light delivery and fluorescence collection; this allows flexibility of sampling location in the engine oil system and could even be implemented in the cylinder-wall oil film, where oil dilution is highest. A low cost 532 nm laser diode is used for excitation. Spectrally resolved fluorescence detection is effected via small fiber-coupled spectrometers. The diagnostic is portable.

Figure 2 shows oil-dilution variations with and without (shaded region) post injection and for various post injection timings. The timing of the additional fuel injection for rich combustion operation was varied while holding constant the minimum air-to-fuel ratio during the rich event. The main injection pulse was kept constant while the additional fuel was added at starting crank angles of 15º, 30º, 45º, 60º, 75º, and 90º past top dead center. Results of the conventional GC analysis are also shown. It is apparent from both the LIF and GC methods that oil dilution increases with post injection. The LIF technique has greater precision and sensitivity than the GC technique, which allows detection of smaller rates of dilution. Although the LIF- and GC-based dilution trends are similar, the magnitude of reported oil dilution differs by a factor of 7. The most likely explanation for the discrepancy is that the LIF technique is based on the dye, which does not evaporate from the oil like fuel components. Observations from this engine work lead to guidance for engineers to minimize fuel dilution during LNT regeneration strategy development and are outlined in SAE paper 2007-01-4108, which describes the diagnostic and engine applications.

Status

The oil-dilution diagnostic has been demonstrated on a Mercedes 1.7 liter engine at ORNL as well as on a partner engine. The methodology and instrument (Figure 3) have been transferred to Cummins. A license to implement the technology commercially has been acquired from ORNL by Da Vinci Emission Services.

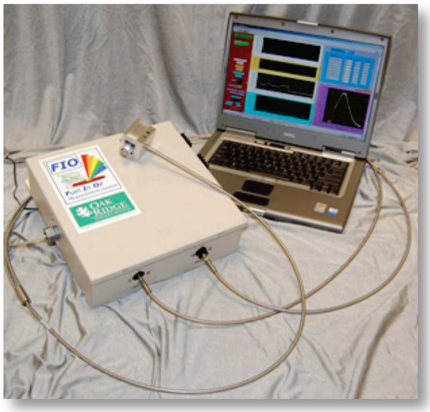

Figure 3: The fuel-in-oil instrument package is transportable and has been licensed for commercial use.

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A Strong Energy Portfolio for a Strong America

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Fuels, Engines, and Emissions

Reduction of Particulate Emissions While Maintaining High Efficiency Using Low-Cetane Fuels

Background

The Fuels for Advanced Combustion Engines (FACE) program was chartered as a working group of the Coordinating Research Council to develop a set of research fuels that could be used by many researchers to investigate advanced combustion technologies. By encouraging the use of common research fuels in many different combustion programs, the U.S. Department of Energy hopes to gain a broad view of the impact of fuel properties on advanced combustion technologies. The FACE working group, composed of stakeholders from engine manufacturers, car companies, energy companies, academia, and the national laboratories, proposed a set of nine diesel fuels (Figure 1) that are now offered for sale to users by Chevron-Phillips Specialty Chemical Company.

Technology

Researchers at Oak Ridge National Laboratory (ORNL) recently conducted a study on the impact of fuel properties using the FACE diesel fuels and a 1.9 liter General Motors diesel engine operating in low temperature combustion mode. The study was conducted at a low-power road-load condition (1,500 RPM and 2.6 bar brake mean effective pressure), and all fuels were evaluated at the same exhaust gas recirculation level.

When the best fuel injection timing was chosen for each fuel from a sweep of start of injection (SOI), the brake thermal efficiency (BTE) data showed that there was little, if any, penalty associated with the use of low-cetane-number fuels under these conditions [Figure 2(a)]. However, the soot levels with the low-cetane-number fuels were near-zero because of the extended mixing time afforded by the relatively long ignition delay [Figure 2(b)]. Oxides of nitrogen emissions were very similar for all the fuels, while use of the low-cetane-number fuels caused increases in hydrocarbon and carbon monoxide (CO) emissions. Comparison of the fuels at a fixed 50% burn location, however, resulted in efficiency penalties and further increases of hydrocarbons and CO associated with the use of low-cetane-number fuels.

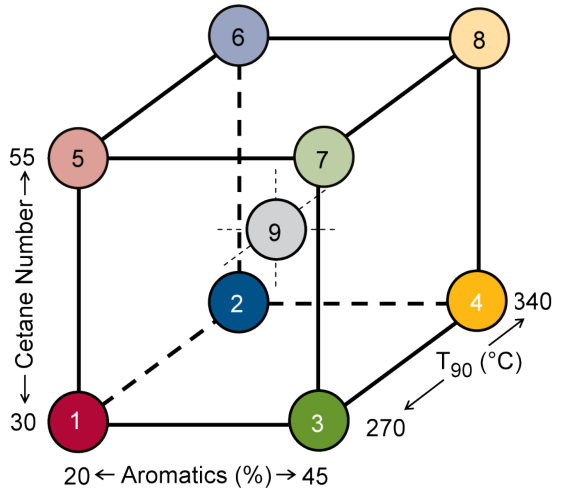

Figure 1: Graphical representation of the FACE fuels showing their relative aromatics (by percent), volatility (T90 in degrees C), and cetane number. FACE fuel 9 (at the center) is representative of an average marketplace fuel.

Benefits

- *It is possible to achieve essentially nonsooting combustion along with high part-load BTE in an engine through the use of low-cetane-number fuels (FACE fuels 1–4).*
- *Small reductions in cetane number may provide improved efficiency through combined optimization of the fuel with the engine and aftertreatment system.*

Status

Research using the FACE diesel fuels to further the understanding of fuel property impacts on efficiency and emissions performance of advanced combustion technology is ongoing.

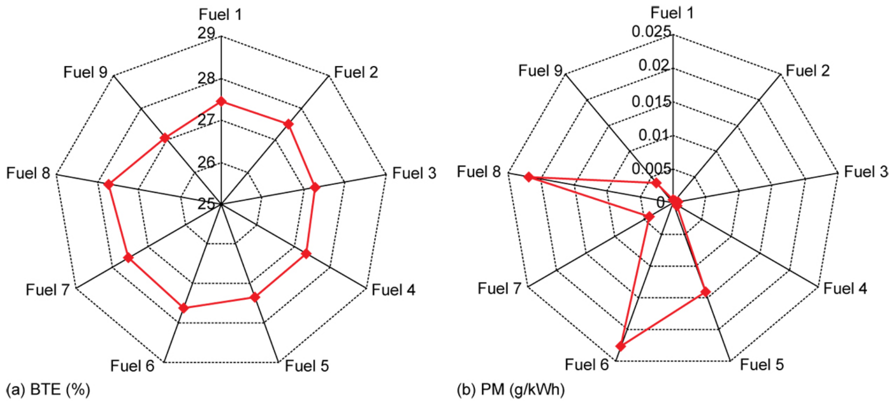

Figure 2: Results of the ORNL study of the FACE fuels showing (a) brake thermal efficiency (BTE) and (b) particulate matter (PM) emissions.

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High Temperature Materials Laboratory

User Projects on Automotive Lightweighting Materials

Background

The High Temperature Materials Laboratory (HTML) at Oak Ridge National Laboratory (ORNL) is a U.S. Department of Energy (DOE) User Facility that specializes in materials characterization and conducts collaborative materials research with industry, universities, and other research organizations. The HTML User Program's mission is to enable the development of materials-based, energy-efficient, and environmentally-friendly highway transportation technologies. As part of this mission, HTML supports the DOE Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program (VTP) automotive lightweighting activity through collaborations with users to characterize structural materials for applications that significantly reduce the weight of passenger vehicles without compromising vehicle performance, safety, life-cycle cost, or recyclability. As a result of these collaborations and the unique measurement and test capabilities at HTML (described below), HTML users are gaining a better understanding of and contributing to the knowledge base on the properties of polymer composites, high-strength steel, carbon fibers, and lightweight metals for automotive and heavy truck components.

User Projects

1. Innegrity LLC, the manufacturer of Innegra S thermoplastic fibers for composite reinforcement, has been working with HTML researchers to characterize and better understand the high strain rate tensile properties of Innegra S yarns and hybrid composite panels fabricated with Innegra S yarns and fiberglass or carbon fibers. The fiber's use as an impact energy enhancing reinforcement in hybrid composite automotive applications is currently being evaluated.

2. Representatives from the Automotive Composites Consortium and Multimatic Engineering Group have been using HTML's test machine for automotive crashworthiness (TMAC) to evaluate the high-rate strength of hybrid steel-composite joints for structural composite vehicular underbodies. The results from these tests are being used to calibrate models being developed by Multimatic. High-rate tensile tests using TMAC will be carried out as a follow-on task for this project (Figure 1).

Figure 1: Test machine for automotive crashworthiness (TMAC).

Benefits

- *Development of models for lightweight structural materials that enable producing lightweight materials with improved properties and 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.*
- *Development of 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.*

3. Plasan Carbon Composites, a leading supplier of carbon fiber parts and assemblies in the United States, is developing an automotive door system using composite materials to reduce weight while ensuring the safety of passengers during side impact collisions. Representatives from Plasan and two potential manufacturers visited HTML to evaluate the effect of fiber architecture and strain rate on the flexural strength of braided composite structures for automotive door systems, using TMAC to perform tests at a constant crosshead speed in a three-point bend configuration (Figure 2). Preliminary results from these tests show that braided structures over foam cores are significantly stronger than plain pultruded composite beams without cores. Plasan expects to redesign their composite beams to take advantage of the lessons learned at HTML. Ultimately the results from this project will facilitate the introduction of these composite structures in automotive applications.

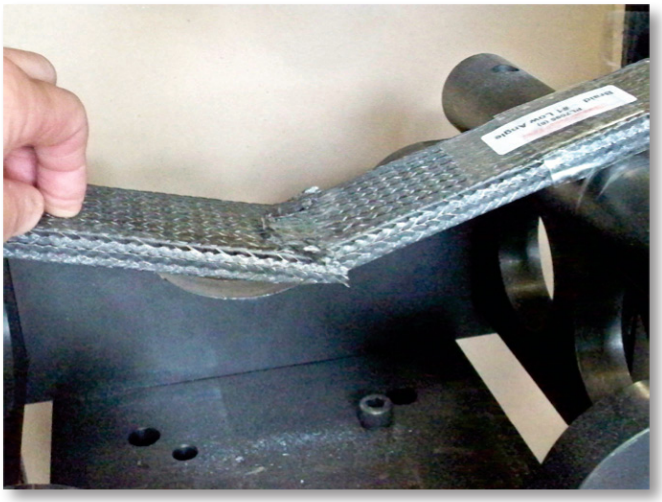

Figure 2: Braided composite after a high-rate impact test.

4. In a project jointly funded by the National Science Foundation (NSF) and DOE through the DOE-NSF cooperative effort known as the Faculty and Student Teams Program, researchers from Michigan State University teamed with researchers from Magna Cosma International and HTML to investigate the impact of shot peening on the fatigue life of an automotive aluminum alloy (A356.2) using HTML's x-ray diffraction residual stress mapping facilities (Figure 3). If the fatigue lives of the shot-peened plates are significantly longer than those for the baseline (not shot-peened) material, then Magna Cosma will use this technique for preparing alloys it supplies to automobile manufacturers.

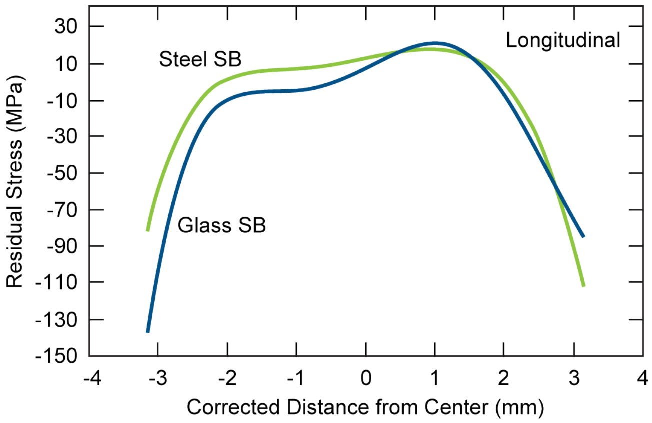

Figure 3: Residual stress results based on the measured d-spacings through the thicknesses of 6.2 mm thick aluminum plates that had been shot-peened with glass and steel beads.

5. Using the Second Generation Neutron Residual Stress Mapping Facility (NRSF2) at ORNL's High Flux Isotope Reactor, researchers from the Mississippi State University Center for Advanced Vehicular Systems are working with HTML's Dr. Cam Hubbard to develop predictive models for spot welding automotive steel sheets (Figure 4). Such models will enable improved control of the entire process, leading to energy savings. A validated model for stresses from spot welding will enable predictions of fatigue life and crack resistance in spot welded panels in vehicles and thus improve reliability. One key finding from the study is that the spot welding process is not symmetrical across welded sheets and, hence, cannot be simply modeled.

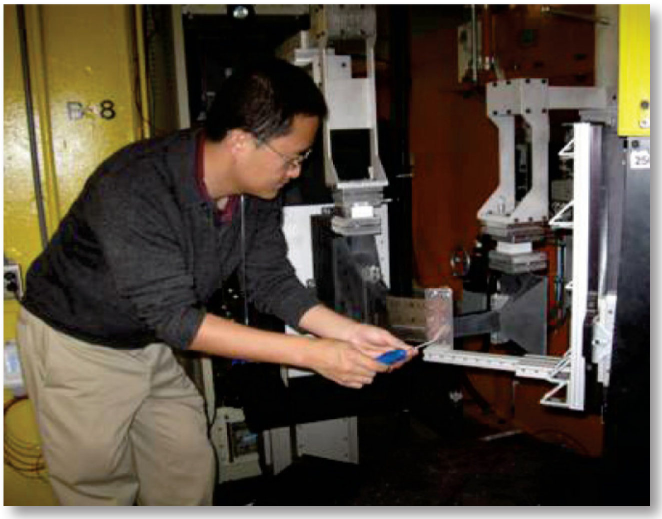

Figure 4: Mississippi State University's Dr. Liang Wang mounts a spot-welded sample at NRSF2.

6. Pratt & Whitney researchers Jim Lin and Gopal Das are working with HTML's Harry Meyer to characterize gamma titanium aluminide (TiAl) for high temperature applications such as turbocharger wheels. Results from this project could lead to greater use of gamma TiAl as a structural material, replacing denser materials, with consequent weight and fuel savings.

7. It has been estimated that substantial use of carbon fiber reinforced composites in automobiles could reduce automotive fuel demand by 20% to 30% per vehicle. However, the current high cost of carbon fibers is one factor limiting their greater use. As part of the DOE VTP Lightweighting Materials program, ORNL researchers are working to reduce the cost of carbon fibers by using lower cost precursors. Over the past year, the compressive elastic modulus of three different carbon fibers, from different precursors, has been investigated. Results indicate that carbon fiber from low cost textile-based precursors or textile grade carbon fiber (CF-T) compares favorably with aerospace grade carbon fiber (CF-A) and commodity grade commercial carbon fiber (CF-C) (Figure 5).

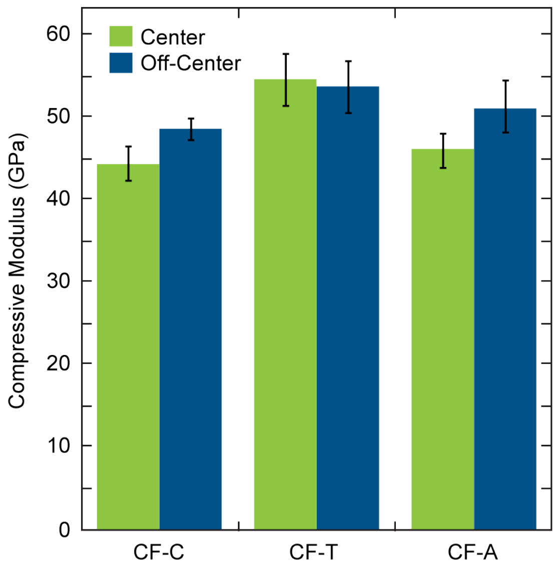

Figure 5: Compressive elastic modulus results for various types of carbon fiber.

8. Understanding different torsional deformation processes and the resulting residual stresses and the ability to predict them will enable design engineers to achieve weight reduction, and concomitant fuel savings, in the structural frames of heavy vehicles and automobiles while maintaining strength and fatigue-resistant properties. To this end, University of Tennessee doctoral student Jeffry Bunn and HTML's Cam Hubbard are using NRSF2 to develop microstructure-based models of deformation changes due to torsion and tension. Their results to date indicate that, when subjected to deformation by tension or torsion, ferritic steels show different intergranular stresses for torsion. This is the first report of different behavior due to the different loading mechanisms and thus will be valuable for developing materials deformation models for ferritic steels. Design engineers ultimately can use such models to predict properties and service life under complex load conditions exceeding yield.

9. As part of a larger project to develop property prediction tools to reduce fracture toughness quench rate sensitivity; to avoid tempered martensite embrittlement; to improve strength, abrasive wear resistance, and fracture toughness; and to lower the cost for wear-resistant, ground-engaging tool and undercarriage steels used in Caterpillar vehicles, Amy Clarke of Caterpillar and HTML's Tom Watkins used x-ray diffraction to determine the kinetics of embrittlement and quantify the amount of retained austenite in medium carbon, low alloy, high silicon steels. Ultimately, this project will help Caterpillar produce tougher, longer lasting, lighter weight parts, resulting in lower warranty costs and better fuel efficiency.

10. In two similar user projects, John Deere and HTML researchers are studying residual stresses—in welded structures and castings—to determine their impact on and improve fatigue life, develop a better understanding of manufacturing processes, and develop better process and prediction models. Ultimately this will enable Deere to lower warranty costs and potentially reduce the weight of vehicle components, thus saving money and reducing fuel needs.

High Temperature Materials Laboratory

User Projects on Lithium-Ion Batteries

Background

The High Temperature Materials Laboratory (HTML) at Oak Ridge National Laboratory (ORNL) is a U. S. Department of Energy (DOE) User Facility that specializes in materials characterization and conducts collaborative materials research with industry, universities, and other research organizations. The HTML User Program's mission is to enable the development of materials-based, energy-efficient, and environmentally friendly highway transportation technologies. In its support of the DOE Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program (VTP) goals, projects in the HTML User Program are 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 the HTML-operated X14A synchrotron beam line at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL), researchers from ORNL and BNL are investigating changes in electronic and crystal structures for both uncoated and carbon-coated (C-) cathode materials, including $LiFe_{1/4}Mn_{1/4}Co_{1/4}Ni_{1/4}PO_4$ and, more recently, C-$LiFe_{0.6}Mn_{0.4}PO_4$, during charge-discharge cycling (Figure 1). Detailed structural analyses of the phase transitions occurring during cycling are under way. These studies will enhance the understanding of the thermal stability of these cathode materials and the effects of their interactions with electrolytes, thereby supporting the VTP goals of safe batteries with improved energy and power density.

2. In a similar program, Massachusetts Institute of Technology (MIT) graduate students Nonglak Meethong and Yu-Hua Kao (Figure 2) are working with HTML researcher Jianming Bai at NSLS to investigate the solubility limits in lithium iron phosphate ($Li_{1-X}FePO_4$) battery cathode materials. The site occupancy location of dopants in alivolavent cation (Mg^{2+}, Al^{3+}, Zr^{4+}, Ti^{4+}, and Nb^{5+}) substituted olivine powders is of particular interest. The average defect structure of the crystallites, including crystallite size and microstrain, will be characterized, and changes in crystal structure with

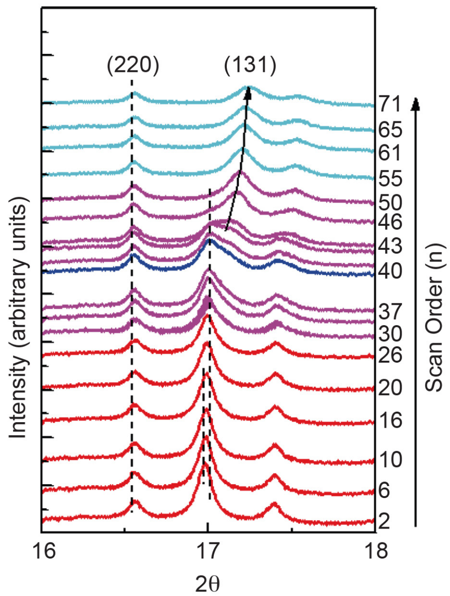

Figure 1: Detailed structure of the x-ray diffraction (XRD) pattern for C-$LiFe_{0.6}Mn_{0.4}PO_4$ during the first charging process. A small change in the XRD pattern of the first phase during the Fe^{2+} to Fe^{3+} oxidation (red lines) and the solid solution region for final phase (the fully delithiated compound) were observed. In contrast to the previously studied C-$LiFe_{1/4}Mn_{1/4}Co_{1/4}Ni_{1/4}PO_4$, no intermediate phase was observed in C-$LiFe_{0.6}Mn_{0.4}PO_4$.

Benefits

- *Improved safety and performance 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.*
- *Development of more durable and reliable batteries for electric vehicles.*

cycling under in situ conditions will be investigated in subsequent phases of the project. The reversibility and stability of such structural transformations determine the energy, power, and life of battery systems based on $Li_{1-X}FePO_4$. In addition, in situ studies may provide details of structural changes and their effect on the electrochemical properties of this class of materials. The knowledge developed from this research is expected to contribute substantially to the development of high performance lithium rechargeable batteries and thus play a major role in the effort to reduce worldwide petroleum consumption and greenhouse gas emissions.

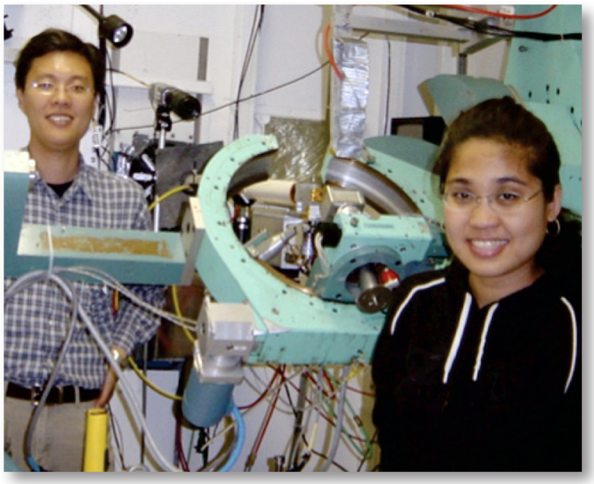

Figure 2: MIT graduate students Yu-Hua Kao (left) and Nonglak Meethong (right) at the NSLS X14A beam line.

3. Although thermal runaway is an important safety and reliability issue for lithium ion batteries, no standardized test methods have been established by battery manufacturers or the automotive industry to induce internal short circuits and assess their effect on the propensity of batteries to thermal runaway. In a cooperative project between ORNL and Motorola Energy Systems Group (MESG), Dr. Hossein Maleki of MESG is working with HTML staff member Dr. Hsin Wang to develop such a test. A particular focus of this project has been thermal diffusivity measurements because battery manufacturers are looking at ways to manage heat generated from internal shorts and are investigating methods to prevent cell temperatures reaching levels that result in thermal runaway. The data gathered from analysis of internal short circuits and thermal runaway (Figure 3) will be applied to developing a safer battery for use in electric vehicles, where a similar cell chemistry is used in large numbers of cells.

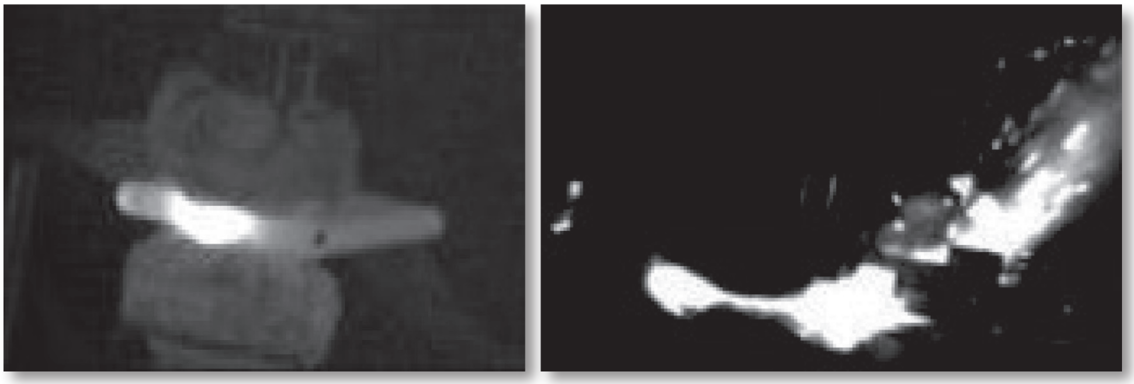

Figure 3: Infrared images of (left) a normal internal short and (right) a thermal runaway.

4. To develop a comprehensive understanding of material degradation and aging mechanisms in lithium ion battery cathodes, a team of researchers from Ohio State University (OSU) and ORNL are participating in an HTML User Project to quantify the thermal diffusivity of cathode materials with different degrees of degradation. The goal of this research is a better understanding of the dynamics of cathode surface aging, which might lead to safer, more durable lithium ion automotive batteries with greater energy and power density.

Figure 4: ORNL researcher Ralph Dinwiddie (left) and OSU graduate student Shrikant Nagpure (right) review data from thermal diffusivity tests of battery electrodes.

5. The electrification of transportation depends on the availability of energy storage devices with high energy and power density, low cost, a high degree of safety, and long service life. For typical electric or hybrid electric vehicles, batteries will be subjected to many charge-discharge cycles, and most of the lithium ion battery systems currently available exhibit a decrease in capacity and durability with cycling. ORNL researcher Claus Daniel, University of Tennessee graduate student Kevin Rhodes, and HTML director Edgar Lara-Curzio are collaborating to characterize the acoustic emissions associated with repeated charge-discharge cycling of lithium ion half cells (Figure 5). The results to date from this investigation have demonstrated the potential of acoustic emission analysis as a tool to monitor the occurrence of damage in lithium ion batteries. Furthermore, this analytical tool provides insights into both the mechanisms responsible for these occurrences and the strategies to mitigate their effects, resulting in the development of more durable and reliable batteries for hybrid and electric vehicles.

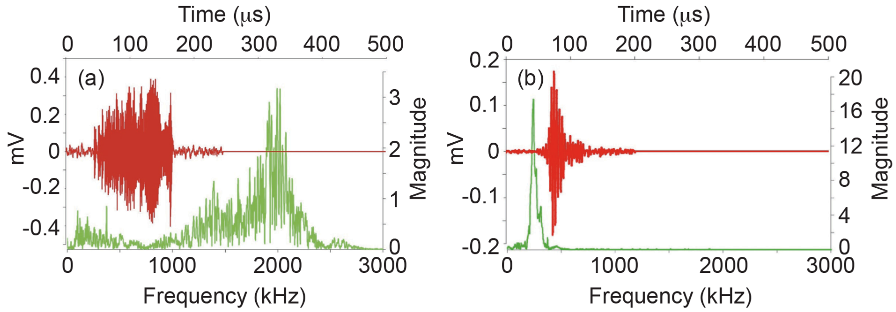

Figure 5: Acoustic emissions associated with charge-discharge cycling of lithium ion cell electrodes. (a) Type I acoustic emissions typically had frequencies above 1 MHz and an amplitude of 27 dB. (b) Type II acoustic emissions had an average frequency of 238 kHz and were associated with the formation of CO_2 bubbles.

High Temperature Materials Laboratory

User Projects on Catalysts

Background

The High Temperature Materials Laboratory (HTML) at Oak Ridge National Laboratory (ORNL) is a U.S. Department of Energy (DOE) User Facility that specializes in materials characterization and conducts collaborative materials research with industry, universities, and other research organizations. The HTML User Program's mission is to enable the development of materials-based, energy-efficient, and environmentally friendly highway transportation technologies. As part of this mission, HTML supports the DOE Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program emissions reduction goals through collaborations with users to characterize catalytic materials used in aftertreatment devices, fuel cell technologies, and biofuel production. As a result of these collaborations and the unique in situ heating and spectroscopic capabilities at HTML (described below), users are gaining a fundamental understanding of the behavior of these materials, which may lead to more effective emissions controls as well as new energy sources.

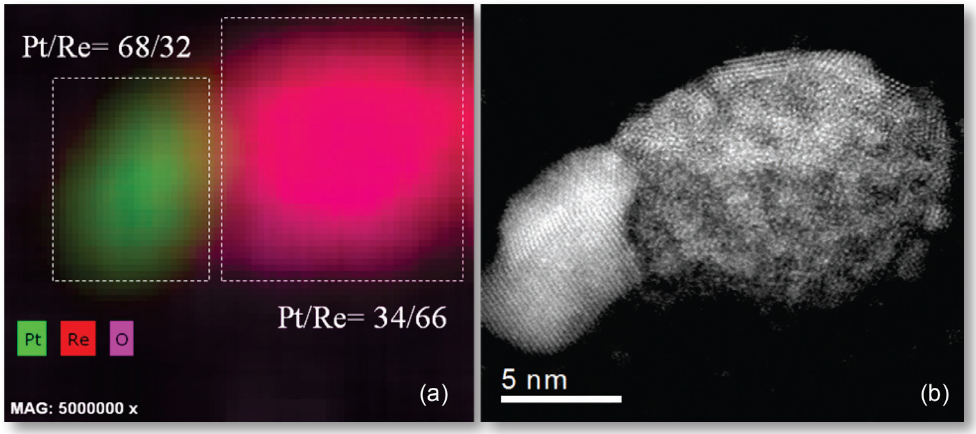

Figure 1: High-resolution x-ray mapping (a) of elements in Pt-Re nanoparticle (b). Oxygen is apparently coupled with the Re-rich side of the nanoparticle.

User Projects

1. A bimetallic platinum-rhenium (Pt-Re) catalyst, based on Pt-Re clusters loaded on novel carbon support (carbon nanotubes and carbon thin film) materials, is a promising candidate for catalytic conversion of biomass-derived liquids because of an enhanced activity which occurs with the addition of Re species. However, the nanostructure of the Pt-Re bimetallic clusters, and thus the underlying reaction mechanics, has not yet been well characterized. Now, Dr. Liang Zhang of the Pacific Northwest National Laboratory has teamed with Dr. Larry Allard at HTML to investigate the atomic structure of Pt Re clusters using HTML's aberration-corrected electron microscope (ACEM), with its

Benefits

- *Development of more effective catalytic materials for use in automotive exhaust aftertreatment devices.*
- *Improved fundamental understanding of the thermodynamics and kinetics of nucleation, growth, and sintering in precious metal catalysts.*
- *Enhanced catalysts for lean-burn diesel engines and their greater use in automotive vehicles.*
- *Development of advanced catalysts for biofuel production.*
- *Development of advanced catalysts for fuel cell applications.*

novel in situ heating capability, and various other spectroscopic tools (Figure 1). Structural characterization of Pt-Re at the atomic level will advance the understanding of interactions within the catalyst system and of aqueous phase reforming, thus contributing to the design and development of advanced catalysts for biofuel production.

2. Lean-burn gasoline and diesel engines hold great promise for improving automotive fuel economy; however, they pose problems for meeting emissions standards for nitric oxide (NO), a potent greenhouse gas. Platinum is generally regarded as one of the best NO oxidation catalysts; however, like other precious metal catalysts, Pt is expensive. A collaboration involving researchers from HTML, the University of Michigan, and the Ford Research Laboratory is using various electron microscopy techniques available at HTML to characterize the properties of these catalysts (Figure 2) and the relationships between morphology and performance to develop better, more economical alternatives for automotive exhaust aftertreatment systems.

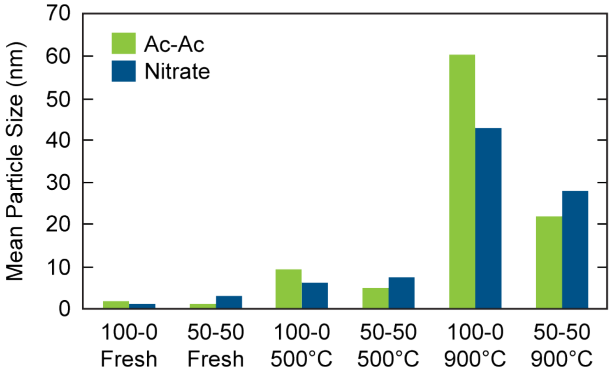

Figure 2: Mean precious metal particle size obtained from transition electron microscope analysis of pure Pt (100-0) and a combination of Pt and palladium (50-50) from either actinium (Ac-Ac) or nitrate precursors.

3. Methanol is a very convenient fuel for delivering hydrogen to fuel cells, and because of its high reactivity and stability, copper-zinc oxide is a popular catalyst for the methanol-hydrogen conversion process. However, the catalyst deactivates rapidly and is difficult to regenerate. Recent work has shown palladium-zinc (PdZn) catalysts to be a viable alternative that is more easily regenerated. Because the deactivation mechanisms of PdZn catalysts are not well understood, Dr. Larry Allard of HTML, Prof. Abhaya Datye from the University of New Mexico, and some of Dr. Datye's graduate students are studying the microstructure of these catalysts using HTML's ACEM. Figure 3 shows images of a PdZn on alumina catalyst after a combination of hydrogen reduction at 500°C and a long-term reaction. These images show that ordered PdZn crystallites are formed after use in this reaction. It appears that these ordered structures may be responsible for the decrease in reactivity. Further work is underway to confirm this hypothesis so that future research can be directed toward developing PdZn catalysts with the optimal amounts of Zn for enhancing methanol steam reforming.

4. In similar projects, researchers from the University of Texas-Austin, Massachusetts Institute of Technology, and HTML are studying platinum alloys for hydrogen fuel cell catalysts in an effort to reduce the amount of precious metals used, thus reducing costs, and extend the life of the catalysts. While research is still underway, team members have identified platinum-cobalt and palladium-platinum-nickel as possible replacement candidates for more traditional precious metal catalysts.

5. Currently there is little understanding of the compatibility of engine emissions control systems with renewable fuels such as biodiesel, which could contribute to reducing the nation's dependence on foreign oil. Will Brookshear, a graduate student from the University of Tennessee, under the guidance of ORNL researcher Todd Toops, used x-ray diffraction at HTML to detect changes in the composition and microstructure of aged diesel catalysts. A better understanding of the deactivation mechanisms of the various catalysts used in emissions control devices will lead to a greater understanding of the impact of biodiesel fuels on these devices and improvements that will extend their efficiency and durability for vehicles operating with biodiesel.

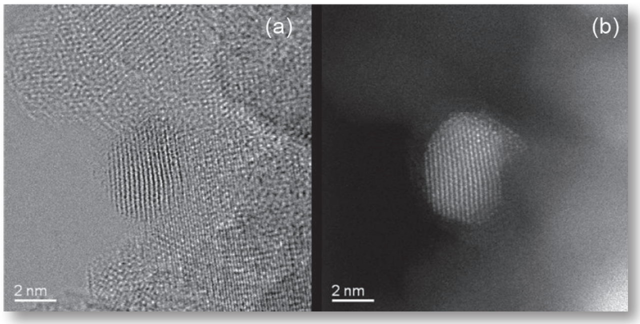

Figure 3: PdZn on alumina catalyst after use in a reactor for 72 hours. The ordered PdZn structures in the center are difficult to distinguish from the alumina support [bright field image, (a)] but can be clearly seen in the ACEM image (b).

High Temperature Materials Laboratory

User Projects on Thermoelectric Materials

Background

The High Temperature Materials Laboratory (HTML) at Oak Ridge National Laboratory (ORNL) is a U.S. Department of Energy (DOE) User Facility that specializes in materials characterization and conducts collaborative materials research with industry, universities, and other research organizations. The HTML User Program's mission is to enable the development of materials-based, energy-efficient, and environmentally friendly highway transportation technologies. As part of this mission, HTML supports the DOE Office of Energy Efficiency and Renewable Energy Vehicle Technologies Program goals by assisting facility users in the development of thermoelectric materials with high figures of merit or efficiency (ZT) for use in waste heat recovery devices for internal combustion engines. Because 35 to 40% of a fuel's energy potential is lost in the exhaust gases, recovering this energy would be one way to improve engine efficiency and increase vehicle fuel economy.

User Projects

1. Researchers from General Motors (GM) are continuing their work at HTML on skutterudite and clathrate materials, concentrating on (1) understanding the effect on transport properties of filling/doping microstructural "cages" with filler atoms and (2) visualizing those filler atoms (Figure 1). The results so far have confirmed that the skutterudites prepared at GM show the highest

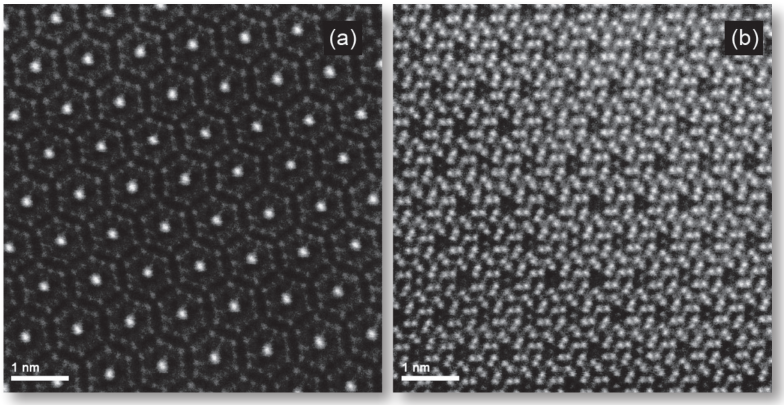

Figure 1: Scanning transmission electron microscope images of (a) a type-I clathrate and (b) a triple-filled skutterudite.

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.*

efficiency (ZT = 1.4–1.5) for n-type materials and provided experimental evidence for theories on filling limits and thermal dynamic stability of skutterudites with different compositions. GM will use the results in follow-on work with single-filled skutterudites and ultimately in the development of improved thermoelectric materials.

2. LAST (lead-antimony-silver-tellurium) is an emerging thermo-electric material system whose outstanding thermoelectric properties make it an excellent candidate for automobile waste heat recovery and similar applications. Researchers from Michigan State University (MSU) are working with HTML staff to characterize the nanostructure of LAST materials as a function of temperature. Future work will focus on the role of nanoscale features such as nanoinclusions and dislocations on thermal properties. A better understanding of the relationship between microstructure and the thermal behavior of LAST materials will enable development of thermoelectric generators for waste heat recovery applications.

3. New candidate thermo-electric materials such as lead-sulfide–lead-telluride (PbS-PbTe) and skutterudite thermoelectrics are being developed by the MSU Chemical Engineering and Materials Science Department. This past year doctoral students Jennifer Ni and Robert Schmidt (Figure 2) visited HTML to work with staff researchers Rosa Trejo, Edgar Lara-Curzio, and Andrew Payzant to characterize the microstructure and mechanical properties of new hot-pressed PbS-PbTe and skutterudite materials. The results of their investigation will enable the development of more durable and reliable thermoelectric materials for waste heat recovery applications.

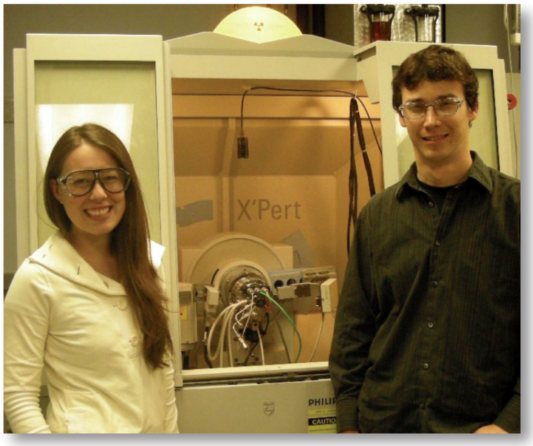

Figure 2: MSU students Jennifer Ni and Robert Schmidt in front of the x-ray diffraction units that were used to identify phases as a function of temperature in candidate thermoelectric materials.

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A Strong Energy Portfolio for a Strong America

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Lightweighting Materials

Advanced Preforming Technologies

Background

Successful deployment of "next generation" highly fuel efficient vehicles is dependent on significant weight reductions in current vehicles. With assistance and direction from the U.S. Department of Energy (DOE) Vehicle Technologies Program, 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 application. Carbon fibers, as the load-bearing components in these composites, offer significant weight saving potential because of their remarkable high strength, high modulus, and low density. Carbon fiber composites have the potential to reduce automotive component weight by as much as 50 to 60%; however, greater use of carbon fibers and composites in automotive applications has been impeded by 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. The goal of this effort is greater understanding of preforming technology so that it can have broader impact in meeting DOE goals for weight/energy savings in vehicle applications.

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 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 Systems, AB, as a baseline for evaluating and pushing development of advanced performing. This machine is commonly referred to as P4, short for "programmable powdered preform process." The process features a robotically actuated machine (Figure 1) that sprays reinforcing fiber (typically carbon fiber or fiberglass) and a matrix material [either a binder (currently in powder form) or a thermoplastic fiber] onto a screen shaped like the final part to create fiber preforms. After being preconsolidated on the preforming machine at elevated temperature, the preforms are subsequently injected with resin (in a structural reaction injection molding or SRIM process when thermoset resins are used) in a mold and consolidated with heat and pressure to create the final part (Figure 2). In this

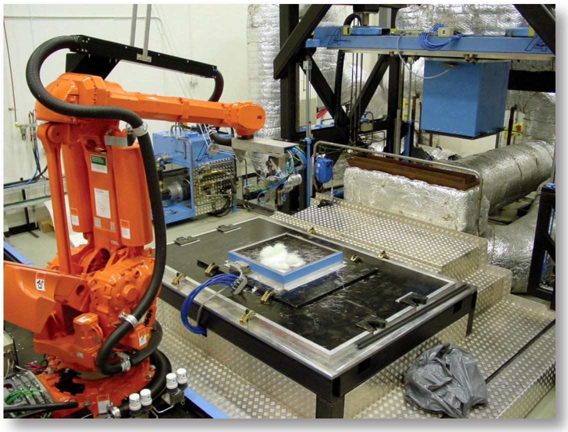

Figure 1: Robotic preforming machine at ORNL.

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.*

manner, automated spraying of carbon or glass fiber could soon provide the most economical way to create preforms for a variety of applications in automobiles, heavy vehicles, and other machinery.

The objective of this next generation program is to develop processing techniques, based on current P4 technology, which will enable the high volume, cost-effective processing of carbon fiber, hybrid glass and carbon fiber, and reinforced thermoplastic preforms. Thermoplastic matrices have rapid cycle times and are attractive for a number of automotive applications. Thinner sections may be possible where thermoplastic fiber for the matrix is blended with the reinforcing fiber before being chopped, thereby minimizing flow requirements for resin injection. Working with ACC and École Polytechnique Fédérale de Lausanne (EPFL), ORNL has demonstrated that preforms manufactured using comingled glass and polypropylene (Twintex) at ORNL and molded at EPFL can be competitive with other more expensive materials.

Such hybrid preforms may be the best way to introduce carbon fiber to automotive production because they would lower the overall cost of materials in a part versus use of all carbon fiber; would require a smaller carbon fiber supplier base with smaller capacity requirements; and would, we believe, provide tailorable and/or synergistic properties. In situ blending should be more cost-effective itself and offers the potential to rapidly evaluate numerous other options. ORNL has demonstrated the capability to blend, chop, preconsolidate, and mold in situ blends of hybrid glass and carbon fiber with polypropylene, although molding limitations have hindered detailed product evaluation. Plans are under way to procure a combination convection-infrared heating system for preheating thermoplastic charges and to implement a recently acquired urethane injection machine for SRIM processing of thermosets to facilitate evaluation of hybrids.

ORNL has also made improvements in chopping techniques. Working with ACC, ORNL introduced an alternative prototype chopper that has been upgraded 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.

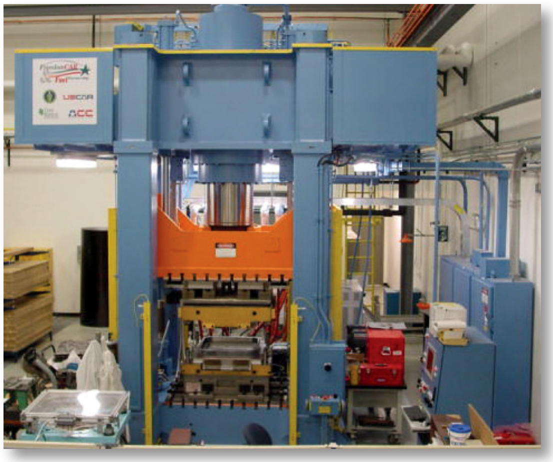

Figure 2: ORNL press and mold for evaluating preform developments.

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A Strong Energy Portfolio for a Strong America

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Lightweighting Materials

Carbon Fiber Technology Center

Background

With the assistance and direction of the U.S. Department of Energy Vehicle Technologies Program, Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for transportation. Carbon fiber reinforced composites are excellent candidates for this application. Carbon fibers offer significant weight saving potential because of their remarkable high strength, high modulus, and low density. However, broader use of carbon fibers is currently restricted by their high cost—$8 to $15 per pound. ORNL is developing new precursors and conversion processes for manufacturing low cost carbon fibers (LCCFs).

Technology

Because we anticipate a future need for the capability to demonstrate scalability of LCCF technology and to produce tons of LCCF for evaluation by composite manufacturers and original equipment manufacturers, ORNL is designing a new, highly flexible, highly instrumented facility for advanced LCCF research (Figure 1). The planned Carbon Fiber Technology Center (CFTC) will support the demonstration and evaluation of new low cost precursors and manufacturing processes at pilot scale; promote successful LCCF commercialization; and enable the United States to develop the necessary infrastructure to support key scientific and engineering breakthroughs in LCCF, thus strengthening the economy and ultimately our security. As envisioned, CFTC will be capable of the following:

- Demonstrating the scalability of the science and technology for lowering the cost of carbon fiber by at least 50%.
- Producing and making available to potential end users and upper-tier suppliers in multiple industries up to 25 tons per year of conventionally converted fibers (made from low cost precursors).
- Accommodating advanced conversion technologies.
- Producing precursor fibers made from a variety of precursor materials (e.g., lignin and polyolefin) on a melt spinning line in sufficient quantity to feed the conversion lines.

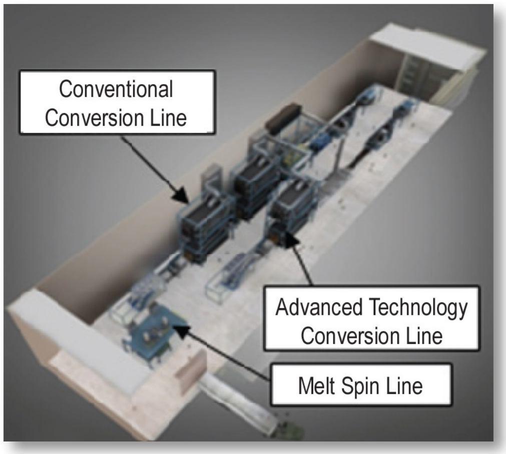

Figure 1: Conceptualization of the new CFTC.

Benefits

- *Demonstrate LCCF scalability.*
- *Produce several tons of LCCF for evaluation by composites manufacturers in multiple industries.*
- *Promote industrial and university collaborations.*
- *Educate and train a highly skilled future workforce.*

- Enabling industrial and university collaborators to effectively leverage the expertise of ORNL personnel in developing low cost manufacturing techniques for carbon fiber components.
- Educating and training a highly skilled future workforce for LCCF implementation.

Status

It is envisioned that CFTC will promote commercialization of all LCCF technologies. Prospective commercialization partners should contact C. David Warren.

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Lightweighting Materials

Fiber-Matrix Interface Adhesion in Low Cost Carbon Fiber Production

Background

With the assistance and direction of the U.S. Department of Energy (DOE) Vehicle Technologies Program, Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for transportation. Carbon fiber reinforced composites are excellent candidates for this application. Carbon fibers offer significant weight saving potential because of their remarkable high strength, high modulus, and low density. As part of DOE's FreedomCAR initiative, significant research is being conducted at ORNL to develop lower cost, high volume technologies for producing carbon fiber. As a result of that work, new precursor materials and processing technologies have been developed which offer the potential for a future type of lower cost, moderate performance, high volume commodity-grade carbon fiber.

In parallel efforts to these low cost carbon fiber programs, ORNL is developing carbon fiber posttreatment technologies and ways of achieving them on an industrial scale that are readily transferrable to current carbon fiber or composite production plants.

Technology

Elucidation of the principles governing the relationship between carbon fiber surface chemistry, morphology, resin type, and environmental conditions and interfacial adhesion is essential to achievement of the ultimate goal of greater use of composite materials in transportation applications. In current industry practice, posttreatments are highly proprietary and are usually targeted at epoxy resins. The result is that fiber-matrix adhesion properties are often deficient for other automotive resins, including polyesters, vinyl esters, and polyurethanes. Furthermore, it is difficult to use carbon fibers from multiple fiber suppliers because the lack of standardization in the field leads to a lack of interchangeability.

However, the tendency in the manufacture of carbon fiber is to stay away from commonly used electrochemical surface activation techniques due to the effluents generated, which must be eliminated posttreatment before discharge to the environment. Additionally,

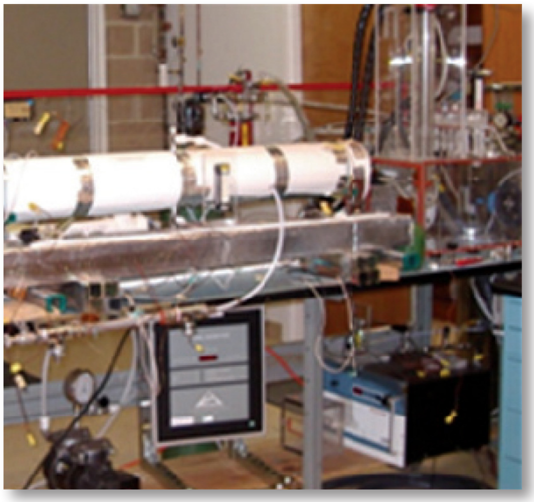

Figure 1: Ozone applicator with support devices.

Benefits

- *Optimized interfacial bonding improves mechanical properties; hence the quantity of carbon fiber required to meet the designed targets is reduced.*
- *Improved adhesion at the carbon-fiber interface will enable the fabrication of thinner parts with comparatively higher mechanical performance, resulting in weight reduction and cost savings.*
- *Developing posttreatment technology addressing low cost carbon fiber will accelerate the use of low cost carbon fiber precursors and technology.*
- *Specialty posttreatment recipes target resin systems of interest to automotive and other emerging energy industries where low cost carbon fiber can be used beneficially.*

the electrochemical method features a sequence of discrete processing steps making this process complicated, difficult, and more prone to process failure. Therefore, ORNL is focusing on developing ozone-based surface treatments, which are clean and require minimal steps. The ozone surface treatment process requires only an ozone generator; a piping system; and an ozone applicator, where the ozone will interact with the carbon fiber, and is easily implemented in current manufacturing plants.

In the course of this project, scientists at ORNL investigated various polymer blends, catalysts, and additives as a means for improving the sizing strength, toughness, and reactivity between the fiber and matrix resin. ORNL research targets the resin systems of interest to the automotive industry.

Status

Development of specific surface treatments and sizing will be geared toward the use of low cost carbon fiber technology.

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Lightweighting Materials

High Strength Carbon Fibers for Hydrogen Storage

Background

With the assistance and direction of the U.S. Department of Energy Fuel Cell Technologies Program, Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for hydrogen storage. Carbon fiber reinforced composites are excellent candidates for this application. Carbon fibers offer significant weight saving potential because of their remarkable high strength, high modulus, and low density. The use of high strength carbon fibers for hydrogen storage is currently restricted by their high cost.

Technology

A significant part of the cost of high strength carbon fiber is attributable to the cost of fiber formation and the processes for conversion into finished carbon fibers. The usual wet spinning process for precursor fiber production is a significant cost factor. Melt spinning is a low cost, high throughput alternative process; however polyacrylonitrile (PAN), a key carbon fiber precursor, decomposes before melting. ORNL researchers in partnership with Virginia Tech are developing advanced chemical and processing approaches to render PAN melt spinnable. The goal is to reduce the mill cost of high strength carbon fibers by at least 25% while achieving minimum mechanical properties of 30 Msi tensile modulus, 650 ksi ultimate tensile strength, and 1.5% ultimate tensile strain.

Virginia Tech has demonstrated the ability to melt spin PAN fibers with 90% acrylonitrile (AN) and 10% methyl acrylate comonomer (Figure 1). This is a significant breakthrough. Researchers continue to work toward melt spinning fibers with higher AN content. The target is ≥ 95% AN content, which is expected to significantly increase carbon fiber strength. ORNL is also developing advanced methods for converting PAN fibers into carbon fibers. These approaches will be tested when melt spun PAN fibers can be made in sufficient quantities to enable continuous processing trials.

Figure 1: Spool of melt spun filaments with 90% AN content.

Benefits

- *Estimated 30% reduction in cost of high strength carbon fibers.*
- *High throughput fiber forming process.*
- *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.*

Status

Melt spun precursor is part of a suite of patented or patent pending carbon fiber technologies that will likely be commercialized together. For more information on our research in this area and how you can partner with ORNL, contact C. David Warren.

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Lightweighting Materials

Infrared Inspection of Resistance Spot Welds

Background

With the assistance and direction of the U.S. Department of Energy Vehicle Technologies Program, 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 economic constraints of the auto production environment. Any weld quality inspection technique must be fast, highly cost-effective, 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, and Chrysler). This project addresses this critical industry need through the development of an infrared- (IR-) based online weld quality monitoring technique. The goal is to provide automakers a low cost nondestructive evaluation tool for weld quality inspection/monitoring on assembly lines.

Technology

Heat generated during the resistance spot welding process can be used to monitor weld quality. Working with the U.S. Council for Automotive Research and automotive original equipment manufacturers, ORNL is developing an online inspection technique using IR thermography. IR thermography detects surface temperature changes due to geometric discontinuity or inhomogeneity. A distinct advantage of IR thermography as a nondestructive evaluation (NDE) tool is its nonintrusive and noncontact nature. This makes IR-based NDE especially attractive for the highly automated body-in-white assembly lines.

The IR inspection technique developed at ORNL combines novel IR system setup and IR signal analysis techniques that overcome the key technical barriers inhibiting IR weld NDE in auto assembly

Benefits

- *Noncontact inspection and potential to be developed into turnkey system.*
- *No interference with assembly-line production.*
- *Low false call 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 need for destructive "pry-check."*
- *Integration with robots and machine vision software to allow rapid feedback and control.*
- *Applicable to high-strength steels in which pry-check does not work well and may cause injuries.*

lines. Both postmortem (post-weld) inspection and real-time detection of weld quality were explored. Both the postmortem and the real-time approaches in Phase I required no further special treatments of the as-welded or as-received surfaces – a key issue that has hindered previous IR inspection attempts.

Postmortem IR inspections using several heating and cooling techniques were carried out to assess weld quality. Working with cold welds (small, undersized, and just below expulsion welds) carefully prepared by ArcelorMittal, ORNL determined that the welds could clearly be distinguished by the selected cooling and heating methods and grouped according to the heat flow through the weld nuggets.

For testing the feasibility of real-time IR inspection, the IR camera was taken to the ArcelorMittal Global Research and Development Laboratory in East Chicago, Indiana. The same set of spot welds was 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 for 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 the IR inspection technique. Future work has been planned to use image processing and new software algorithms to improve the inspection speed.

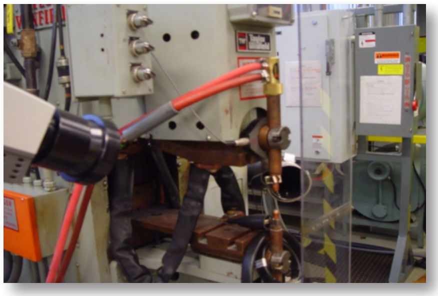

Figure 1: IR imaging of resistance spot welding.

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.

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Lightweighting Materials

Lignin-Based Precursors for Lower Cost Carbon Fibers

Background

With the assistance and direction of the U.S. Department of Energy Vehicle Technologies Program, Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for transportation. Carbon fiber reinforced composites are excellent candidates for this application. Carbon fibers offer significant weight saving potential because of their remarkable high strength, high modulus, and low density. However, broader use of carbon fibers is currently restricted by their high cost—$8 to $15 per pound. ORNL has developed the baseline technology necessary to use lignin, a by-product from the cellulosic ethanol fuel production and paper making processes, as a very low cost feedstock material for making carbon fiber precursors. The key to this process is the ability to isolate lignin with the appropriate chemistry, physical properties, and level of purity for melt spinning into a precursor fiber suitable for carbon fiber production.

Figure 1: Lignin is a renewable resource available from cellulosic ethanol production from switchgrass.

Technology

To help achieve programmatic goals, polymer compounding, pelletizing, and melt spinning equipment was installed at ORNL. The equipment is used to establish process conditions for melt spinning precursor fiber tows from lignin materials from various sources, including pulping of hard and softwoods for paper production and, more recently, production of cellulosic ethanol fuel from wood and switchgrass. The focus in FY 2009 has been on scaling up the conversion of lignin precursor fiber into carbon fiber and transitioning the process from batch furnaces to a continuous, laboratory scale conversion line. In addition, work was implemented on identifying suitable polymers for use as alloying agents to enhance manageability of the precursor fiber as well as mechanical properties of the finished carbon fiber. These tasks will be continued through FY 2010. New tasks will include the evaluation of lignin materials of much higher molecular weight with the objective of enhancing the lignin glass transition temperature and, ultimately, carbon fiber properties.

Benefits

- *Lignin-based precursors are less than half the cost of traditional precursors.*
- *Melt spinning is less expensive than solution spinning; no solvents are used.*
- *Total savings in carbon fiber costs could exceed $2 per pound (reduced unit investment cost).*
- *Lignin is a renewable resource; it is readily available from domestic forest products and in the future will be available from cellulosic ethanol production from wood and switchgrass.*

As lignin materials of the required purity level became available, work on the purification of lignin was terminated and the effort refocused on the production of carbon fiber from an organosolv-pulped hardwood lignin, Alcell, furnished in bulk by Lignol Innovations and a kraft-pulped softwood furnished by Kruger Wayagamack. The purity levels of these lignins compared to those of a hardwood lignin furnished by a supplier of commercial kraft lignin products are shown in the table below. Elimination of the purification step is a significant economic benefit.

Lignin Material[a]	**Impurities**					
	C (%)	S (%)	Na (ppm)	K (ppm)	Ca (ppm)	Ash (%)
HWL	59	2.45	19,000	1,770	650	2.800
HWL-Aq	65	1.48	73	70	255	0.030
HWL-Org	65	1.40	1,160	104	76	0.010
SWL-K2	67	1.18	2,390	100	78	0.200
Alcell	66	0.05	17	44	163	0.001

[a]Acronyms and abbreviations: HWL = kraft hardwood lignin as received from commercial supplier; HWL-Aq = same kraft hardwood lignin purified by ORNL (aqueous procedure); HWL-Org = same kraft hardwood lignin purified by supplier (organic procedure); SWL-K2 = kraft softwood lignin as received from Kruger Wayagamack; Alcell = organosolv lignin as received from Lignol Innovations.

Status

Lignin precursor development is being conducted as part of a collaborative agreement between Lignol Innovations (Canada), Kruger Wayagamack (Canada), Innventia (Sweden), and ORNL. Those interested in more information and/or partnering with ORNL should contact C. David Warren.

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Lightweighting Materials

Polyolefin-Based Precursors for Low Cost Carbon Fibers

Background

With the assistance and direction of the U.S. Department of Energy (DOE) Vehicle Technologies Program, Oak Ridge National Laboratory (ORNL) is conducting research and development into lightweight materials for transportation. Carbon fibers offer significant weight saving potential because of their remarkable high strength, high modulus, and low density. Greater use of carbon fibers in such applications 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 precursors. Currently, common commodity grade carbon fibers are produced from polyacrylonitrile- (PAN-) based precursors. PAN-based textile precursor is a potential candidate for low cost carbon fibers, with the projected cost savings being around $2 per pound of finished carbon fiber. At present, however, there are no domestic producers of textile PAN; therefore, supply and price stability may become an issue. Polyolefin-based fibers (polyethylenes and polypropylene) are industrially produced in the United States and are very low cost commodity plastic fibers ($0.50–0.65 per pound). The cost of these precursor fibers is less than half that of the PAN-based precursor fibers.

However, since polyolefin fibers are melt spun, a stabilization route (to prevent melting) needs to be developed before carbonization of the precursor fiber. In the past, conversion of polyolefin precursors was attempted by a few research groups via sulfonation of the precursor fibers. Although the reported practical carbon yield was very high for the polyolefin fibers (~78%) in comparison to that of the PAN-based fibers (~50%), unfortunately the residence time required for the stabilization step was very high. Recently, ORNL researchers have developed a potentially patentable conversion technology for polyolefin precursors that requires only 1 h stabilization time and includes direct carbonization without an oxidation step.

Technology

A systematic investigation is under way to optimize the conversion parameters with an overarching goal to produce polyolefin-precursor-based lower cost carbon fiber that can be used for automotive

Figure 1: Spool of polyolefin fiber.

Benefits

- Polyolefin-based precursors are significantly lower in cost compared to PAN-based precursors.
- Melt spinning is less expensive than solution spinning.
- Fibers can be spun at high speed.
- Total savings in carbon fiber cost could exceed $2 per pound.
- Unit investment cost can be reduced.
- Melt spun polyolefin fiber is available in the commercial market.
- Polyolefins offer significantly higher carbon yield (60–75%).

applications. A novel accelerated route of stabilization for the polyolefin fibers is also being developed at ORNL. The conversion of polyolefin fibers requires only 1 h stabilization time and direct carbonization without any further oxidation step. This stabilization route would replace the 75–120 min oxidative stabilization step in conventional carbon fiber manufacturing from PAN-based fibers. To render polyolefin fibers infusible at an accelerated rate (before carbonization), modified polyolefin fibers were developed. The fibers were then melt spun in collaboration with an industrial melt spinning equipment manufacturer in the United States (Figures 1 and 2).

Status

Polyolefin-based precursor development is being conducted at ORNL. Prospective commercialization partners should contact C. David Warren.

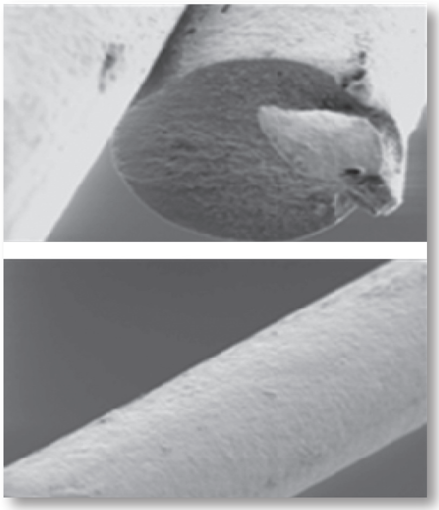

Figure 2: Scanning electron microscope images of polyolefin-based fibers.

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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 (DOE) Vehicle Technologies Program, the Automotive Composites Consortium, and the American Plastics Council, Oak Ridge National Laboratory (ORNL) is 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 costs and good mechanical properties. These materials have already been used for semistructural applications and are now candidate materials for structural applications to reduce vehicle weight. Long-fiber thermoplastics produced by injection molding present the additional advantage of low cost part production because conventional injection molding equipment can be modified to produce long-fiber thermoplastic parts.

Use of reinforced plastics and polymer composites in automotive structural applications 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 shaped components are being developed to address this shortcoming.

Technology

A collaborative program by ORNL, Pacific Northwest National Laboratory, 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. Structural analysis code ABAQUS is interfaced with Moldflow in order to use the material microstructure information for mechanical property prediction of molded components. New processing and structural models are being incorporated in the coupled processing-structural predictive framework.

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.*

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, 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-PA66 [polyamide (nylon) 6,6] 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 PA66 to remain on exposed fibers on the fracture surface (Figure 2).

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

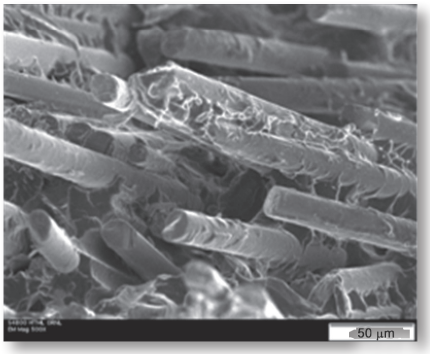

Figure 2: Matrix material residuum on exposed fibers after fracture.

Current and future work is focused on development and validation of models for creep, fatigue, and impact response of long fiber thermoplastics. The resulting suite of tools will accelerate the use and reduce the cost of lightweight composite components in automotive applications.

Status

Predictive models are being implemented in commercially available and supported packages. Moldflow Corporation is an active team member in this project. Others interested in partnering on this project should contact C. David Warren.

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Lightweighting Materials

Textile-Grade Precursors in Low Cost Carbon Fiber Production

Background

With the assistance and direction of the U.S. Department of Energy (DOE) Vehicle Technologies Program, 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 application. 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 greater than that of steel at approximately the same stiffness and ~1/5 of steel's density. If carbon fiber composites were used in passenger automobiles, it is estimated that vehicle structure weights could be reduced up to 50%.

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 typically 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. As indicated previously, 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-grade polyacrylonitrile (PAN) fiber (Figure 1) 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 commercialize this precursor to make it available to current and potential carbon fiber manufacturers.

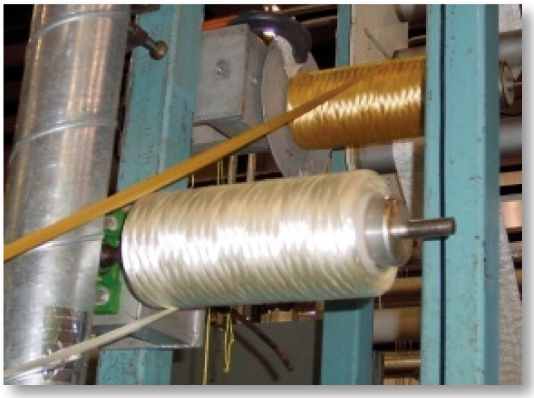

Figure 1: Textile-grade PAN precursors.

Benefits

- *Textile-grade PAN precursors are less than half the cost of traditional 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 savings in carbon fiber costs could exceed $2 per pound.*
- *Higher speed conversion of the precursor into carbon fiber yields additional cost savings.*

Technology

A collaborative international program by ORNL and FISIPE S.A. is under way to render textile-grade PAN 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 per pound in the finished carbon fiber manufacturing costs.

Recently the two organizations have defined several textile formulations that could yield suitable carbon fibers, and they are modifying materials that can be oxidized near conventional oxidation temperature. 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.

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. Mechanical properties now well exceed the program requirement, as shown in Figure 2.

Oxidative stabilization is the low speed bottleneck in the carbon fiber conversion process. The oxidative stabilization of the modified textile precursors requires only ~70 minutes compared to an average time of 80–120 minutes for conventional carbon fiber precursors. 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 parallel efforts under way to develop new production technologies that will enable manufacturers to develop high volume, commercial carbon fiber plants that use textile-grade PAN precursors along with other advanced manufacturing methods. Prospective commercialization partners should contact C. David Warren.

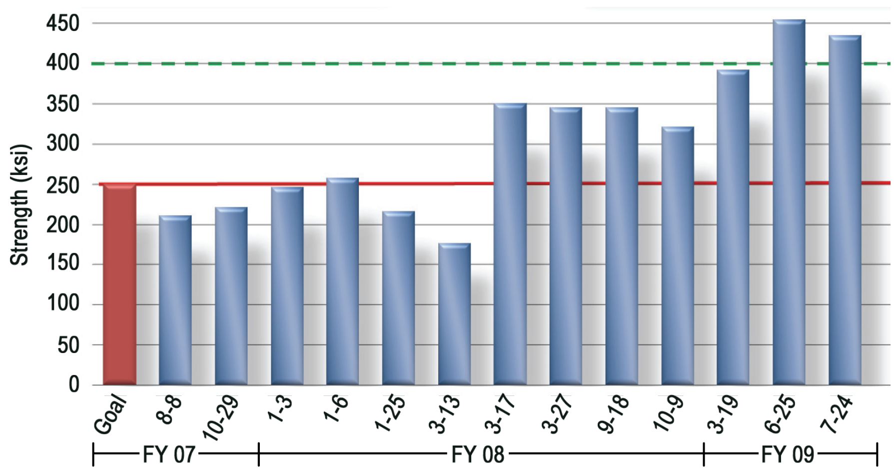

Figure 2: Improvement in fiber strength during the project.

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Medium Truck Duty Cycle

Instrumentation and Launch of Six Instrumented Class-6/Class-7 Vocational Vehicles to Collect Vehicle Performance Data

Background

The Medium Truck Duty Cycle (MTDC) Project is a follow-on to the Heavy Truck Duty Cycle (HTDC) Project that was completed in FY 2008. Data collected within the HTDC and MTDC efforts come from commercial fleets operating in real-world environments. Special data analysis tools have been developed, in prototype form, which allow parsing of the data to support modeling and fuel efficiency analysis needs. The Duty Cycle Generation Tool (DCGenT) prototype was developed to generate a characteristic duty cycle from multiple database segments that meet user specified criteria. The MTDC Project is collecting 60 channels of data from two of four Class-6/Class-7 vocations (combination tractor-trailers owned by H.T. Hackney and local transit buses operated by Knoxville Area Transit Authority) in the 2009–2010 time frame and the other two vocations (utility truck and wrecker) in the 2010–2011 time frame. Data and information from this project will be useful for (1) supporting development and evaluation of the heavy and medium truck modeling efforts; (2) generating customized, real-world-based data for the heavy truck energy efficiency research community; (3) conducting real-world-based energy efficiency studies related to heavy truck performance-shaping factors; and (4) making investment decisions. In early FY 2009, six Class-6/Class-7 vehicles from two vocations were instrumented, tested, and launched for data collection purposes.

Technology

The MTDC Project uses the six data collection platforms developed in the HTDC portion of the program. Improvements in the platforms include the ability to wirelessly download the collected data on a daily basis (as opposed to a download weekly or twice per month) and the ability to access near-real-time data for any of the instrumented vehicles. Improvements in the DCGenT were also achieved through the addition of conditional probability sampling from duty cycle histograms of velocity and accelerations in the generation of a single characteristic duty cycle.

Signing the Memorandum of Understanding for the MDTC project between, left to right, ORNL's Dana Christensen, DOE's Lee Slezak, H. T. Hackney's Ed Meyer, Knoxville Area Transit Authority's Si McMurray at the National Transportation Research Center, Knoxville, Tennessee, July 10, 2009.

Benefits

- *Provides a fundamental understanding of the operations of selected Class-8, Class-7, and Class-6 vocations to support future energy efficiency technology investment decisions.*
- *Provides real-world data as a baseline for assessing the benefits of new and emerging truck-based energy efficiency technologies.*
- *Provides data sufficient for characterizing duty cycles associated with the selected Class-8, Class-7, and Class-6 vocations.*
- *Provides a real-world-based data source for evaluating and validating models of engine and vehicle performance.*

Status

Nearly 8 months of data collection for two vocations have been completed. Data are being collected on 60 performance measures sampled at 5 Hz, providing information related to the vehicle, driving, and its situation. In addition, the U.S. Department of Transportation's Federal Motor Carrier Safety Administration is partnering with the MTDC effort to collect 20 additional performance measures related to tire pressure and brake usage for the combination tractor-trailer vocation. Data collection for the first two vocations will be completed in February 2010. Additionally, selected data analysis has been completed on the HTDC data. The primary topic was fuel efficiency due to the use of wide-based single tires in comparison to standard dual tires. The study involved an investigation across payload and speed. In all instances, the wide-based single tires offered a statistically significant (6%–10%) fuel efficiency gain and provided more than a 10% gain for fully loaded Class-8 tractor-trailers. Similar analyses are being planned for the Class-6/Class-7 data.

Planning efforts for a Large Scale Duty Cycle feasibility study were also conducted. This study will be initiated in FY 2010 and will collect a reduced set of duty-cycle-based performance measures from a significantly enlarged set of tracked vehicles in multiple vocations. The use of existing communications providers (e.g., PeopleNet and QUALCOMM) will be investigated.

Instrumented H. T. Hackney and Knoxville Area Transit test vehicles at the National Transportation Research Center, Knoxville, Tennessee.

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Propulsion Materials

Advanced Materials Development through Computational Design for HCCI Engine Applications

Background

Interest in homogeneous charge compression ignition (HCCI) combustion has grown in recent years because of its potential to improve engine efficiency and reduce emissions. The use of HCCI combustion, however, will subject components to significantly higher temperatures and pressures. The temperatures for diesel engines will reach more than 1,600˚F and pressures may reach 2,000 psi—up to twice that of a regular combustion engine. Therefore, materials performance must improve before the advantages of HCCI combustion can be realized. This project deals with the identification of material requirements for HCCI engines in automotive and truck applications and the development of advanced, yet cost-effective, materials through computational design.

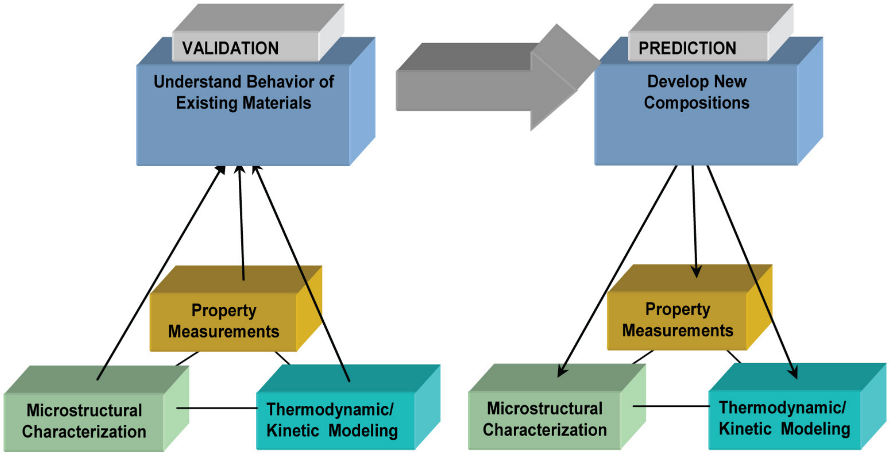

Figure 1: ORNL's overall approach for computational design of materials (materials-by-design).

Technology

"Materials-by-design" is an Oak Ridge National Laboratory (ORNL) concept that encompasses a variety of materials-related techniques including modeling, correlation, and materials modification (Figure 1).

The premise behind the materials-by-design approach is that mechanical properties can be correlated to microstructure and phase compositions. Microstructures and phase compositions can be achieved through variations in alloy chemistry; thermal treatment at high temperatures; and thermal-mechanical processing techniques such as quenching, rapid casting solidification, or mechanical working. The observed microstructural characteristics can be correlated with mechanical properties and predictions from equilibrium thermodynamic and kinetic modeling through advanced correlation techniques. Results from such correlations allow untested compositions or treatments to be modeled so that desirable trends

Benefits

- *Targeted, "on-demand" development of new materials for specific applications.*
- *Reduced development cost due to selective experimental alloy development work.*
- *Cost-effective design of suitable materials with varying alloying element additions.*

in microstructure and phase compositions can be rapidly established. Small heats of targeted materials can then be processed to confirm the modeled properties and to broaden the correlation database.

Status

Based on discussions with various companies, exhaust valves were identified as one of the highest priority components. New valve materials are needed to operate at temperatures up to 1,600˚F, significantly higher than the current value of 1,400˚F. Using rotating beam fatigue tests, we identified high temperature fatigue life as the critical property of interest for the valve materials at the temperature of interest.

Several candidate nickel-based alloys with the potential to have required high temperature properties at 1,600˚F were identified for further testing and evaluation. Fatigue properties of these alloys have been measured using fully reversed fatigue tests at 1,600˚F (Figure 2). Based upon the relationships between fully reversed fatigue life and rotating beam fatigue life developed at ORNL, several commercial alloys have been identified as strong candidates for use in exhaust valves at temperatures of 1,600˚F. Using these alloys as a base, several new alloys have been designed and prepared in small laboratory-sized batches and their properties are being evaluated. In the future, one alloy with the required properties and lowest cost will be subjected to further industrial scale development.

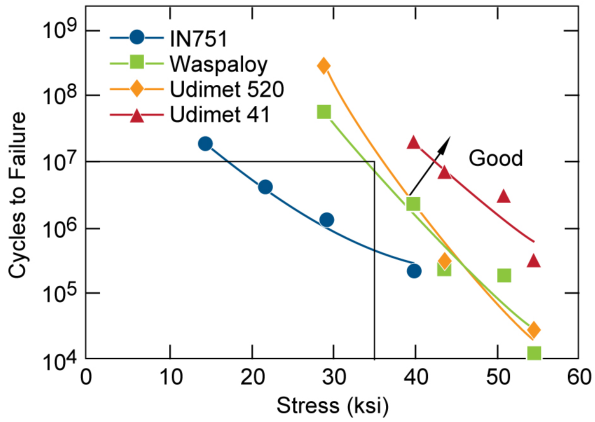

Figure 2: Several commercial alloys with desirable fatigue properties have been identified using fully reversed fatigue tests.

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Propulsion Materials

Design Optimization of Piezoelectric Multilayer Actuators for Heavy Duty Diesel Engine Fuel Injectors

Background

Use of piezoelectric stack actuators in diesel fuel injectors can reduce emissions such as nitrogen oxide and particulate matter by 30%, fuel consumption by 15%, and engine noise by 6 dB. These stacks are susceptible to frequent malfunctions, especially in high temperature, high humidity environments where both fatigue and premature breakdown have been observed previously in laboratory and field tests. The application is confronted with a substantial challenge in root cause analysis of failure as a piezoelectric stack typically consists of hundreds of alternating lead zirconate titanate (PZT) and internal electrode layers, termination, bus wire, and encapsulant. Moreover, each of these components plays a unique role in the application. The robust performance and effective interaction of the various stack components, as well as the coupling between different physical fields, call for an effective design optimization with regard to all involved parameters, which can only be achieved through testing and characterization of the various elements composing the piezoelectric stacks and the stacks themselves under identified, controlled conditions.

Technology

At Oak Ridge National Laboratory (ORNL), we are working toward design optimization of piezoelectric materials through testing and characterizing candidate components and devices. PZT piezoceramics research here is focused at the component level, where various experimental approaches such as ball-on-ring and four-point bend tests are used to measure fracture stress and investigate strength limiters (Figures 1 and 2). In the future, these experimental studies will be extended to include the effects of electric field, temperature, and humidity under specifications defined by a Cooperative Research and Development Agreement (CRADA) with Cummins Inc.

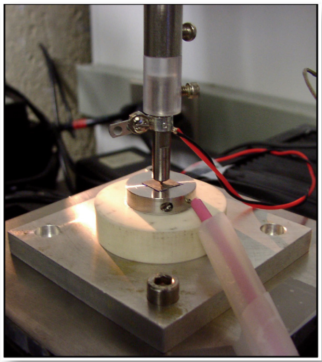

Figure 1: Ball-on-ring setup is used to study the mechanical strength of PZT and electrical effects.

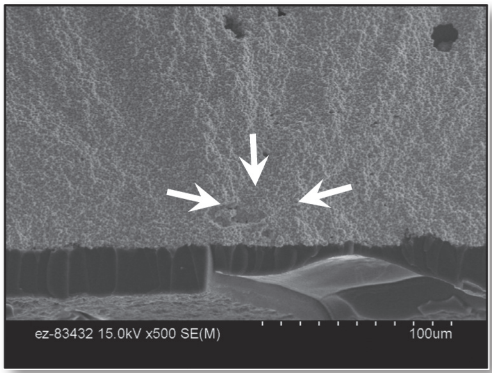

Figure 2: Failure origin featuring a volume pore in as-extracted PZT. Ball-on-ring setup was with 10 mm polymer ring and 2 mm steel ball; rate was 0.01 mm/s and failure stress was 60 MPa.

Benefits

- *Findings can be integrated into probabilistic component design and fabrication procedures to produce robust piezoelectric stacks with long-term reliability and durability.*
- *Findings are transferable to other piezoceramic applications.*
- *Results demonstrate the ORNL piezostack accelerated fatigue facility can provide key complementary and cost-effective approaches to help diesel engine companies identify life-limiting factors and thus significantly improve the long-term reliability and durability of advanced diesel engine fuel injectors.*

Parallel testing on PZT stacks is also proposed as an important strategy to achieve design optimization. Work on stack level characterization at ORNL focuses on accelerated cyclic fatigue with controlled operational parameters, which is different from and complementary to the work conducted under the Cummins CRADA. The ORNL piezostack accelerated fatigue facility has been modified to accommodate this stack level testing and characterization, which is being pursued at both the macrolevel and microlevel. Mechanical strain, charge density, and hysteresis are characterized during the fatigue cycle and microstructure damage and evolution after the fatigue cycle are analyzed through a set of advanced characterization tools developed at ORNL. Stack level characterization will be conducted on two main candidates that are being considered for use in heavy diesel engine systems, EPCOS and Kinetic Ceramics stacks, and will also be extended to include the environmental factors within the test matrix.

Status

Previous work on the commercially available PZT-5A and PZT-5H multilayer PZT stacks available from Piezo Systems, Inc., revealed a host of strength-limiting flaws; the role of polarization was also characterized.

The piezoceramic characterization conducted within the framework of our CRADA with Cummins has validated the ORNL piezostack accelerated fatigue facility and the test methods we are developing, including fast Fourier transformation for macroresponse and sequential polishing techniques for detailed microstructure analysis.

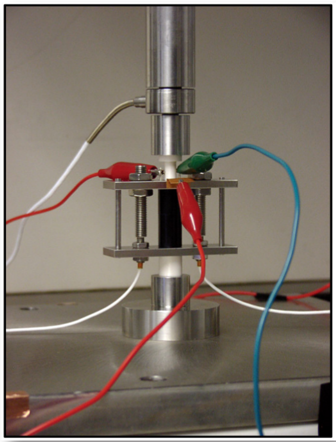

Figure 3: ORNL piezostack accelerated fatigue facility has been modified to accommodate stack level testing and characterization to evaluate the long-term reliability of commercial PZT stacks.

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Propulsion Materials

Electronic Structure and Transport Theory for Thermoelectric Materials

Background

Developments in electronic structure and transport theory allow direct calculation of properties of thermoelectric materials, including thermopower, based on knowledge of their structure and composition. These methods have been applied to predict the transport properties of materials and their doping levels and temperature dependencies to find improved thermoelectric compositions that can be used in waste heat recovery applications in vehicles. These calculations have been used to assess different potential new thermoelectric materials and to map out the doping level dependence of their properties. In this way the composition and doping range where high thermoelectric performance is likely can be determined before experimental synthesis and characterization.

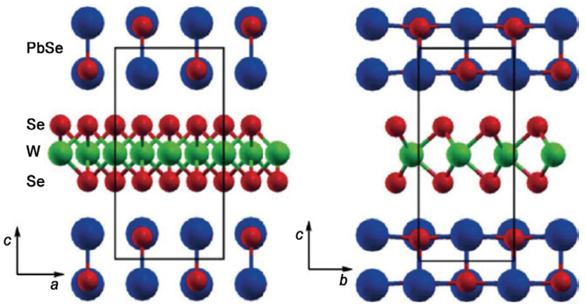

Figure 1: Relaxed structure for a coherent approximant structure of the simplest 1:1 PbSe-WSe_2 intergrowth compound as obtained from density functional calculations.

Technology

The studies described here are based on the use of the computer code "BoltzTraP," which was developed in a collaboration between Oak Ridge National Laboratory and the University of Aarhus (Denmark). This code calculates thermopowers and other electrical transport functions of materials directly from their electronic structures as produced by standard density functional methods. The code has been tested and validated for a wide variety of thermoelectric materials including both conventional and oxide thermoelectrics.

Status

Transport calculations for La-Te high temperature thermoelectrics analyzed in relation to experimental data obtained at the California Institute of Technology showed how high thermoelectric performance can arise from a mixture of heavy and light band structure features in a material. This understanding led to a potentially important observation in the context of PbSe-based thermoelectrics. These were investigated as potentially high performance, low cost materials as compared to PbTe. The work was motivated by reports of very low thermal conductivity in layered intergrowth compounds of PbSe and WSe_2 (Figure 1). The calculations showed an enhanced thermopower in these materials, especially at high doping levels and high temperatures, similar to

Benefits

- *Screening potential thermoelectric materials allows focus on the most promising compositions.*
- *Calculations of thermopower and its dependence on temperature and doping levels are yielding information about whether further optimization of specific thermoelectric materials is likely to give significant performance improvements.*
- *Transport calculations can be used to determine whether the peak performance of specific materials can be shifted to match the temperature conditions in waste heat recovery applications.*
- *Results provide insight into the origins of high thermoelectric performance which can be used to guide the search for promising new compositions.*

La-Te. This motivated a reexamination of the thermoelectric properties of bulk PbSe in terms of its electronic structure. It was found that PbSe could become a high performance thermoelectric material in the temperature range appropriate for waste heat recovery if it were doped at the 1% level and appropriately nanostructured (Figure 2). This is a consequence of the nonparabolic band structure, which takes on heavier characteristics at higher energy. Estimates of the length scale for which nanostructuring would be beneficial were made based on the results. The calculations show that control of the doping level in PbSe will be critical to obtaining high performance. These results are of importance because tellurium availability may be a barrier for widespread deployment of PbTe-based thermoelectrics in vehicles and therefore a selenium-based alternative is desirable.

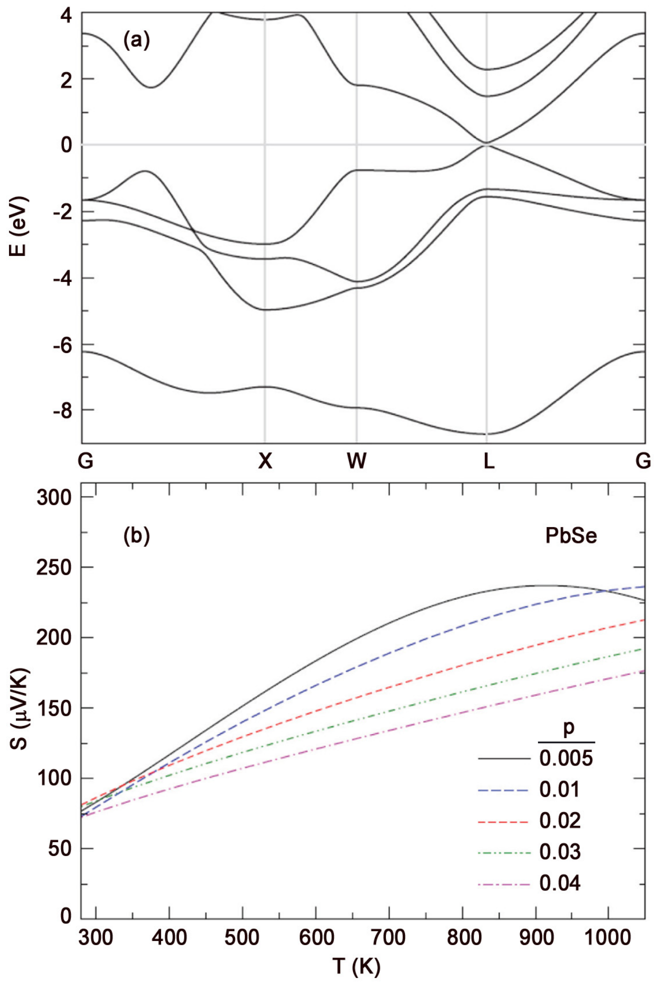

Figure 2: Band structure including spin-orbit interactions (a) and calculated thermopower as a function of temperature and doping (b) for p-type PbSe. Note that the thermopower in the temperature regime relevant to waste heat recovery does not decrease as rapidly as might be expected with doping showing that the best performance may be at higher doping levels than previously thought.

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Propulsion Materials

Friction and Wear Reduction in Diesel Engine Valve Trains

Background

Heavy truck diesel engine designers face two important challenges: (a) to improve fuel efficiency and (b) to meet increasingly strict emissions regulations while at the same time keeping manufacturing and maintenance costs affordable to owners and operators. Technologies such as homogeneous charge compression ignition, advanced engine control systems, and exhaust gas after-treatment are being used to meet these challenges, but such approaches can affect the mechanical, thermal, and chemical environments to which engine materials are exposed. In specific cases, current materials and surface treatments fall short of meeting the requirements for those more aggressive environments, leading to unacceptable durability and surface degradation. The objective of the effort described here was to optimize the selection and use of durable exhaust valves for diesel engines. The effort drew on past studies, wear-oxidation experiments, and the simulation of valve wear conditions in a custom-designed laboratory system. In FY 2009, the final year of this project, this work has led to the development of a multiparameter valve seat wear model.

Technology

The seating surfaces of exhaust valves are exposed to one of the most severe contact environments in diesel engines. They must resist repetitive contact pressure, fine-scale sliding motions, and high temperatures from the exhaust gas (see Figure 1). Engine designers can change contact conditions by adjusting such things as combustion timing and seat insert angles, but the materials must stand up to such changes. To provide key information to enhance material selection for exhaust valve applications, the current project included both an experimental and a modeling effort. Over the course of this project we have used information from published research, consultations with diesel manufacturers, and experimental work using test apparatus built specifically to simulate contact environments to gain a better understanding of wear-oxidation processes and to develop a model to represent the wear of valve and seat surfaces as a function of the number of contact cycles of operation.

Figure 1: Deposit on the faces of a used exhaust valve showing a combination of wear and oxidation.

Benefits

- *Achieved an improved understanding of the role of the synergistic effects of oxidation and wear as applied to exhaust valve materials for diesel engines.*
- *Designed and built a unique, HTRI testing system for simulating wear damage on exhaust valve and seat surfaces.*
- *Developed a multiparameter wear model for the recession of valve and seat surfaces under combined deformation and abrasion.*
- *Measured friction of high performance alloys as a function of temperature to support model development.*

Status

In project years 1 and 2, using representative iron, nickel, and cobalt alloys, experiments were conducted on the effects of mechanical surface damage on oxidation of surfaces at exhaust valve temperatures. Results were published in several refereed journals, leading to an invited presentation at an international conference on tribocorrosion. During this time, a unique, high temperature, repetitive impact (HTRI) testing system was designed and built (see Figure 2). Experiments conducted on the HTRI system produced mixed metal-oxide layers like those seen on engine components. During the current, and final, year of this effort, information on oxidation, layer formation, and mechanical response was integrated to produce a nonlinear, multiparameter model to portray the dimensional changes on valve-seat contact surfaces. A sample plot showing valve and seat wear is given in Figure 3. This project will conclude with the publication of the final report which contains a detailed derivation and rationale for the valve wear model, a bibliography of past research on valve wear, and several examples of model output. The report will be distributed to engine manufacturers, high-performance materials suppliers, and the tribology community in general.

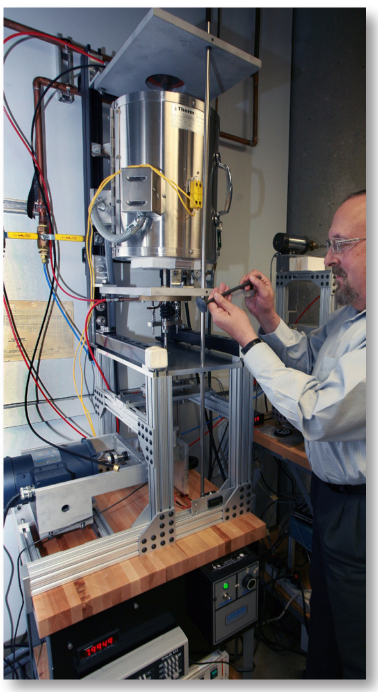

Figure 2: HTRI testing system that simulates wear damage on valve and seat surfaces. It is capable of reaching temperatures as high as 850°C.

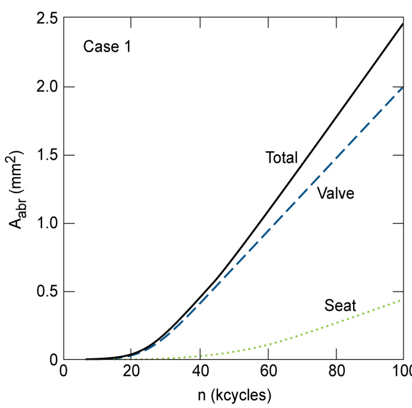

Figure 3: Sample output from the valve wear model in which the combined material loss of the valve and seat are plotted versus thousands of cycles of contact.

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Propulsion Materials

Materials-Enabled High Efficiency Diesel Engines

Background

Oak Ridge National Laboratory (ORNL) recently signed a Cooperative Research and Development Agreement (CRADA) with Caterpillar Inc. to investigate the potential of materials enabled technologies to improve diesel engine performance, efficiency, and emissions. The primary objective of this activity is to achieve and demonstrate 55% brake thermal efficiency in a heavy duty diesel engine through materials-enabled improvements in the combustion process and thermal management of the engine and reductions in friction and parasitic losses. Caterpillar has provided ORNL with two dc motoring dynamometers and a dynamometer-ready 2004 C-15 advanced combustion emissions reduction technology (ACERT) engine. The engine is equipped with a user accessible controller allowing for manipulation of critical engine parameters such as fuel injection timing, duration, and pressure. Engine and materials science experts at ORNL and Caterpillar are working together to develop, implement, and assess the performance of advanced materials on engine performance and emissions. The near-term effort will focus on using advanced material coatings for improved management and use of thermal energy, which is normally discarded to the environment. A modeling activity is also under way to guide experimental activities and identify potential fuel efficiency opportunities. Through the use of internal funds, ORNL has supported the development of a new engine laboratory in support of this CRADA activity.

Technology

The engine is now operational with a user accessible controller that allows manipulation of many engine parameters including full control of fuel injection events. The engine is fully instrumented to measure the temperature, pressure, and mass flows at critical locations in the setup. This information will be used in support of modeling work and in identifying and characterizing potential efficiency opportunities. The combination of experiment and model to perform a component-by-component assessment of thermodynamic losses and opportunities is expected to be critical for fully understanding and realizing the maximum potential of materials-enabled technologies. Future instrumentation will include in-cylinder pressure and intake/exhaust valve temperature measurements. Engine instrumentation is summarized in Figure 1. Another key technical component is the use

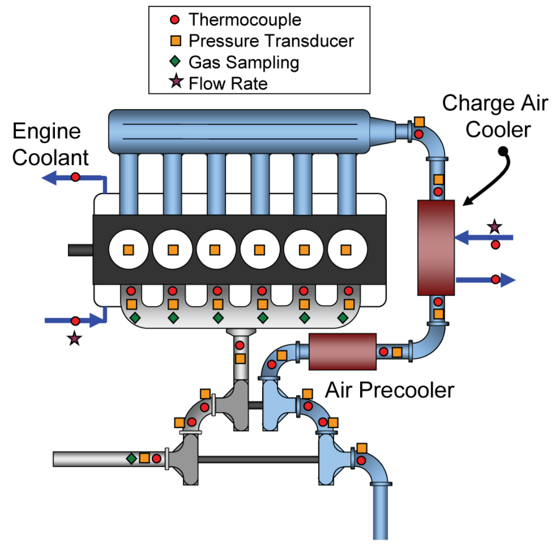

Figure 1: Diagram of sensor layout on engine.

Benefits

- *This CRADA bridges engines and materials teams at Caterpillar and ORNL to make better use of and improve upon the integration of advanced materials for improved performance and emissions.*
- *The integration of advanced materials from a thermodynamics perspective for improved engine efficiency and thermal management is critical to achieving 55% brake thermal efficiency in heavy duty diesel engine applications.*
- *Collaboration with Caterpillar ensures that successful technology advances made in this project are relevant and transferable to industry.*

of the advanced materials characterization and analytical tools available at the ORNL High Temperature Materials Laboratory. The capabilities of the ORNL materials science staff are critical in assessing material and component performance and expediting the use of advanced materials in engine systems.

Status

An engine research cell has been developed and commissioned at the ORNL National Transportation Research Center in support of this CRADA. The engine laboratory was constructed from the ground up and required significant infrastructure modifications including the installation of a control room, cooling water system, fuel supply system, cell ventilation, and power for the dc motoring dynamometer. The cell infrastructure, dynamometer, C-15 ACERT engine, and data acquisition systems have been commissioned as shown in Figure 2. Baseline experiments are also under way and are expected to be complete by the end of FY 2009.

Materials related engine experiments are expected to start in early FY 2010 and will be focused on the evaluation of a low cost thermal barrier material for improving the availability or quality of exhaust thermal energy.

Figure 2: Photograph showing installed engine and dynamometer.

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Propulsion Materials

Modeling/Testing Environmental Effects on Power Electronic Devices

Background

A complex relationship exists between the environment (temperature, humidity, and vibration) and the performance and reliability of the material constituents within automotive power electronic (PE) devices and support systems. There is significant interest in developing more advanced PE devices and systems that are capable of sustained operation to 200˚C for transportation applications [e.g., electric vehicles (EVs) and hybrid electric vehicles (HEVs)]. Advances in packaging materials and technology can achieve this but only after any service limitations they might impose are better understood via modeling and testing.

Technology

Interest exists in operating PE devices at temperatures up to 200˚C for EV and HEV applications. However, many contemporary devices such as insulated gate bipolar transistors cannot sustain continuous operation above 125˚C because of the limits of their material constituents.

Additionally, accurate life prediction and accelerated test methods are not available to the PE device community, and this hinders more rapid development of devices. This is important because contemporary PE devices will need greater ruggedness and improved thermal management for continued development and use.

Finally, other electronic components in EVs and HEVs (e.g., permanent magnetic materials used in motors) are too expensive or are increasingly scarce. Some could be more efficiently designed to lessen weight and volume. Therefore, there is a need to identify and develop alternative material constituents that help overcome those limitations.

Status

A patent was issued for a direct cooled ceramic substrate. The development was a consequence of a collaboration of Oak Ridge National Laboratory Advanced Power Electronics and Electric Machines and Propulsion Materials Programs and the National Transportation

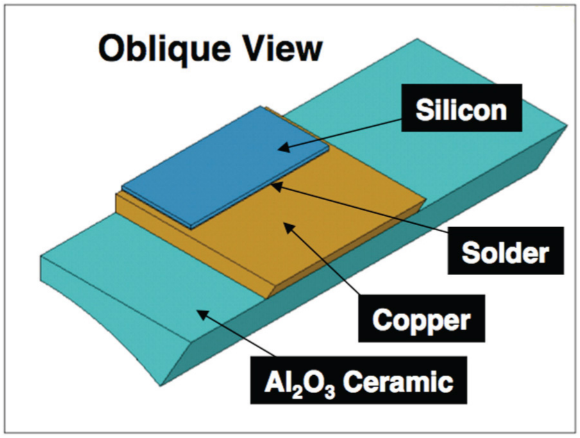

Figure 1: Finite element model of direct cooled ceramic substrate package.

Benefits

- *PE devices capable of operation at higher temperatures.*
- *More reliable PE devices.*
- *Alternative methods to achieve improved thermal management.*

Research Center. Thermomechanical analysis of candidate ceramics was performed using finite element and material strength probabilistic analyses. The finite element model is shown in Figure 1. The ceramic [aluminum oxide (Al_2O_3)] substrate, solder layer, copper layer, and silicon chip are shown in a model with one-twelfth symmetry. Examples of the resulting service and temperature profile and stress field are shown in Figures 2 and 3, respectively. The analyses were used to iteratively redesign the ceramic substrate until the maximum tensile stress in the Al_2O_3 substrate was minimized.

As a second primary effort, numerous properties of $Nd_2Fe_{14}B$ permanent magnetic materials from motors from three different hybrid vehicles were quantified. Property measurements included coefficient of thermal expansion, density, elastic modulus, Poisson's ratio, hardness, phase analysis, and elemental analysis.

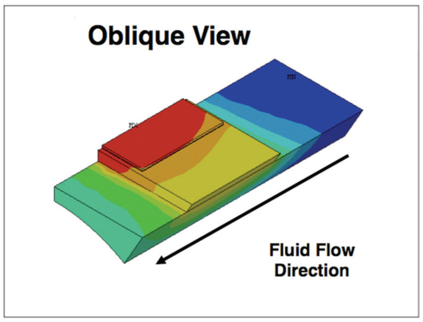

Figure 2: Resulting temperature profile from heat-producing silicon chip and cooled interior.

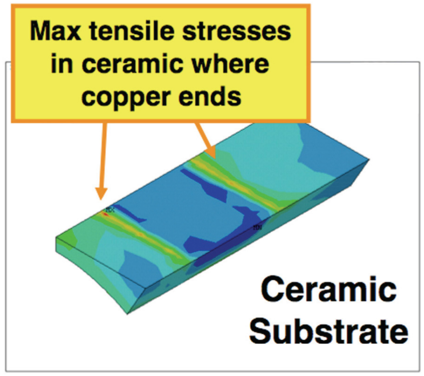

Figure 3: Resulting stress profile in the ceramic substrate from the temperature profile.

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Propulsion Materials

Ultrahigh Resolution Electron Microscopy for Catalyst Characterization

Background

Ultrahigh resolution electron microscopy using the High Temperature Materials Laboratory's (HTML) aberration-corrected electron microscope (ACEM) at Oak Ridge National Laboratory 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 unique microelectromechanical systems- (MEMS-) based chip heater technology introduced by Protochips Inc. (Raleigh, North Carolina), with whom we are collaborating by leveraging funding through a Work for Others project. In FY 2008 we demonstrated the ability to achieve single-atom imaging resolution on catalyst samples at temperatures as high as 1,000˚C. Because 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, the information provided by in situ heating is an important step toward this goal. In FY 2009, we have made further progress in extending the Protochips heating technology by incorporating a capability for gas reaction studies via an environmental cell (or E-cell) approach. With modifications to the ACEM pumping system, we have also enabled the capability to perform gas reactions (primarily reductions) at atmospheric pressure within the specimen airlock of the microscope, essentially a pseudo-ex situ approach that has initially given useful results (not detailed here). The E-cell technology and an example of the initial imaging with the E-cell are described in the following paragraphs.

Technology

Protochips' Aduro heating chips comprise a thin ceramic membrane suspended over a hole in a silicon chip that is both the heater (e.g., current passed through the membrane can heat it to >1,000˚C in 1 ms) and the support for the catalyst powder sample to be heated. In a first generation (Gen 1) E-cell design, one of these heating chips was sandwiched between two similar silicon chips that supported thin amorphous silicon nitride windows [Figure 1(a)]. However, this three-chip design proved to be too thick (1.7 mm) to fit appropriately within the thin gap (2 mm) of the objective lens

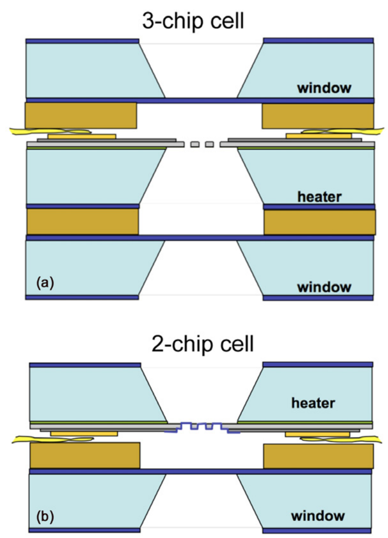

Figure 1: E-cell geometry. (a) = Gen 1 three-chip design; (b) = Gen 2 two-chip design.

Benefits

- *Subångström resolution microscopy provides unique information leading to fundamental understanding of how catalysts behave at the atomic level.*
- *In situ gas reaction techniques via an E-cell developed using Protochips' Aduro technology gives us a unique capability to study the kinetics and mechanisms of catalyst behavior.*
- *Attraction of top catalyst researchers in the country eager to collaborate with the U.S. Department of Energy.*

of the microscope. The solution was a second generation (Gen 2) design comprising only two chips [Figure 1(b)] with the upper chip serving as both the window and the heater. The new holder we fabricated, shown in Figure 2, was only 1.38 mm thick.

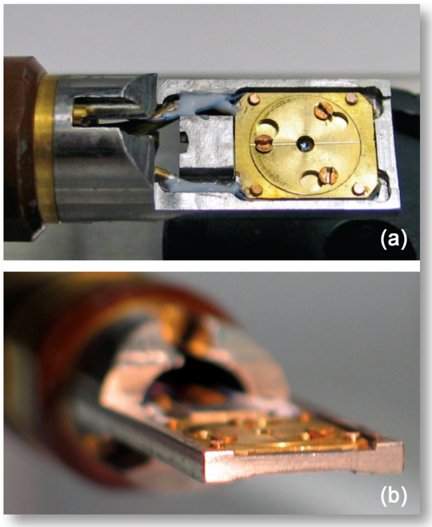

Figure 2: Top (a) and end (b) views of the Gen 2 E-cell holder showing 1.38 mm thickness.

Status

An example of imaging through a currently achievable window material is shown in Figure 3. The sample is deposited on the inside surface of a 25 nm thick amorphous silicon nitride window, which models the upper (heater) chip. The catalyst material is imaged with the electron beam passing first through this window material. A gold (Au) on iron oxide (FeO_X) catalyst with 2 nm Au nanoparticles was imaged using high-angle annular dark-field techniques. The Au species also show as a near-atomic dispersion within the bulk of the FeO_X crystals and coat the inner surfaces of voids in the oxide. Figure 3(a) shows the latter case, and Figure 3(b) shows the well-resolved crystal structure of a surface nanocrystal. This result offers great promise for the success of our future E-cell development.

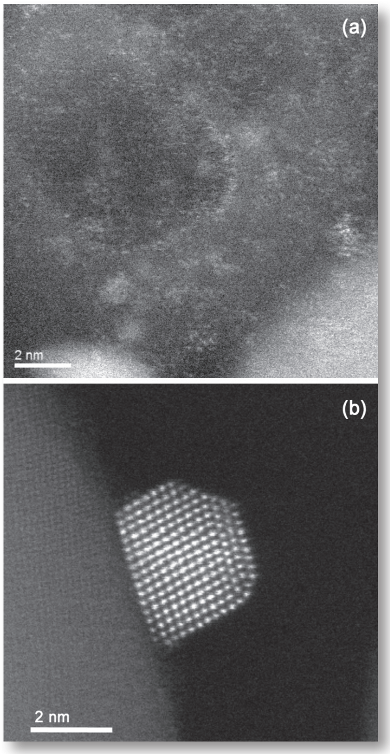

Figure 3: Imaging examples. (a) = single Au atoms decorating voids in Au-FeOX catalyst imaged through 25 nm silicon nitride window; (b) = Au nanoparticle showing crystal lattice imaged through the same window.

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Vehicle Systems

Development of Models for Advanced Engines and Emission Control Components

Background

Accurate predictions of the fuel efficiency and environmental impact of advanced vehicle propulsion and emissions control technologies are vital for making informed decisions about the optimal use of research and development resources and U.S. Department of Energy (DOE) programmatic priorities. One of the key modeling tools available for making such predictions is the Powertrain System Analysis Toolkit (PSAT) maintained by Argonne National Laboratory. A distinctive feature of PSAT is its ability to simulate the transient behavior of individual drivetrain components and their combined performance effects under realistic driving conditions. However, the accuracy of PSAT simulations ultimately depends on the accuracy of the individual component submodels or maps. In some cases of leading-edge technology, such as with engines using high efficiency clean combustion (HECC) and lean exhaust particulate and nitrogen oxide (NO_X) controls, the availability of appropriate component models or the data to construct them is very limited.

Technology

Oak Ridge National Laboratory (ORNL) is building stoichiometric and lean exhaust aftertreatment component models for vehicle systems simulations using proven approaches for simulating transient chemical reactors. As much as possible, the descriptions of the internal reaction and transport processes are simplified to account for the dominant effects and physical limits while maintaining execution speeds acceptable for typical PSAT users. For example, there are no cross-flow (i.e., radial) spatial gradients accounted for in the devices, and the kinetics are defined in global form instead of elementary single reaction steps. This in-between level of detail still allows for faithful simulation of the coupling of the aftertreatment devices to both upstream and downstream components (arranged in any desired configuration). With the above information it is also possible to determine both instantaneous and cumulative systems performance for any desired period.

Due to the greater complexity of engines, it is not practical to develop models with the same level of dynamic detail as in the aftertreatment component models. Instead, the usual approach for engine modeling relies on tabulated “maps” developed from steady-state or pseudo-steady-state experimental engine-dynamometer data. Recently, it has been possible to develop maps that extend over both conventional and HECC operating ranges. A key feature that will be added in the future is an engine control submodel that determines how the engine should operate (e.g., make transient shifts in combustion regime) to accommodate the needs

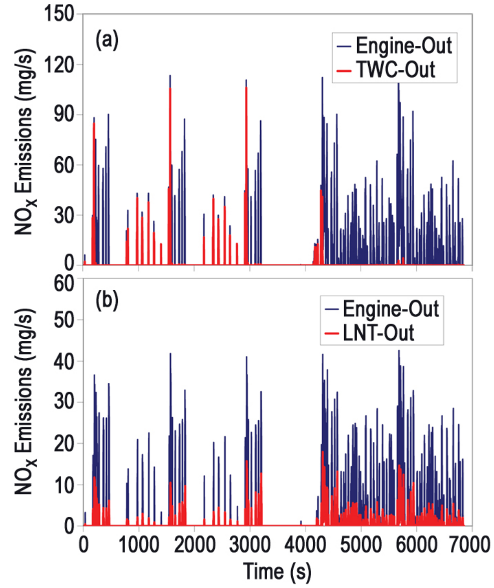

Figure 1: Simulation of engine-out and tailpipe NO_X emissions from gasoline-powered and diesel-powered PHEVs over five consecutive Urban Dynamic Driving Schedule cycles beginning with a cold start.

Benefits

- *Provides a fundamental understanding of the potential energy efficiency benefits of different advanced vehicle system power generation and emissions control options that can support technology investment decisions by DOE and industry.*
- *Provides real-world data as a baseline for assessing the benefits of new and emerging passenger vehicle and truck energy efficiency technologies.*
- *Provides tools sufficient for predicting the impact of alternative fuels and control strategies on vehicle system component interactions and global efficiency.*
- *Provides a real-world-based data source for evaluating and validating models of engines, aftertreatment systems and components, and vehicle performance.*

of aftertreatment devices downstream. This will also involve development of sensor models that indicate the state of the aftertreatment devices.

Status

ORNL has developed a methodology for modifying steady-state engine maps to account for cold- and warm-start transients that has been successfully demonstrated for multiple light duty engines, including both gasoline and diesel engines similar to those expected to be used in advanced hybrid vehicles. An idealized, full-range HECC exhaust map for a 1.7 L Mercedes diesel engine was developed and used to estimate the potential impact of full HECC operation on hybrid vehicle fuel economy and emissions. For gasoline hybrid vehicle simulations, a preliminary three-way catalyst aftertreatment model has been improved and validated with experimental data from multiple sources. For diesel hybrid simulations, a catalyzed diesel particulate filter (DPF) aftertreatment model was developed from the noncatalyzed DPF model developed previously, validated with data from the literature, and implemented in PSAT simulations of hybrid vehicles. A diesel oxidation catalyst aftertreatment model was also developed and validated to a limited extent to account for oxidation of carbon monoxide, nitric oxide, and hydrocarbons. To evaluate the effects of waste heat recovery, a coolant thermal storage component model (e.g. to supply heat for more rapid aftertreatment catalyst "lightoff") has been developed and implemented in plug-in hybrid electric vehicle (PHEV) system simulations.

PHEV simulations comparing diesel- and gasoline-powered vehicles equipped with appropriate NO_X emissions controls indicate that diesel vehicles will have modest efficiency advantages, but these are reduced from what is ultimately possible due to emissions control fuel penalties. Example comparison simulations of gasoline and hybrid vehicle NO_X emissions and fuel consumption are illustrated in Figures 1 and 2.

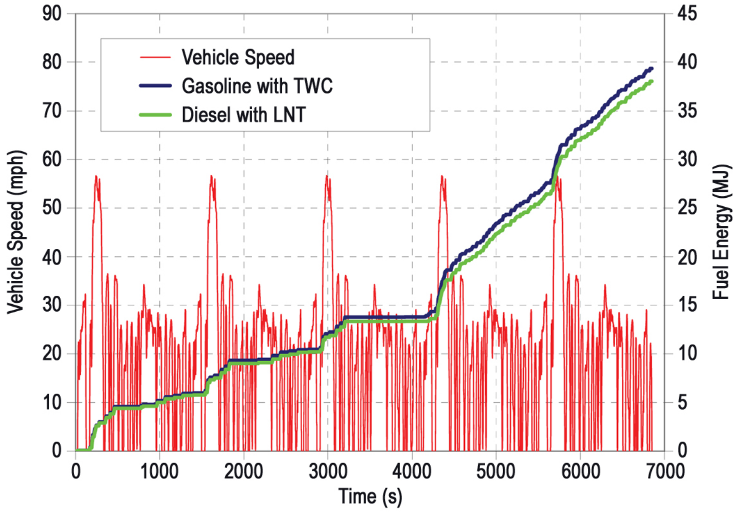

Figure 2: Simulation of fuel energy consumption for gasoline-powered and diesel-powered PHEVs over five consecutive Urban Dynamic Driving Schedule cycles beginning with a cold start.

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