USDRIVE

DRIVING RESEARCH AND INNOVATION FOR
VEHICLE EFFICIENCY AND ENERGY SUSTAINABILITY

U.S. DRIVE Highlights of Technical Accomplishments 2013

March 2014

U.S. DRIVE
Highlights of Technical Accomplishments Overview

Through precompetitive collaboration and technical information exchange, U.S. DRIVE partners are accelerating the development and availability of clean, efficient automotive and energy technologies.

The U.S. DRIVE Partnership (*Driving Research for Vehicle efficiency and Energy sustainability*) is a voluntary government-industry partnership focused on precompetitive, advanced automotive and related infrastructure technology research and development (R&D). Partners are the United States Department of Energy (DOE); the United States Council for Automotive Research LLC (USCAR), a consortium composed of Chrysler Group LLC, Ford Motor Company, and General Motors Company; Tesla Motors, Inc.; five energy companies, (BP America, Chevron Corporation, Phillips 66 Company, ExxonMobil Corporation, and Shell Oil Products US); two electric utilities, DTE Energy and Southern California Edison; and the Electric Power Research Institute.

By providing a framework for frequent and regular interaction among technical experts in common areas of expertise, the Partnership accelerates technical progress, helps to avoid duplication of efforts, ensures that publicly-funded research delivers high-value results, and overcomes high-risk barriers to technology commercialization.

U.S. DRIVE partners selected the technical highlights in this document from many hundreds of DOE-funded projects conducted by some of the nation's top scientists and engineers. Each one-page summary represents what DOE and automotive, energy, and utility industry partners collectively consider to be significant progress in the development of advanced automotive and infrastructure technologies. The report is organized by technical area, with highlights in three general categories:

Vehicle Technologies
- Advanced Combustion and Emission Control
- Electrical and Electronics
- Electrochemical Energy Storage
- Fuel Cells
- Materials
- Vehicle Systems and Analysis

Crosscutting Technologies
- Codes and Standards
- On-board Hydrogen Storage
- Grid Interaction

Fuel Infrastructure Technologies
- Fuel Pathway Integration
- Hydrogen Delivery
- Hydrogen Production

More information about U.S. DRIVE, including prior year accomplishments reports, is available on the DOE (www.vehicles.energy.gov/about/partnerships/usdrive.html) and USCAR (www.uscar.org) websites.

Advanced automotive and energy infrastructure technologies are entering the market in increasing numbers, and technologies that were only concepts less than a decade ago are now approaching initial commercial readiness. These advancements are the result of partners working together to achieve a common goal. With continued progress resulting from the joint efforts of government, industry, and academic experts, the U.S. DRIVE Partnership is helping to increase the competitiveness of American industry and secure U.S. leadership in an increasingly competitive global market to enable a clean and sustainable transportation energy future.

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VEHICLE TECHNOLOGIES

Advanced Combustion and Emission Control

2013 U.S. DRIVE Highlight

Lean Downsized Boosted Engine Projected to Improve Combined-cycle Fuel Economy by 25%

Project identifies potential of lean stratified combustion with intake pressure boosting, air motion control, and EGR to improve efficiency while maintaining power and torque.

General Motors, Ricardo, Bosch, Umicore

Researchers studied the improvement in engine efficiency with lean (excess air) stratified gasoline fuel, exhaust gas recirculation (EGR), intake pressure boosting, and reduced displacement. Lean operation with EGR improved efficiency at light to medium loads. Boosting extended the efficiency improvements to higher loads and enabled the reduction in engine displacement while maintaining the maximum power and torque.

The engine components consisted of direct fuel injection into the combustion chamber formed with a specific piston design. The fuel was injected in multiple pulses to improve fuel-air mixing. Cooled EGR was added to control engine-out NOx emissions. Air motion was controlled and augmented with a port throttle to reduce combustion variations at lean conditions. A turbocharger increased the air flow mass since lean operation required larger air flow than typical for the engine size. With these technologies, the four-cylinder engine displacement was reduced from 2.4 to 1.4L.

The engine was tested using an engine dynamometer at 12 key points representing U.S. city and highway driving. Relative to the 2.4L port-injected engine with stoichiometric homogenous gasoline fuel, the brake-specific fuel consumption (BSFC) was improved by up to 35%, as shown in Figure 1. Using the measured data, the projected improvements in city and highway fuel economy were 26% and 12%, respectively for a mid-sized passenger car. The projected combined cycle fuel-economy improvement was 21%. A vehicle implementation would include a system to stop the engine when the vehicle stops (stop/start), which improves fuel economy by 5%. Including stop/start, the projected combined cycle fuel economy improvement was 25%.

This engine was installed in a mid-sized car and demonstrated with stop-start. Researchers developed a passive selective catalytic reduction (SCR) aftertreatment system combined with active urea control. The passive SCR enabled significant reduction in urea consumption. This aftertreatment system demonstrated partial zero-emission vehicle emission capability with the first-generation lean naturally aspirated engine developed as part of this project.

		Speed (RPM)	Load (n-m)	BSFC Improvement
City	Idle	700	19	0%
	Zone 2	1335	27	30%
	Zone 3	1565	28	31%
	Zone 4	1805	29	35%
	Zone 5	1530	95	7%
	Zone 6	1821	80	9%
	Zone 7	2250	101	7%
Highway	Zone 8	1410	51	16%
	Zone 9	1669	60	14%
	Zone 10	1461	114	3%
	Zone 11	1692	100	6%

Projected FE Improvement by Engine	**City**	26%
	Highway	12%
	Combined	21%
Stop/Start FE Improvement		5%
Projected Vehicle FE Improvement		25%

Figure 1. BSFC improvements at 12 key points and projected fuel economy improvements for lean, downsized boosted engine.

Fundamental Differences between Gasoline and Diesel Fuel Sprays Revealed

New theoretical description of fuel injection process is developed, which points the way to advanced injection and combustion models.

Sandia National Laboratories

The combination of advanced theory and high-fidelity large eddy simulation (LES) has provided new insights into direct injection processes at high-pressures. LES directly resolves most of the turbulent structures in the flow and models the remaining unresolved very small flow features. Research has previously shown that under some high-pressure conditions, the presence of discrete two-phase flow processes becomes diminished. Under such conditions, liquid injection processes transition from classical sprays with droplets to dense-fluid jets, with no drops present. Why and under what conditions this transition occurs, however, was not understood until now. The new theoretical description is one of the first to explain and quantify this phenomenon, and it has important implications for the development of validated predictive models for engine design.

A key output from the theory is a regime diagram such as shown in the left of Figure 1. It quantifies the pressure-temperature conditions where classic atomizing sprays (white region) transition to dense-fluid jets (grey region). Researchers corroborated trends predicted by the regime diagram using microscopic imaging to zoom in on the detailed features of dense-fluid jets (top right image, which shows no presence of distinct fuel droplets) and classical spray processes (bottom right image, which shows fuel droplets near the spray boundary). The analysis, contrary to conventional wisdom, suggests that for almost all diesel conditions, fuel enters the cylinder as a dense-fluid jet without drop formation. Classical spray processes, however, occur under current gasoline spark-ignition engine conditions. Advanced models must account for both extremes.

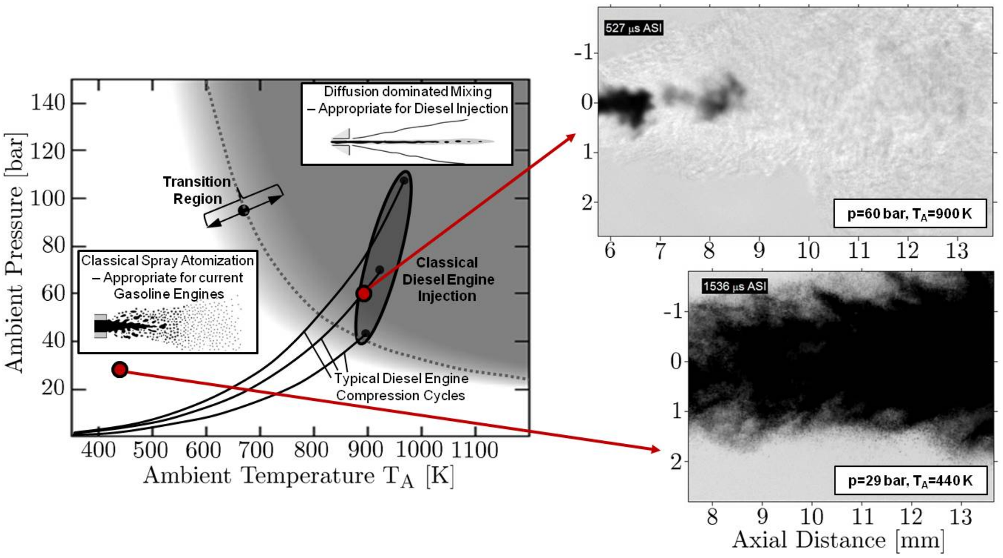

Figure 1. Regime diagram on the left for n-dodecane injected into nitrogen suggests the presence of dense supercritical jets (grey region) under diesel conditions (dark grey highlighted area) without drop formation. Classical spray atomization processes (white region) occur under gasoline engine conditions. High-speed imaging of both a dense jet (top right) and a spray (bottom right) corroborates the theory.

2013 U.S. DRIVE Highlight

Optical Engine Reveals How Post Injections Reduce Soot and Unburned Fuel for Efficient Diesel Combustion Options

Laser/optical techniques show that post-injections displace soot or enriched mixtures to allow better oxidation of soot and fuel, knowledge critical to designing multi-pulse injections for clean, high-efficiency engines.

Sandia National Laboratories

Post injections of fuel, which are small pulses of fuel split off from the main injection, can reduce soot and unburned fuel emissions while maintaining efficiency. The processes inside the engine are unclear, however, so design of post-injections for maximum benefit is limited. Recent research in optical engines is helping, by revealing how post-injections affect combustion and pollutant formation. Figure 1 shows how exhaust soot emissions increase with engine load for single injections (black squares). Adding a small (<20% of fuel) post-injection after the premixed burn can reduce soot by 55% (blue circles). The image view up through the piston shows the post injection displacing soot (red) out of the bowl (yellow arrows), and improved oxidation by OH (green).

Figure 2 shows that adding a post-injection (blue squares) can also reduce unburned fuel emissions by 27% compared to a single injection (black squares). Optical-engine images show that the post-injection (right) enriches the near-injector region relative to a single injection (left), causing a greater extent of burned fuel (green), leaving less unburned fuel (red).

Both strategies use close-coupled injections to maintain good combustion phasing for efficiency. With this improved understanding of how post-injections work, better strategies to take full advantage of multi-pulse injections can be devised.

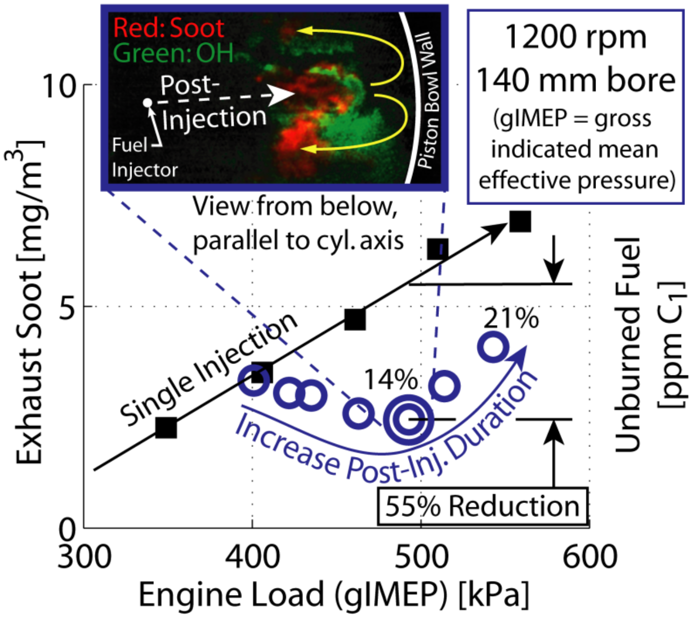

Figure 1. Exhaust soot emissions for single injection (solid black squares) and with post-injection (open blue circles), showing 55% reduction with a post-injection. Image at top shows the post-injection displacing soot (red) to the left, away from the bowl wall (curved line).

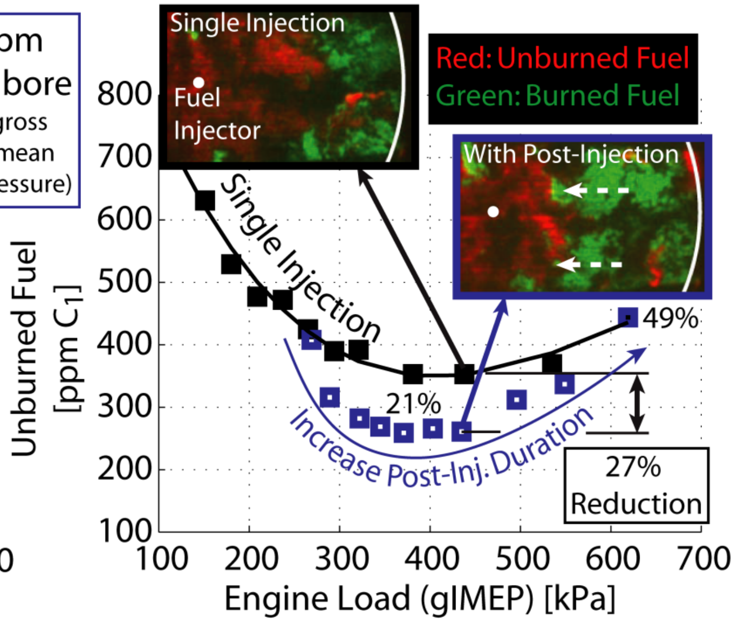

Figure 2. Unburned fuel emissions for single injection (solid black squares) and 27% reduction with post-injection (open blue squares). Top images show more unburned fuel (red) with single injection (left), and fuel burning extending leftward (green) with post-injection (right).

2013 U.S. DRIVE Highlight

Research Clarifies Chemistry of Negative Valve Overlap Fueling for Control of Gasoline Auto-ignition

Novel approach to combustion control expands high-efficiency, clean operation to broader range of engine operating conditions.

Sandia National Laboratories

The underlying chemistry enabling enhanced control of gasoline auto-ignition has been characterized by recent experiments. The research focuses on negative valve overlap (NVO) which, through early exhaust valve closing, traps and recompresses residual gases from the previous engine cycle. Fuel can be injected during NVO and reformed prior to main compression, providing both thermal and chemical energy that can be used to control main combustion on a cycle-by-cycle timescale. This strategy enables low-temperature gasoline combustion (with resulting low emissions) at moderate loads while maintaining high efficiency.

Sandia National Laboratories' experiments indicate that NVO fuel-injection timing is an important control parameter, as illustrated in Figure 1. Retarding the NVO injection increases the apparent heat release (AHR) and advances the phasing (CA10, or 10% burn point) of main combustion. Experiments have demonstrated that while thermal effects contribute to the enhancement of main combustion, chemical effects can be equally important. A recent full-cylinder gas-sampling campaign provided crucial NVO chemistry details.

Several measured NVO species are shown in Figure 2. Concentrations of the parent fuel, iso-octane (C_8H_{18}), are consistently high, but are not strongly affected by NVO injection timing. Three other species—carbon monoxide (CO), hydrogen (H_2), and acetylene (C_2H_2)—are important for several reasons. First, their abrupt upturn correlates with the enhanced main heat release seen in Figure 1. Second, all are products of rich combustion, consistent with optical-engine observations of pool fires associated with late NVO injection. Finally, seeding experiments and chemical kinetics simulations confirm that such concentrations of hydrogen and acetylene will contribute to advancing auto-ignition.

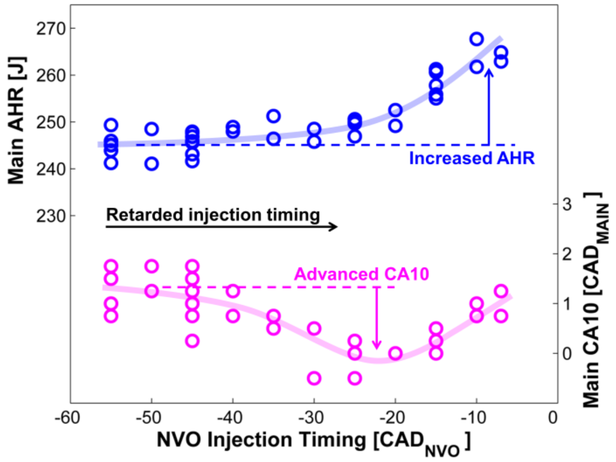

Figure 1. Main combustion enhancement by NVO fueling. Axes units = Crank Angle Degrees after top center of NVO or Main portion of cycle.

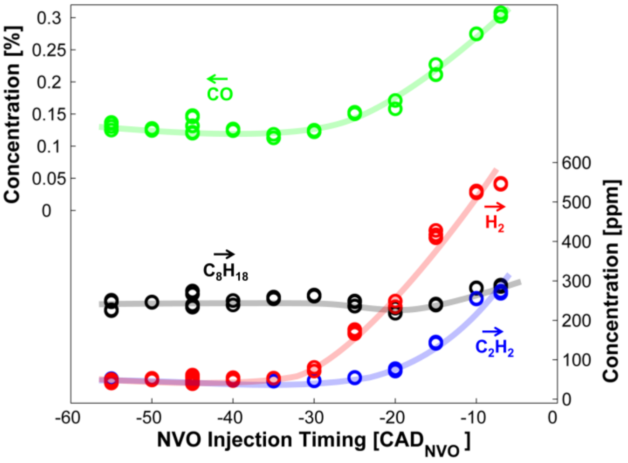

Figure 2. Key NVO product species profiles measured as a function of NVO injection timing.

2013 U.S. DRIVE Highlight

EGR Probe Enables Improved Model-based Engine Design

On-engine crank-angle and spatially resolved CO_2 measurements allow assessment and improvement of intake architectures, control strategies, combustion uniformity, and numerical design tools.

Oak Ridge National Laboratory and Cummins, Inc.

A cooperative research and development agreement project between Oak Ridge National Laboratory and Cummins, Inc. has developed and applied an exhaust gas recirculation (EGR) probe. It provides for crank-angle and spatially resolved carbon dioxide (CO_2) measurements throughout the intake manifold and has been used for advancing a wide range of technologies related to developing advanced-efficiency engine systems. These include improvement of intake architectures, mixing physics, control strategies, cylinder-to-cylinder and cycle-to-cycle combustion uniformity, and numerical design tools (e.g., computational fluid dynamics).

The instrument is based on mid-infrared laser absorption, uses a single-port probe, and allows for simultaneous measurement from four separate probes. The probe requires only a single access port and minimal modification of the stock hardware. This allows for broad measurement applications on developed and advanced-packaged engines where access can be limited. EGR distributions can be resolved via multiple access points and probe translation. The spectroscopic approach allows for simultaneous measurement of CO_2 concentration and pressure, to differentiate fluctuations associated with mixing and combustion versus density. Four-point multiplex measurements allow for fast and extensive system mapping. The system is capable of resolving transients within individual valve events, and throughout the cycle.

The EGR probe was applied to improve an EGR mixing model used for engine-system design. The EGR probe was used to characterize the temporal EGR dynamics associated with a certain mixer design and engine condition, as shown by the red curve in Figure 1. Compared to these measurements, the original mixing model predicted significantly different EGR dynamics, as shown by the green curve. The blue curve shows predicted EGR dynamics from an improved mixing model, which was tuned using the EGR probe measurements. Specifically, both the amplitude and shape of the improved-model predictions better match the measurements. For example, the amplitude of the predicted EGR dynamics was reduced from 59% to 22% CO_2, which more closely matched the 20% CO_2 measured value, and represented a 63% improvement over the original mixing model results. Through such improvements, model-based engine design is enhanced, which in turn hastens development of high-efficiency, low-cost, and durable engines.

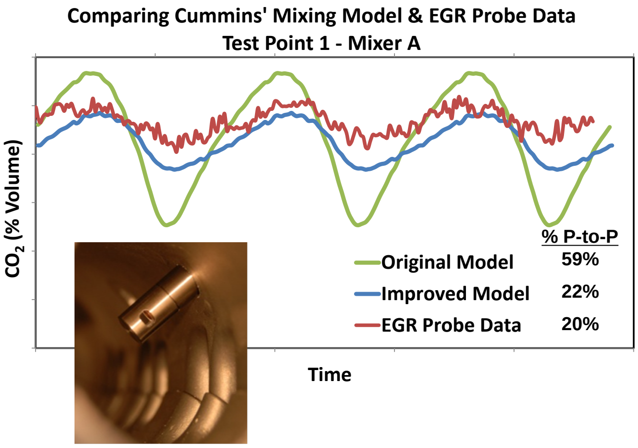

Figure 1. Design model improved using EGR probe measurements. The inset shows the EGR probe in an intake manifold.

2013 U.S. DRIVE Highlight

Bimetallic Catalysts Reduce Emissions Associated with Low Temperature Exhaust from Fuel Efficient Engines

A bimetallic catalyst based on Au and Cu achieves oxidation of CO and NO at lower temperatures, which can enable higher efficiency engines to meet U.S. emission regulations.

Oak Ridge National Laboratory

Improvements in the efficiency of advanced combustion engines are creating challenges for emission control systems due to the fact that greater fuel efficiency is leading to lower exhaust temperatures. Oxidation of carbon monoxide (CO) and other pollutants by catalysts becomes more difficult at lower temperatures, but a new type of catalyst developed at Oak Ridge National Laboratory (ORNL) is enabling improved low temperature performance.

A bimetallic catalyst composed of gold (Au) and copper (Cu) discovered in ORNL's Basic Energy Sciences program has unique properties that vary with exhaust conditions. Under rich conditions, an intermetallic nanoparticle of Au and Cu forms. Under lean conditions, a core-shell particle forms with Au on the inside core surrounded by a Cu oxide shell. This core-shell nanoparticle exhibits improved low temperature oxidation.

In studies on a bench flow reactor in simulated exhaust environment with nitric oxide (NO), CO oxidation over the Au-Cu catalyst was inhibited. However, by physically mixing a platinum (Pt) based catalyst with the Au-Cu catalyst, the combined catalyst demonstrated synergistic performance benefits and overall improvement in low-temperature oxidation as compared to both the traditional Pt-based and unique Au-Cu catalysts (Figure 1). CO oxidation performance "light-off" was attained at 30°C lower temperature than the Pt-based catalyst, and NO oxidation efficiency was doubled. Hydrocarbons currently inhibit the catalyst performance, and ongoing research is aimed at addressing hydrocarbon-induced limitations. However, the combination of Au-Cu and Pt catalysts shows benefits when hydrocarbon emissions are minimal. The improved catalytic performance will enable advanced combustion engines to meet challenging emission regulation levels.

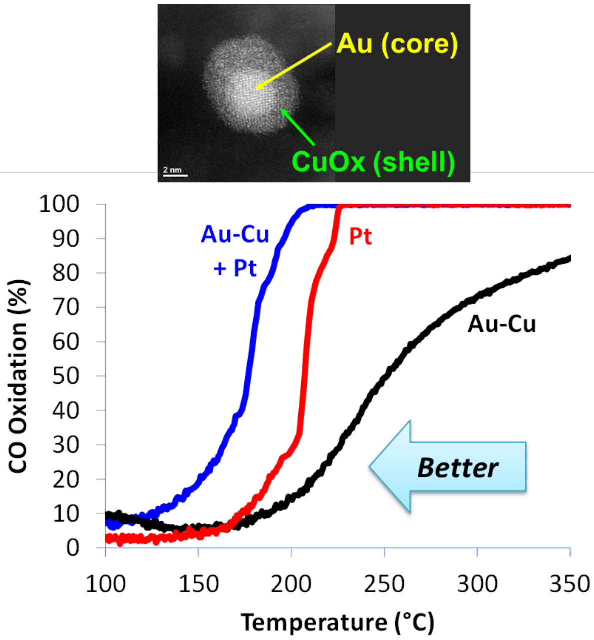

Figure 1. Micrograph of Au-Cu core-shell catalyst nanoparticle (upper) and CO oxidation efficiency vs. temperature for Au-Cu, Pt, and Pt and Au-Cu mixed catalysts in presence of CO and NO (lower).

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Emissions Control System Exposed to 20% Biodiesel-level Metals Meets Full Useful Life Emission Standard

System passes aggressive aging test that will help accelerate the introduction of higher levels of biodiesel from B5 to B20.

Oak Ridge National Laboratory and National Renewable Energy Laboratory

Introducing greater levels of domestically-produced renewable fuels is of high interest to increase energy security and lower greenhouse gas emissions. However, small impurities can have a significant impact on the emissions control system over the lifetime of the vehicle and need to be investigated. Currently, diesel fuel is limited to 5% biodiesel (B5), although some vehicles have been certified up to 20% biodiesel (B20). Small concentrations of metal impurities are introduced from chemicals in the biodiesel production process. These metals include sodium (Na) from sodium hydroxide, potassium (K) from potassium hydroxide, and calcium (Ca) from water. Current standards limit the combined Na+K content in biodiesel to 5 ppm; the Ca+magnesium (Mg) limit is also 5 ppm.

To study the impact of these metals on emission controls systems at a B20 level, researchers initiated an accelerated aging study. Researchers performed a full-useful life metal exposure and on-vehicle evaluation assuming use of B20 with 5 ppm metal for the entire 150,000 mile lifetime. Figure 1 shows the nitrogen oxide (NO_x) emissions during catalyst aging. The vehicle passes the NO_x emissions standards at the end of the test. However, elevated emissions at interim points highlighted the need for closer examination of the catalysts.

During materials characterization of the aged catalysts at Oak Ridge National Laboratory, a previously unknown deactivation mechanism was observed for the Na- and K-aged selective catalytic reduction (SCR) catalysts. A thin layer of copper oxide (CuO) formed on the surface of the washcoat (Figure 2). During aging, Na and K displace the copper (Cu) from the zeolite exchange sites. The Cu migrates to the surface of the washcoat in the form of CuO. This degradation mechanism did not eliminate the overall reactivity of the SCR catalyst at the 5 ppm exposure level, but higher levels of Na or K will cause the SCR catalyst to eventually fail the emission test. This phenomenon is unique to Na and K and was not observed in the catalyst aged with ultra-low-sulfur diesel (ULSD) or biodiesel with Ca.

Vehicles with up to B20 that meet the 5 ppm Na+K standard can meet the required emission regulation. Strict adherence to the metal content in biodiesel fuel standards is critical to avoid inducing Cu migration, which eventually degrades SCR catalyst performance.

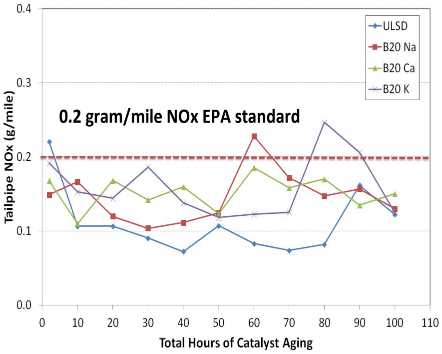


Figure 1. Tailpipe NO_x during accelerated aging with ULSD and B20 with three different metals. Each of the complete systems met the emissions standard at the end of the full-useful life durability evaluation.

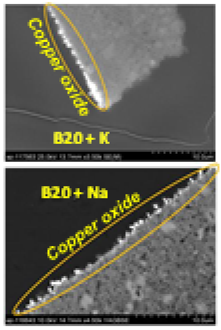


Figure 2. Micrographs showing the Na- and K-aged samples with an inactive CuO layer that originated from the Cu-zeolite SCR sites.

2013 U.S. DRIVE Highlight

New Method Developed to Assess Engine Efficiency Opportunities

New method uses 1st and 2nd laws of thermodynamics and experimental data to estimate potential efficiency opportunities of advanced engine technologies.

Oak Ridge National Laboratory

Increasingly stringent fuel economy regulations are driving innovative approaches to improving the efficiency of internal combustion engines. Typically, less than half of the energy released during combustion supplies work to the piston with the remainder consumed by inefficient processes including friction, pumping, heat loss, and hot exhaust leaving the tailpipe. The relationships between these processes are highly interdependent such that reducing one loss often increases another. Achieving significant increases in engine efficiency requires a thorough understanding of these interdependencies and multiple, concurrent approaches to reduce losses and concentrate the released energy where it can provide useful work.

Researchers at Oak Ridge National Laboratory (ORNL) have developed a method to account for the interdependent nature of energy usage in an engine and assess the potential benefits of various efficiency-improvement strategies from a purely thermodynamics basis without regard to cost, feasibility, or practicality. The approach begins with a complete 1st and 2nd law thermodynamic analysis of experimental or simulation data to evaluate the distribution of energy consumption within the engine. The potential efficiency benefits of given strategies are then evaluated by applying thermodynamics-based, multiplicative factors to estimate reductions in energy consumption and predict how that recovered energy may be redistributed among the other energy pathways. Determining proper values for these factors is difficult and subject to opinion. However, the mathematically simple approach makes it easy to perform sensitivity and uncertainty analyses for a given approach and provide a statistical range of potential benefits for a given strategy.

ORNL is working closely with industry stakeholders to apply this new technique to experimental data from state-of-the-art engine platforms to define pathways toward maximizing efficiency for light-duty applications. As an example, Figure 1 shows engine loss areas and the potential opportunities to improve their efficiencies for a light-duty diesel engine. The values of efficiency opportunity prioritize the areas of efficiency improvement. Future work is required to identify their cost, feasibility and practicality.

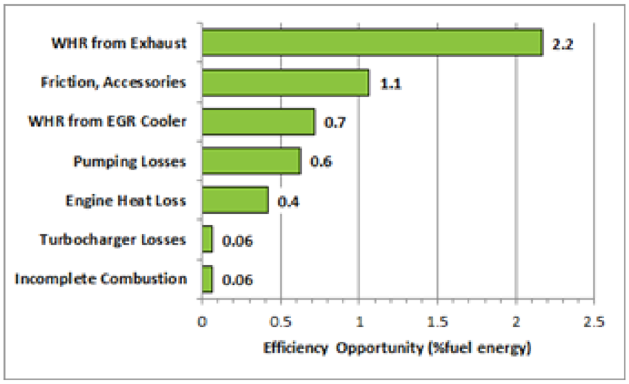


Figure 1. Example scenario for a light-duty diesel at part load showing potential opportunity for efficiency gains by reducing or recovering lost energy.

Study of GDI PM Size, Shape, and Composition Highlights Control Challenges that Differ from Diesels

New techniques to quantify particulate matter offer insight to increasing efficiency of gasoline direct-injection engines.

Oak Ridge National Laboratory

Elevated particulate matter (PM) emissions have become a challenge as direct-fueling replaces port-fuel injection in gasoline engines to boost fuel economy. Control of gasoline direct-injection (GDI) PM emissions involves in-cylinder combustion control and/or aftertreatment with gasoline particulate filters (GPFs). A better understanding of the origins of GDI PM can improve in-cylinder control and lessen GPF requirements, thus preserving fuel economy gains.

Using conventional particle sizing, Oak Ridge National Laboratory (ORNL) found that GDI soot spanned a much wider size range than diesel soot. Using exhaust from a 2.0L turbocharged GDI engine operating on 100% gasoline, ORNL collected a representative sample with a transmission electron microscopy (TEM) grid sampler designed to collect the full spectrum of particle sizes. Researchers analyzed resulting TEM images with a new technique that quantitatively measures the particle sizes and shapes. Diesel soot is made up of aggregates (chain-like structures) of tiny, spherical particles known as "primary" particles typically 20-25 nm diameter. Diesel PM uniformity arises from the high injection pressures and uniform atomization. In contrast, GDI soot morphology was found to vary greatly (Figure 1). Aggregates of nanoparticles were most common, but, unlike diesel, aggregates consisted of a broad size range of primary particle sizes. Next most abundant were single spheroids, followed by nascent soot with a thick, low volatility film, and the smallest fraction composed of irregular volatile particles.

The broad range of GDI particles indicates incomplete fuel and air mixing in-cylinder. Fuel impingement on surfaces leads to locally fuel-rich zones that produce large nanoparticles. The soot precursor compounds, the film on the nascent soot, indicates incomplete formation of the primary soot particle and fuel-rich conditions. In locally lean zones, small particles are formed. Within the soot cake of an exhaust filter (GPF), packing and pore penetration of small nanoparticles will reduce porosity and increase backpressure, affecting fuel economy. Quantitative studies of particle size and shape can potentially help engine design for in-cylinder control of GDI PM and GPF design for efficiency.

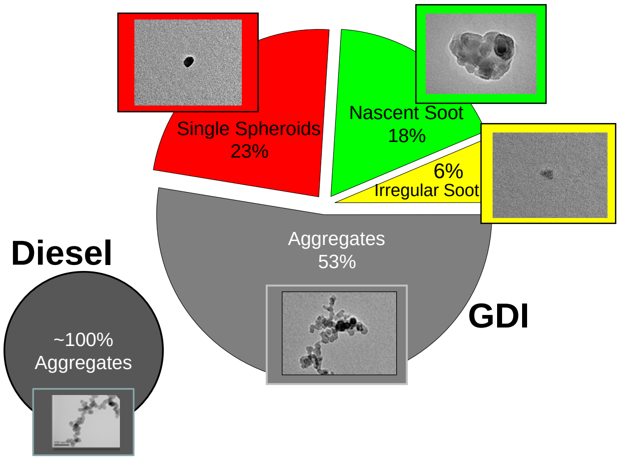


Figure 1. While diesel PM (lower left) is composed of nearly all aggregates, GDI PM (upper right) is composed of a complex mixture of aggregates, single spheroids, nascent soot, and irregular soot. Scales for the GDI TEM images are the same.

Electrical and Electronics

2013 U.S. DRIVE Highlight

Inverter Achieves DOE’s 2015 Goals

Delphi developed, tested, and demonstrated an inverter (55 kW peak) that meets U.S. Department of Energy’s 2015 cost, weight, and volume targets when manufactured in quantities of 100,000 units/year, and operates in a higher temperature environment.

Delphi Automotive Systems, LLC

Delphi’s high temperature inverter with integrated controller achieved the U.S. Department of Energy’s (DOE) 2015 research and development targets. Support tasks from industry partners and national laboratories included: power semiconductor development and characterization, capacitor development and testing, power device packaging, system modeling, thermal and heat exchanger experiments, interface material characterization, and inverter system testing.

Technology innovations developed during this project (low-loss world-class semiconductors and packaging, thermal stack-up and materials, and inverter level packaging concepts) have been incorporated in an inverter planned for production in mid-2015 (Figure 1).

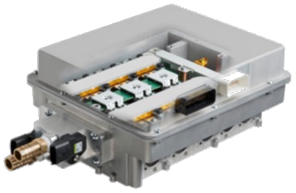


Figure 1. Delphi prototype production inverter incorporating DOE inverter innovations.

Delphi’s solution is also scalable across the range of 55 kW to 120 kW peak through the use of different die sizes and thermal materials. The Delphi/DOE inverter demonstrated its capability to operate with a standard 105˚C coolant system in a 140˚C ambient environment to eliminate the separate cooling loop typically required for today’s inverters.

A primary enabler for the inverter’s higher temperature capability was a direct current (DC)-link capacitor developed by General Electric, using polyetherimide (PEI) film as the dielectric. The newly developed PEI film has a permittivity that is 50% better than the polypropylene (PP) film used in today’s DC-link capacitors, and is capable of 200˚C operation versus PP’s 85˚C. Additionally, a roadmap was created to show a path to a smaller, lighter, lower cost PEI capacitor (Figure 2). Delphi also teamed with Argonne National Laboratory to develop a lead lanthanum zirconium titanate (PLZT) ceramic capacitor. The resulting sol-gel version of this capacitor exhibited benign failure, a permittivity about thirty times greater than today's baseline PP capacitor, and relatively high breakdown voltage. The team identified low-cost solutions for producing a high-temperature capable PLZT capacitor 90% smaller than today’s baseline PP DC-link capacitor.

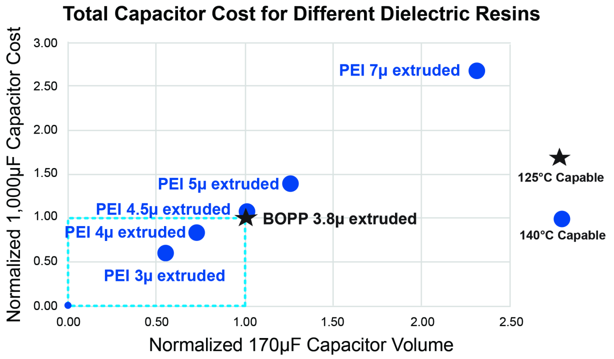


Figure 2. Roadmap to a lower cost, smaller dc-link capacitor with high temperature capability.

Key to the project’s success was Delphi’s development of a silicon (Si) dual-side cooled power device package, which involved collaboration with the National Renewable Energy Laboratory on thermal modeling and characterization. Delphi also worked with Dow Corning to develop a wide bandgap (WBG) power semiconductor platform and determined that cost parity with Si occurs when WBG current density reaches twice that of Si. Simulations from Oak Ridge National Laboratory showed that WBG (versus Si) devices can significantly reduce losses.

2013 U.S. DRIVE Highlight

Improved DC Bus Capacitors Using Glass Dielectrics

Commercial flat panel display glass has the potential to replace polypropylene for high temperature and high ripple current direct current bus capacitors used in electric drive vehicles.

Pennsylvania State University

Current direct current (DC) capacitors, made from polypropylene, do not have the high temperature performance required for use in future electric drive vehicle systems. However, glass is a high temperature, high dielectric constant material and can be incorporated into a capacitor. Thin glass sheet production has grown substantially with strong demand from the flat panel display industry and a large investment in the development of new glass fabrication methods. Glass manufacturers have developed a continuous sheet casting process that creates significant lengths of thin flexible sheet. This enabled Pennsylvania State University to prototype glass capacitors assembled in a similar manner to current polymer film capacitors, demonstrating that flat panel display glass is a viable material for high-temperature DC bus capacitors used in electric drive vehicles.

Flat panel display glass has shown stable capacitance and low loss values up to temperatures of 140°C and is a promising material for DC bus capacitors (Figure 1); however, the long-term material reliability is unproven. A series of electrical tests has demonstrated that the materials can withstand high voltage and temperature operation conditions for the life of the vehicle. Figure 2 shows the characterization of life through a test chamber at 400°C and overall life prediction relative to DOE's 13,000 hour target using this data.

Further testing of glass capacitors under high frequencies and at high temperatures has also yielded positive results. At 150°C and 10 kHz frequency, losses were measured an order of magnitude below DOE targets for DC bus capacitors, and remained low across a representative temperature and frequency range. Since typical polypropylene capacitors are limited to 125°C operation, these glass capacitors could also be used alongside wide bandgap semiconductors. This prototype capacitor fabrication and positive test results confirm the validity of flat panel display glass as a potential substitute for polypropylene in electric drive vehicle systems. With new manufacturing methods and materials for the display industry, glass holds promise for use in new applications, such as in electric drive vehicles.

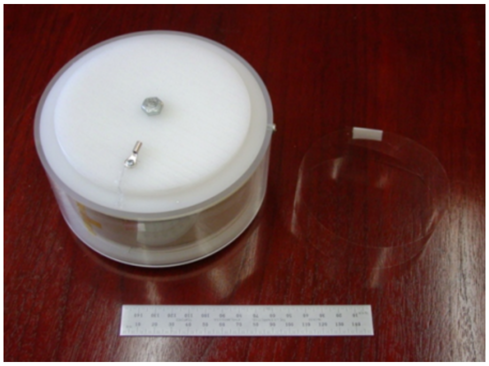


Figure 1. Coiled glass capacitor fabricated and tested at Penn State University using NEG 50 µm thick glass ribbon.

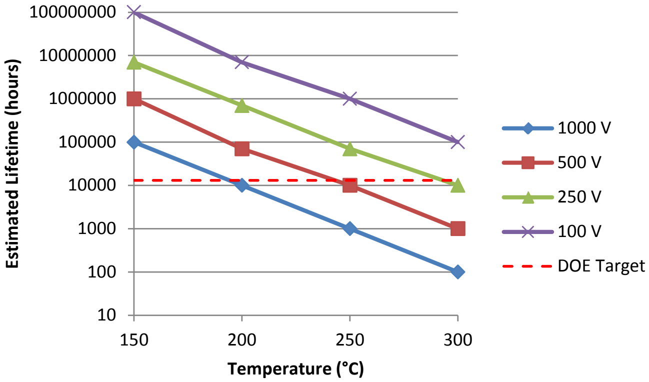


Figure 2. Reliability testing at high temperature is used to predict performance for DC bus capacitors in electric drive vehicles.

2013 U.S. DRIVE Highlight

Thermoplastics Show Excellent Reliability for Power Electronics Packaging

Thermomechanical reliability characterization for power electronics substrate-to-base plate bonded interface materials (BIMs) showed that high-thermal performance thermoplastic BIMs have the potential for meeting 15-year automotive life requirements.

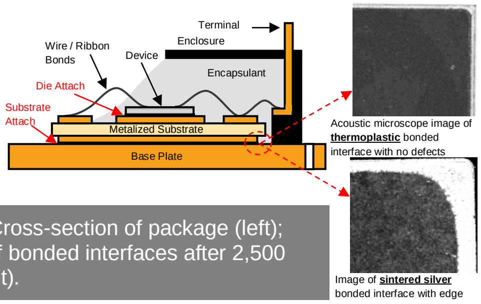
National Renewable Energy Laboratory

In automotive power electronics packaging, there is an industry trend towards high thermal performance bonded interfaces at the die and substrate attach layers. However, the reliability of emerging interface materials has not been proven for substrate-to-base plate attachments (see Figure 1).

The National Renewable Energy Laboratory, in collaboration with industry partners Btechcorp and Semikron, completed a thermomechanical reliability characterization and analysis for bonded interface materials (BIMs) based on thermoplastic/polyamide adhesive with embedded near-vertical aligned carbon fibers, sintered silver, and solder as a baseline. This rigorous characterization showed that thermoplastics have superior reliability than solder and sintered silver for substrate-to-base plate attachment for power electronics in electric-drive vehicle applications (less than 175°C junction temperature). Thermoplastics-based BIMs also provide efficient pathways for heat removal in the package.

Substrate-to-base plate bonded samples (50 mm X 50 mm footprint) were cycled between -40°C and 150°C. The ramp rate was 5°C/min with dwell times of 10 minutes at the maximum and minimum temperatures. Any degradation in the bonded sample was checked via acoustic microscopy every 100 cycles. Figure 1 shows the microscopy images of the bonded interface after 2,500 cycles. The BIM thermomechanical modeling has shown highest strain energy density per cycle at the perimeter, which is the reason for perimeter defect initiation and propagation. Btech thermoplastic samples underwent 2,500 temperature cycles, and no defects were observed. Figure 2 also illustrates that sintered silver is more reliable than solder. Sintered silver is on cost parity with solder, and Btechcorp is continuing work to further reduce the cost of thermoplastics to bring them on par with solder/sintered silver.

In collaboration with partners, future work with sintered silver material will focus on minimizing defects by optimizing processing conditions. The work will support future power electronics designs using wide bandgap devices for higher temperature operation (>200^{0}C). Improved reliability of automotive power electronics will contribute to cost reduction and wider market penetration of electric drive vehicles.



Acoustic microscope image of **thermoplastic** bonded interface with no defects

Image of **sintered silver** bonded interface with edge fracture defect

Figure 1. Cross-section of package (left); condition of bonded interfaces after 2,500 cycles (right).

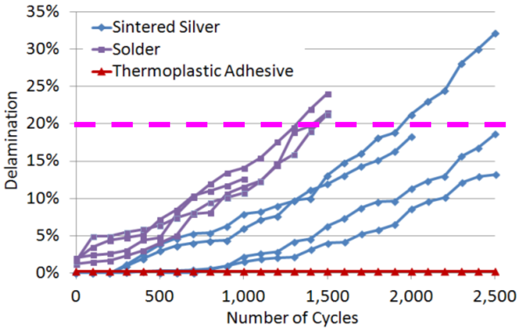


Figure 2. Delamination percentage of initial bonded area for the tested materials. The dashed line shows a common definition of package failure (~20% delamination).

2013 U.S. DRIVE Highlight

Integrated Heat Exchanger for Power Electronics

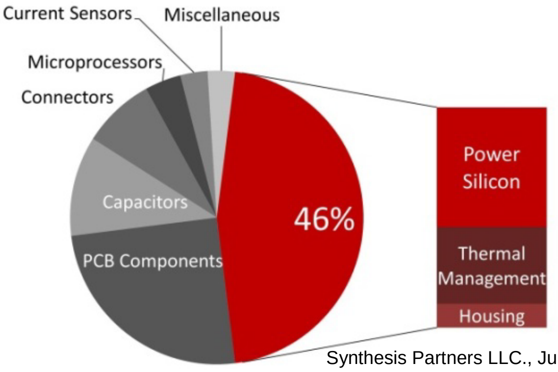
An advanced integrated heat exchanger was developed with thermal performance improvements leading to smaller, lighter, and lower-cost power electronics.

National Renewable Energy Laboratory

The National Renewable Energy Laboratory (NREL) developed and patented a novel heat exchanger integrated with the power semiconductor package for cooling the power electronics module. As shown in Figure 1, the power silicon, thermal management and housing account for almost half of the inverter cost. As compared to a high-performance commercial baseline (Lexus LS 600h inverter), the developed heat exchanger prototype (Figure 2b) doubles the heat rejection capability per silicon area. The result is increased power per silicon area, resulting in reduced cost per inverter power. The improved power capability enables inverter system cost reductions of 8%.

The concept optimizes the passive and active heat transfer paths to increase the die heat rejection capability. Unlike conventional cooling approaches dominated by one-dimensional (1-D) heat transfer (Figure 2a), the new design incorporates multiple heat transfer paths to enhance cooling (Figure 2b), while enabling less aggressive and lower-cost cooling technologies. NREL built an extruded aluminum design in close collaboration with an industry partner, Sapa Extrusions North America, and tested using water-ethylene glycol (WEG) coolant. The open channels (Figure 2b) reduced the number of internal voids resulting in a 25% tooling cost reduction. As compared to castings, which are typically used, extrusions have lower initial tooling cost. By enabling use of alloys with 36% higher thermal conductivity, extrusions also yield better thermal performance than castings. The design approach enables use of less effective coolants (air, transmission fluid), which would allow integrating the power electronics cooling with other vehicle systems, thereby eliminating a separate WEG coolant loop.

Future work will involve implementing this concept in a power module/inverter in collaboration with industry partners. The concept will also enable future wide bandgap packaging configurations. Improving power capability and reducing automotive power electronics costs will significantly contribute to making electric drive vehicles more affordable.



Synthesis Partners LLC., July 2011

Figure 1. Inverter cost drivers (Synthesis Partners LLC).

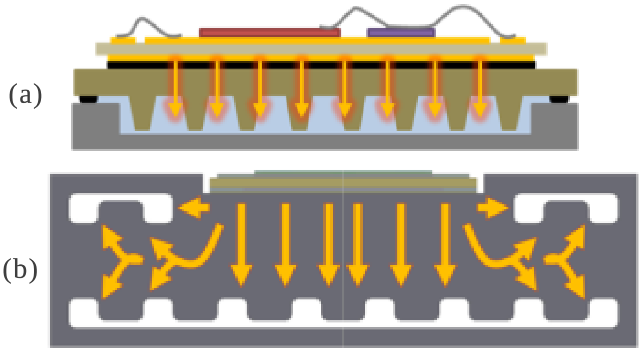


Figure 2. (a) Conventional 1-D cooling; (b) prototype heat exchanger showing multiple heat transfer paths.

Electrochemical Energy Storage

2013 U.S. DRIVE Highlight

High Energy NMC /Silicon Alloy Li-ion Automotive Cell

3M demonstrates a 50% increase in energy over nickel manganese cobalt oxide (NMC)/graphite cells using matched core-shell NMC cathode and silicon alloy anode.

3M Company

Vehicle electrification is fast becoming a reality around the world. Reducing battery cost is one of the keys to success. In order to reduce the cost of the battery ($/Wh), new active materials (anodes and cathodes) are needed to increase battery energy. These new active materials need to be matched carefully to enable the highest energy density. With U.S. Department of Energy support, 3M has integrated new cathode materials, anode materials, and electrolytes that can increase cell energy by 50% over typical high volume consumer electronics lithium (Li) nickel manganese cobalt oxide (NMC)/graphite cells.

3M™ Core-Shell (C/S) NMC Cathode: 3M's cathode materials are mixed nickel (Ni), manganese (Mn), and cobalt oxides with a high Ni core (for high energy) and high Mn shell (for high voltage stability). These materials have high capacity, high voltage, and good cycle stability.

3M™ Silicon (Si) Alloy Anode: 3M's Si alloy anode materials enable high energy density and have proper structure (amorphous active phase), particle morphology, and surface chemistry leading to controlled volume expansion upon lithiation and good cycling.

The Importance of the System: New cathode materials that have energy densities beyond traditional NMC materials invariably operate at higher cell voltages. To maximize the energy of the system, the cathode irreversible capacity should also match the irreversible capacity of the anode. In addition, for optimal cell balance and control of lower cut-off cell voltage, the irreversible capacity of the composite cathode must be slightly larger than that of the anode. The electrolyte and separator must be stable against the two electrodes and across the complete cell voltage range, to mitigate parasitic reactions. The 3M™ C/S high-energy cathode material has an effective usable energy 35% higher than typical NMC cathode materials.

When this cathode is combined with 3M™ Si anode, a 50% improvement in energy (Wh/L) in the wet laminate electrodes is demonstrated, as shown in Figure 1.

Next Steps: Cycle life optimization is underway and will be reported in the future. The process for high volume production of the 3M™ Si alloy anode material has been defined and is ready for implementation. Cathode materials have been scaled to the kilogram level.

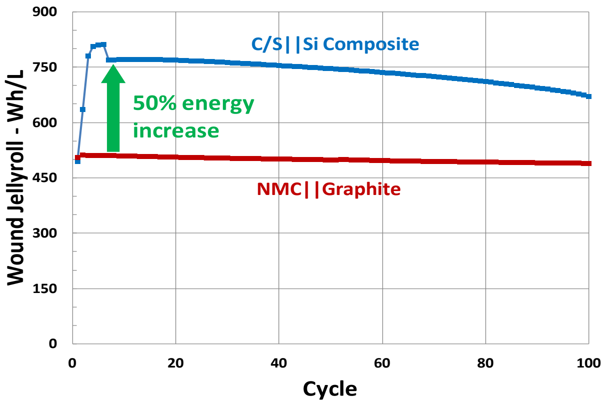


Figure 1. 18650 cylindrical cell data (scaled to reflect jellyroll volume) demonstrating 50% energy improvement of C/S||Si.

2013 U.S. DRIVE Highlight

Voltage Fade and Hysteresis Mechanisms in LMR-NMC Composite Electrodes

Voltage fade and hysteresis, key barriers in advancing high-energy cathode material implementation, are found to be correlated phenomena.

Argonne National Laboratory

Issues such as voltage fade and hysteresis in $x\mathrm{Li_2MnO_3}$•$(1-x)\mathrm{LiMO_2}$ (LMR-NMC) materials represent major barriers to success for these high-energy lithium-ion cathodes. Thus, intense research to understand the mechanisms is underway. The model developed in this project represents a potential major advance in our understanding of degradation mechanisms in LMR-NMC and layered electrodes in general.

Cycling studies have revealed that charging above ~4.2 volts (V) followed by discharging below ~3.2V significantly accelerates voltage fade. These voltage limits correspond to the onset of a strong hysteresis, as illustrated in Figure 1 (top), showing that a portion of the lithium is withdrawn from the cathode at a higher voltage (~4.3V) than it is inserted back into the cathode (~3.3V). X-ray absorption spectroscopy has shown that the local structure and oxidation state of transition metals (TM), or the nickel, cobalt, and manganese in the cathode, is different on charge and discharge, even at equivalent states of charge over the hysteresis window. The above observations imply that lithium does not have access to the same sites on charge versus discharge and that a structural mechanism is at play. A model (Figure 1 bottom) that explains these data involves migration of cations to tetrahedral sites in the lithium layers during charge, which in turn block insertion of lithium into the surrounding octahedral sites on discharge. Once a sufficient driving force is established on discharge (~3.2 V), lithium may be reinserted into the "blocked" sites by driving tetrahedral cations back to their original sites, resulting in an energy penalty in the form of a hysteresis. Alternatively, cations may be driven into octahedral sites of the lithium layers thereby changing the local structure and potential for lithium insertion/extraction resulting in voltage fade. The hysteresis mechanism is only partly reversible and thus decays with cycling as the voltage fade grows.

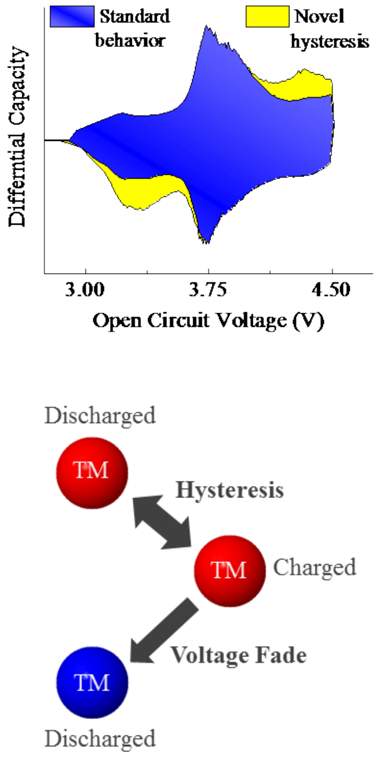


Figure 1. (Top) Hysteresis overlaid on standard behavior. (Bottom) Proposed mechanism of hysteresis and voltage fade.

2013 U.S. DRIVE Highlight

Effect of Coatings on the Voltage Fade Challenge in Layered/Layered Cathodes for High-energy Batteries

Team of researchers has evaluated the impact of cathode particle coatings on voltage fade in high-energy layered/layered cathode materials and found that coatings had no significant effect on this issue.

Argonne National Laboratory

Layered cathode materials in the lithium (Li)-manganese (Mn)-rich portion of the Li-nickel (Ni)-Mn-cobalt (Co)-oxide phase diagram are the focus of much development work because they display a reversible capacity of more than 230 mAh/g (>50% higher than commercial cathodes) and consist mostly of Mn, a relatively inexpensive metal. The Li-Mn-rich, Li-Ni-Mn-Co oxides (LMR-NMC) are structurally integrated composites of Li_2MnO_3 and $Li(Ni,Mn,Co)O_2$.

When cells containing LMR-NMC materials are cycled, however, their impedance rises, and the shape of the voltage vs. capacity curve changes, as shown in Figure 1. In the literature, the continuous change in the shape of the discharge and charge curves has been attributed to the formation of a spinel-like phase. As a result of the loss in potential, there is a loss in energy, limiting the utility of these materials in energy-demanding applications.

Coatings, surface modifications, and additives of many descriptions have been used to stabilize the capacity of cathode materials and enhance cycling ability, enhance rate capacity, lessen their thermal reactivity, lessen their reactivity towards the organic electrolytes, and promote secondary electrolyte interface layer formation on the cathode.

Thus, three national laboratories, Argonne National Laboratory, the National Renewable Energy Laboratory, and Oak Ridge National Laboratory, are collaborating to devise methods to arrest this voltage fade. This project investigated the effects on voltage fade of cathode coatings like aluminum oxide, lithium aluminate, zirconium dioxide, titanium dioxide, aluminum phosphorus quadoxide, and lithium phosphorus oxynitride, and electrolyte additives such as 3-hexylthiophene and lithium bis(oxalato)borate.

The results from the present work indicate that using interface-modifying materials or electrolyte additives had little-to-no effect on voltage fade. Under the cycling conditions used in these experiments, voltage fade appears to derive from an intrinsic property of the LMR-NMC material itself, such as thermodynamic instability, and proceeds at a rate of a few millivolts per cycle. Adjusting the cycling window (e.g., to a lower Vmax and a higher Vmin) was found to be one practical approach to reducing voltage fade, although it also reduces the usable energy available from the cell.

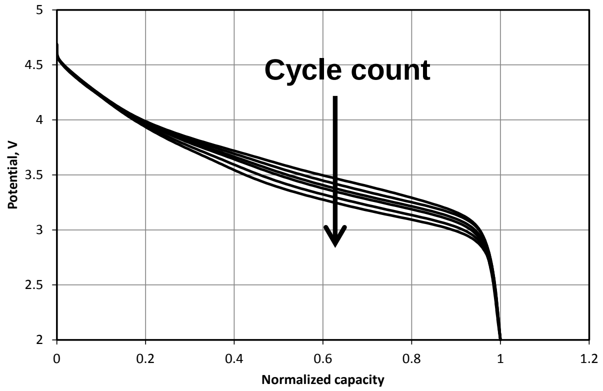


Figure 1. Cell potential vs. normalized capacity for a lithium-ion cathode containing a typical LMR-NMC material in a half cell, showing changes in voltage response with cycling at 30°C.

2013 U.S. DRIVE Highlight

Process Development and Scale-up of Advanced Cathode Materials for High-energy Batteries

Scale-up process development is a key link between basic research and commercialization and provides kilogram quantities of advanced cathode materials for R&D use and industrial evaluation and advances understanding of true mass-market commercialization potential and challenges.

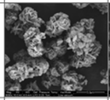
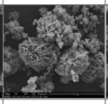
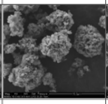
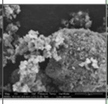
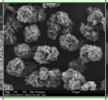
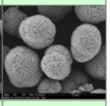
Argonne National Laboratory

Process development and scale-up of advanced cathode materials is a critical step between discovery of advanced battery materials, market evaluation, and high-volume manufacturing. This project produces larger quantities of lab-scale candidate materials with equal or better quality. The performance of cathode material, such as capacity, tap density, and life, etc., can be strongly affected by the synthesis process, even with identical material compositions. Additionally, development of cathode synthesis processes that are economically feasible is important to minimize the cost of the full battery.

A high capacity/voltage cathode development project at the National Aeronautics and Space Administration/Jet Propulsion Laboratory (JPL) had produced a cathode ($Li_{1.5}Ni_{0.16}Mn_{0.68}Co_{0.16}O_{2.5}$) with high capacity (~230 mAh/g) and high tap density (>1.7 g/cc), as shown in Table 1 - column 4, at the bench scale, but JPL had difficulties scaling the material up to kilogram quantities for commercial evaluation. Toda America has produced this composition (HE-5050) at high capacity (~250 mAh/g) but at a much lower tap density (~1.0 g/cc), as shown in Table 1 – column 1-3. In fiscal year 2013, Argonne National Laboratory's (ANL) cathode scale-up program was tasked to produce high capacity, high tap density material for evaluation. The target properties were:

- Composition: $Li_{1.5}Ni_{0.16}Mn_{0.68}Co_{0.16}O_{2.5}$
- Tap density: >1.5 g/cc
- Capacity: ~240 mAh/g (1st discharge)
- Cycle life: ~200 cycles

The first approach was to optimize a hydroxide-based process to synthesize the material. A higher tap density than the Toda hydroxide-based material was achieved but with the tradeoff of lower capacity—not meeting the JPL specifications. Efforts focused on a carbonate-based approach that exceeded capacity and tap density specifications, producing kilogram quantities of material for evaluation. The precursor and cathode materials were produced by a reproducible, scalable process (with performance as shown in Figure 1) and were delivered to ANL's Materials Screening team and JPL for evaluation.

	Toda-HE5050 B#1 5-P767	Toda-HE5050 B#2 P1407	Toda-HE5050 B#3 P2564	JPL pristine	ANL scale-up JPL hydroxide ES-20131004	ANL scale-up JPL carbonate ES-20130924
	Commercial	Commercial	Commercial	Bench scale	Pre-pilot	Pre-pilot
①						
②	3.1/5.3/9.2	1.1/5.2/11.3	2.0/4.9/10.4	1.2/11.1/29.3	3.0/5.1/9.0	4.0/6.7/11.4
③	1.03	1.16	1.07	1.70	1.23	1.82
④	255.3	261.8	254.5	228.2	237.7 *	292.0 *

** Under optimization*

Table 1. Comparison of 6 cathode materials with same composition: ① SEM (8000x), ② D10/D50/D90 (μm), ③ tap density (g/cc), ④ initial discharge capacity at C/20 (mAh/g).

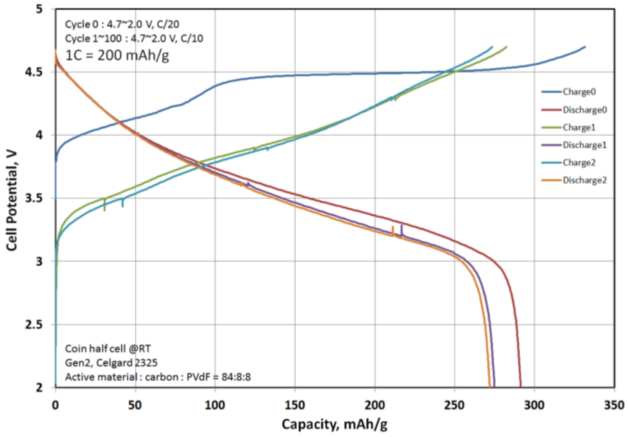


Figure 1. Voltage profile of ANL scaled-up JPL carbonate material.

2013 U.S. DRIVE Highlight

Lowering the Cost and Improving the Performance of Separators for Lithium-ion Batteries

Development and installation of advanced manufacturing processes and research into new material formulations have resulted in improved separator quality and lower cost.

ENTEK Membranes LLC

In 2009, the American Recovery and Reinvestment Act (ARRA) provided $1.5 billion in funding to support the establishment of lithium (Li)-ion battery manufacturing facilities in the United States. One goal of this investment was to reduce the battery cost for plug-in electric vehicles (PEVs). It was recognized that an important step for the electrification of the nation's light-duty transportation sector is the development of more cost-effective, long lasting, and abuse-tolerant PEV batteries.

The separator is a critical battery component that impacts both performance and safety. The thin (≤25 microns), microporous membrane provides an electrically non-conductive barrier between the positive and negative electrodes and a network of pores that can be filled with electrolyte to allow ionic flow between the electrodes. In addition to preventing contact between the electrodes, the separator enhances safety by collapsing its pores and shutting down ion flow when the battery temperature rises to a hazardous level.

The cost of the separator membrane has been a significant portion of a Li-ion battery's material cost. Depending on the battery design, the separator may be 25% or more of the materials cost of a cell. Thus, a reduction in separator cost is necessary to help meet the U.S. DRIVE battery research target of $125/kWh by 2020.

ENTEK's separator is made by what is known as a wet process, where a polymer film containing a plasticizer is extruded with transverse and machine direction stretching followed by extraction to remove the plasticizer and then drying to create the needed porosity. With the assistance of ARRA funding, ENTEK has made improvements to one of its existing production lines and constructed an entirely new line with advanced process capabilities and higher throughput (see Figure 1). The ENTEK production facility has state-of-the-art online characterization equipment and a clean room for slitting master rolls. These improvements have contributed greatly toward meeting U.S. DRIVE's aggressive cost targets of less than $1/m² for high volume purchases.

ENTEK has also received funding through the United States Advanced Battery Consortium for developing an inorganic-filled separator. The material produced from this work has a new formulation that has demonstrated improved high voltage stability, improved power capability, and improved thermal stability compared to standard microporous polyethylene separators. The higher power capability can contribute to lower battery costs by reducing the size of batteries needed to meet low temperature performance requirements.

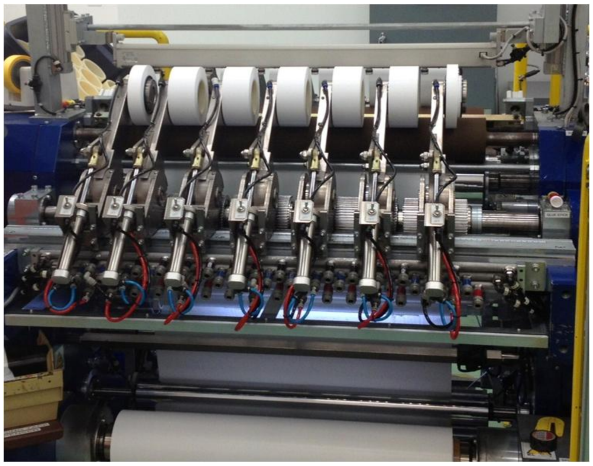


Figure 1. Nishimura slitter installed in ENTEK's new separator production facility as a result of ARRA funding.

2013 U.S. DRIVE Highlight

Silicon Anodes in High-energy Vehicle Batteries

Effective progress has been made by several Batteries for Advanced Transportation Technologies Program investigators in addressing issues with various silicon anode technologies.

Lawrence Berkley National Laboratory

High-energy anodes hold one of the keys to next-generation high-energy vehicle batteries. Graphite, the current active anode material, has a theoretical capacity of 372 mAh/g. Comparatively, silicon (Si) offers a high theoretical capacity of 4,200 mAh/g and is abundant and inexpensive. Further, Si has possible abuse tolerance benefits compared to graphite, as its voltage plateau is slightly higher, potentially reducing risks of lithium plating under abuse. However, numerous technical hurdles remain for Si anodes. Many challenges are associated with the expansion and contraction of Si upon lithium insertion and de-insertion. Particle disintegration can thus occur upon cycling, leading to loss of contact between particles, electrode delamination from the current collector, and electrolyte consumption, all leading to rapid capacity fade and cell failure.

Several institutions (University of Pittsburgh, Binghamton University, The Pennsylvania State University, Stanford University, Pacific Northwest National Laboratory (PNNL), and National Renewable Energy Laboratory (NREL)) are exploring various approaches to mitigating silicon's volume expansion/contraction problem, including use of Si nanoparticles or nanotubes, mixing Si with graphene or carbon nanotubes to absorb volume fluctuations, and using porous secondary particles in which the large amount of pore volume can absorb the volume changes. Key progress metrics are listed in Table 1. Note that each of these approaches has had success in cycling lithium in and out of the Si anode while maintaining the integrity of the Si particles. The progress achieved here in addressing the Si disintegration issue has resulted in the program moving on to some of the remaining issues impeding Si anode use.

Laboratory management has formed five Focus Groups whose objective is to tackle the basic underlying questions that need to be addressed. They are:

1. What is the mechanism of the first cycle loss and what are the specific contributing mechanisms (led by University of California-San Diego).
2. What cycling efficiency is needed in a full cell to insure commercial viability (led by LBNL).
3. What is the role of electrolyte additives in Si anodes and what is their impact on solid electrolyte interface formation and cycling efficiency (led by University of Rhode Island).
4. What is the mechanism of action of coatings on particles and electrodes (led by NREL).
5. What technical barriers need to be addressed to develop electrodes with commercially viable loadings, between 3 and 4 mAh/cm2 (led by LBNL).

Institution	Technical Approach	Loading mg/cm2	Specific Capacity mAh/g	Initial Areal Capacity mAh/cm2	Final Areal Capacity mAh/cm2	Number of Cycles
U. of Pittsburgh	Hollow Si nanotubes	0.8	775	0.62	0.56	150
SUNY Binghampton	Spherical nano Si	2.5	1500	3.7	3	60
Penn. State U.	Si-C nanocomposites	1.7	975	1.6	1.45	160
PNNL	Porous silicon	2.0	750	1.5	1.2	300
Stanford	Conducting hydrogel on Si nanoparticles	0.4	1900	0.75	0.70	1,000
NREL	Si nanoparticles/coating	0.8	1500	1.2	0.9	150

Table 1. Program progress in cycling high energy silicon anodes.

2013 U.S. DRIVE Highlight

Electrolytes Based on Imide Salt Solutions in Fluorinated Solvents with Improved Abuse Tolerance

Electrolytes that are up to 85% by weight non-flammable components were developed. NFi ™ electrolytes demonstrate improved abuse tolerance, long cycle life, good rate, and low temperature performance.

Leyden Energy, Inc.

Regular lithium (Li)-ion cells use electrolytes based on solutions of Li hexafluorophosphate ($LiPF_6$) in organic solvents, which may be ignited under abuse conditions. Previous attempts to formulate non-flammable electrolytes included ionic liquid formulations or the addition of a flame retardant to regular solvents. Neither approach resulted in one formulation with both improved abuse tolerance and fast Li transport that allows quick charge and discharge over a wide temperature range.

Leyden Energy's approach was to use Li imide salt solutions in non-flammable solvents. Imide salts have significantly higher solubility in fluorinated solvents compared to regular salts such as $LiPF_6$, Li tetraflurorborate ($LiBF_4$) and Li bis(oxalato)-borate (LiBOB). This approach allowed Leyden to formulate electrolytes with up to 85% non-flammable components by weight. Small amounts of carbonates are preserved in the electrolyte for efficient solid electrolyte interface formation; limited amounts of esters or linear carbonates assist rate and low temperature performance.

Electrolytes were extensively tested in 18650 and pouch cells (Figure 1) and demonstrated long cycle life at up to 60°C, discharge capability at as low as -30°C, rate up to 5°C and improved abuse tolerance. Electrolytes did not ignite when the cells vented; cell improvements were seen in overcharge, hot box, nail and impact tests.

Leyden's findings and results of the development were independently verified by Mobile Power Solutions' test lab and Exponent failure analysis. In addition to UN and Underwriters Laboratories (UL) testing, tests included cone calorimetry measurement, when a fully charged battery is burned and the amount of heat generated by this process is recorded, as shown in Figure 2. Remarkably, total heat release is about half of the heat released by the same cell with a regular electrolyte such as 1M $LiPF_6$ /Ethylene Carbonate:Di-ethylene Carbonate 1:2.

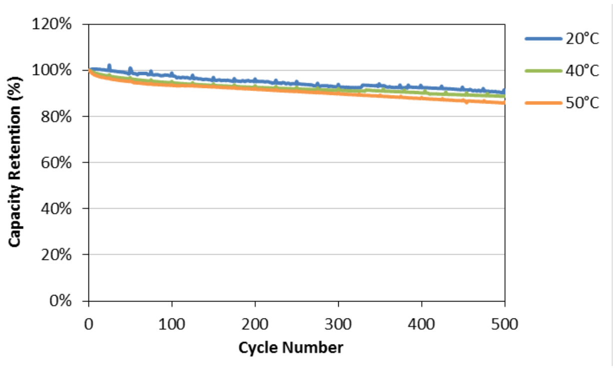


Figure 1. Cycle life of 2.0Ah NCM pouch cell with NFi™ electrolyte.

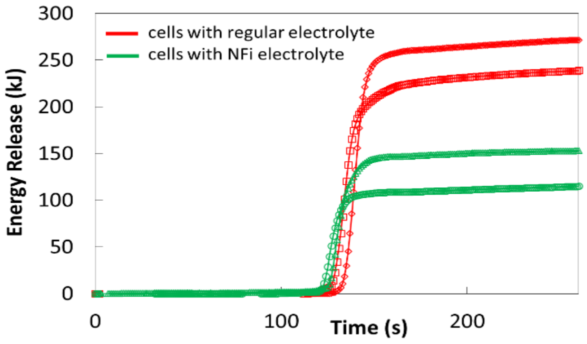


Figure 2. Heat release measured by cone calorimetry in 2.0 amp hour nickel manganese cobalt oxide cells.

2013 U.S. DRIVE Highlight

Reducing Electrode Coating Process Costs Using Light Cured Binders

A new process for manufacturing lithium-ion battery electrodes may significantly reduce electrode coating process costs. Ultraviolet binder cures in less than a second, thus offering a route to significantly reduced capital and operating costs relative to typical drying oven/solvent recovery.

Miltec UV International

Ultraviolet (UV) and electron beam curable binders and the associated curing technology have enabled the production of durable 75 micrometer thick electrode coatings at curing speeds up to 200 feet per minute. This technology has the potential to dramatically increase process speeds and significantly reduce capital costs, operating costs, energy requirements, and environmental emissions from electrode coating by virtually eliminating volatile organic compounds.

During fiscal year 2013, Miltec UV researchers formulated UV curable binders (patents pending) and used them to successfully make lithium-ion battery anode and cathode coatings. Electrode coatings have been made that retained physical integrity after immersion in pure electrolyte at elevated temperatures for extended periods.

Coin cells using UV curable binder anodes and cathodes have been made and tested. The long term room temperature cycling results of full coin cells made with a purely UV cured binder cathode and conventional anode are shown in Figure 1. These efforts culminated in the delivery of eighteen 500-mAh pouch cells for independent laboratory testing made with UV cured binder cathodes and anodes with the goal of having cycle performance equal to or greater than conventional cells.

A slot die coater and reel to reel conveyor have been installed on a Miltec UV multiple lamp UV curing system, shown in Figure 2. The system is capable of accommodating a 10” current collector foil and an 8” coating width.

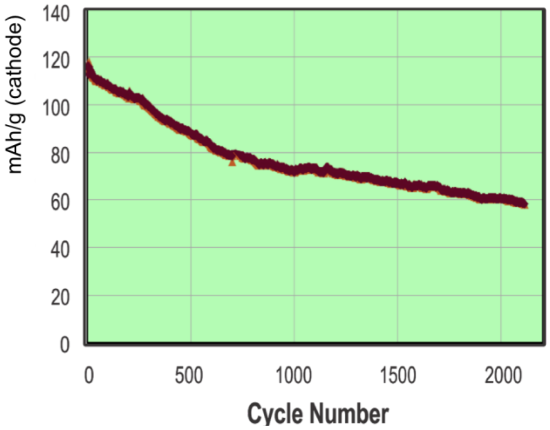


Figure 1. Durable UV binder lasts over 2,000 cycles in nickel manganese cobalt oxide cathode in full cell 100% DOD cycle life testing.

Figure 2. 10” wide slot die press with UV curing shrinks the length of electrode coating operation to 4.2 meters. This eliminates coating ovens and solvent recovery from electrode coating processes.

2013 U.S. DRIVE Highlight

Innovative Cell Materials and Designs for High-energy Electric Vehicle Batteries

Innovative silicon-graphite composite anode powders provide high energy density in lithium-ion cells while demonstrating significant cycle life capability.

Nanosys, Inc.

Interest in plug-in electric vehicles (PEVs) is on the rise. Many industry analysts believe that batteries based on lithium (Li)-ion technologies are the optimal solution for PEVs. Nanosys has developed a novel silicon (Si) composite anode (SiNANOde™) and composite cathode that demonstrate a significant potential advance from the current state-of-the-art in Li-ion technologies.

The specific capacity of SiNANOde can be controlled in a range of 500 to 1,800 mAh/g (compared to 300 mAh/g for currently used graphite) by tuning the amount of Si nanowires grown on graphite powders as needed. By optimizing Si nanowire coverage and distribution on the graphite surface, as well as by optimizing electrolyte and binder chemistry, cycle life has been greatly improved. Cycle life of more than 1,000 cycles with 80% capacity retention were demonstrated for full cells with an electrode loading of 9.6mAh/cm^2 (double sided) (Figure 1 Top), which is in line with today's consumer cells and with electric vehicle battery cycle life requirements. Almost 100% utilization of Si capacity has been realized even in the high capacity cells. Initial coulombic efficiency (ICE) has been improved up to 92% for all the SiNANOde products (Figure 1 Bottom). SiNANOde can match various cathode chemistries, such as lithium cobalt oxide (LCO), nickel aluminum oxide, and nickel cobalt manganese oxide.

Pouch cells have achieved 250 Wh/kg using 550 mAh/g baseline SiNANOde and LCO baseline cathode. Finally, we have demonstrated the feasibility of using SiNANOde and high-energy cathode materials (>255 mAh/g) to make full cells providing 300~400 Wh/kg. The pouch cells exhibit a thickness increase of <14% over 500 cycles, which is critical for module and pack stability (smaller thickness increase results in less pressure build up in a module or pack) and is a marked improvement over many other Si anode full cell cycling results.

SiNANOde development on different graphite substrates has been extensively explored, which will be used to identify the most cost-effective production route.

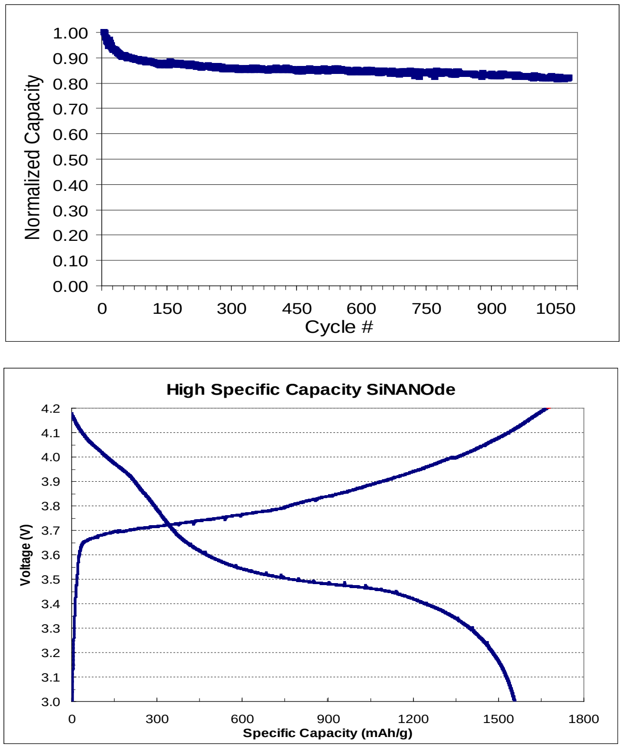


Figure 1. (Top) SiNANOde full cell with >1,000 cycles at 80% capacity retention. (Bottom) High specific capacity SiNANOde with >1600 mAh/g and ICE of >92%.

2013 U.S. DRIVE Highlight

Isothermal Battery Calorimeters: Crucial Tools for Advancing Electric Drive Vehicles

R&D 100 Award-winning instruments provide precise thermal measurements needed for longer-lasting and more cost-effective electric drive vehicle batteries.

National Renewable Energy Laboratory

Advanced energy storage devices, such as lithium-based batteries, are very sensitive to operating temperature. High temperatures degrade batteries faster and increase potential safety concerns, while low temperatures decrease power and capacity. The isothermal battery calorimeters (IBCs) developed by the National Renewable Energy Laboratory (NREL) are the only calorimeters in the world capable of performing the precise thermal measurements at the sample scale needed for longer-lasting and more cost-effective batteries for the next generation of electric drive vehicles (EDVs).

Recently recognized with an R&D 100 Award, the IBCs are the most accurate devices of their kind—able to determine heat levels and battery energy efficiency with 98% accuracy. The IBCs make it possible to precisely measure the heat generated by EDV batteries, analyze the effects of temperature on battery systems, and pinpoint potential thermal management paths for improved performance and life. See Figure 1.

Capable of testing a wide size range of samples, the calorimeters can determine the heat generated by battery cells, modules, sub-packs, and even some full-size packs. The IBCs also evaluate system heat generation, from the individual cells within a module, the inter-connects between the cells, or the entire battery system.

The cell/module version of the IBC has the capacity to test more than 95% of EDV energy storage cells and many small modules. The IBCs can also be used to test a variety of cell formats (i.e., pouch, cylindrical, and prismatic), as shown in Figure 2.

The incredible precision of the IBCs can be attributed to patent-pending features that deliver advanced thermal isolation and highly sensitive temperature readings across a wide range of conditions. NREL has licensed the IBC technology to NETZSCH Instrument North America LLC, a leading provider of thermal analysis instruments, for commercial production and distribution.

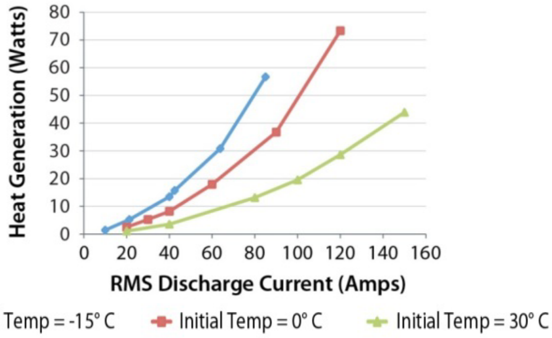


Figure 1. Efficiency curves for a plug-in hybrid electric vehicle battery at various discharge currents and temperatures. This critical information helps in battery thermal management design by identifying conditions resulting in temperature spikes.

Figure 2. The Netzsch IBC-284 has the capacity to test more than 95% of EDV energy storage cells and many small modules. *Photo: Jean-Francois Mauger/Netzsch*

2013 U.S. DRIVE Highlight

Water-based Lithium-ion Battery Electrode Manufacturing

Water-based electrode processing promises to reduce the cost of lithium-ion batteries while increasing the associated manufacturing sustainability.

Oak Ridge National Laboratory

The U.S. DRIVE research target for electric vehicle batteries is $125/kWh by 2020. Meeting this goal requires substantial progress in cost reduction of both materials and associated processing, which comprise over 80% of the total costs of lithium (Li)-ion electric vehicle batteries. Today's electrodes are manufactured using fluorinated polymers and N-methyl-2-pyrrolidone (NMP) as the binder and solvent, respectively. NMP is expensive, flammable, of environmental concern, and requires the use of costly solvent recovery processes. Oak Ridge National Laboratory (ORNL) is investigating aqueous processing techniques for Li-ion battery electrode manufacturing, in which NMP (>$2.25/L) solvent is replaced with deionized water ($0.015/L). The raw materials and associated processing complexity are significantly reduced and the need for recovery and treatment of NMP is eliminated.

Aqueous processing for the graphite anode is mature and has been commercialized by many battery manufacturers, which speaks to the cost and environmental effectiveness of the approach. However, aqueous processing remains challenging for the diverse array of cathodes. ORNL is approaching the challenge by understanding the colloidal chemistry of each cathode component for effective dispersion, screening water soluble binders for superior adhesion and electrode integrity, optimizing mixing protocols for uniform suspensions, improving surface energy of the aluminum current collector for better wettability of cathode dispersions, developing drying procedures for effective moisture removal, and quantifying the effect of residual moisture on battery performance. An example of this work is shown in Figure 1, where rate performance of $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ (NMC 532) cathodes with various water soluble binders from aqueous processing is compared to that with the conventional PVDF binder from NMP-based processing. The NMC 532 cathodes from aqueous processing demonstrate superior rate performance, which indicates that switching the manufacturing from conventional NMP-based processing to aqueous processing not only may reduce process complexity, but may also deliver comparable or improved power capability. Future work will be devoted to demonstrating comparable calendar and cycle life of these electrodes.

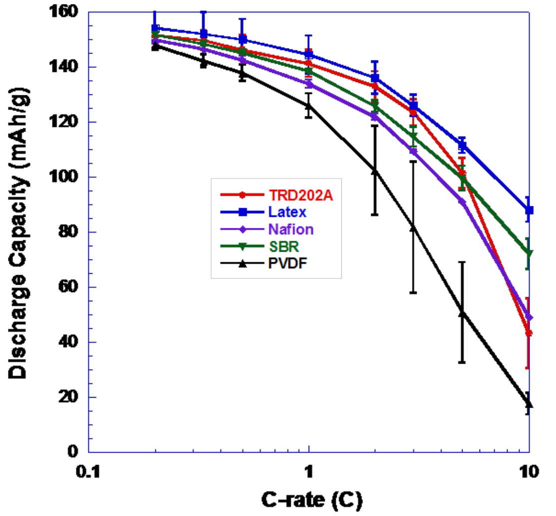


Figure 1. Comparison of rate performance of NMC 532 cathodes using aqueous and NMP-based processing. More information: U.S. Patent pending US 2013/0108776 A1, pub. May 2, 2013.

2013 U.S. DRIVE Highlight

Electrolyte Additives Enabling High-voltage Cathodes

Researchers have identified dominant failure mechanisms in cells with the high voltage spinel cathodes and demonstrated additives that mitigate associated capacity fade.

University of Rhode Island

One of the promising cathode materials for use in plug-in electric vehicles is the high voltage lithium (Li)/nickel (Ni)/manganese (Mn) spinel, $LiNi_{0.5}Mn_{1.5}O_4$, or LNMO. This 5-volt (V) cathode material offers a significant improvement in energy over existing 4V cathodes, and, due to its mechanical stability at high voltage, provides a good test material to evaluate high voltage electrolytes and additives.

Novel additives have been prepared that improve the performance of graphite/LNMO cells cycled to 4.8 V with a standard electrolyte of $LiPF_6$ in ethylene carbonate/ethyl methyl carbonate at elevated temperature. Figure 1 shows the cycling performance of the graphite/LNMO cells with baseline electrolyte and electrolyte containing the additive lithium bis(oxalato)borate (LiBoB) at room temperature (RT), elevated temperature (ET, 55°C), and RT, again. The initial discharge capacity of the cells with 1.5% and 2.5% additive are slightly lower than the cells with baseline electrolyte. This difference is ascribed to the irreversible decomposition of the LiBoB on the electrode surface. However, after 30 cycles at 55°C, the cell with baseline electrolyte suffers significant capacity loss, only delivering 24% of the original capacity. The cells with 1.5% and 2.5% LiBoB showed improved cycling stability at 55°C: 63% and 69% capacity retention, respectively. After cycling at 55°C the cells were cycled at RT. The cell with baseline electrolyte had continued capacity fade, while the cells with LiBoB additive exhibited better stability.

Ex situ surface analysis of both the anode and the cathode extracted from the cells was conducted via a combination of spectroscopy and microscopy (XPS, SEM, TEM with EDX, and ICP-MS) to better understand the role of the LiBoB in capacity retention. Incorporating the additive results in the generation of a thin cathode surface film that inhibits both the deposition of poly(ethylene carbonate) and the dissolution of Mn and Ni at the cathode surface during cycling at 55°C. The additive also inhibits damage to the anode surface with less Mn and Ni deposition on the anode surface and less damage to the anode solid electrolyte interphase.

The improved cycling performance is attributed to the inhibition of electrolyte decomposition at the electrode surfaces and inhibition of Mn and Ni dissolution from the cathode and deposition on the anode. The additives will next be used in cells with other high energy, high voltage cathodes to test whether they improve cycling stability as well.

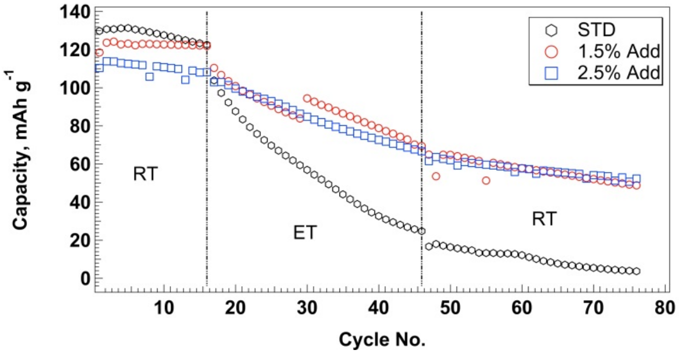


Figure 1. Cycling performance of graphite/$LiNi_{0.5}Mn_{1.5}O_4$ cells with standard and 1.5% & 2.5% LiBoB-containing electrolyte at room temperature(RT), 55°C(ET), and again at room temperature.

2013 U.S. DRIVE Highlight

Advanced Lithium-ion 12V Start-Stop Automotive Battery Meets Performance Requirements

Purpose designed lithium-ion battery for the 12 volt start-stop automotive application shows promising progress toward replacing antiquated lead-acid batteries.

Leyden Energy and U.S. Advanced Battery Consortium

Start-stop technology can provide significant fuel savings using lower cost batteries than those used in standard hybrid cars. The principle behind start-stop systems is simple: in traffic when a car comes to a complete stop, the engine shuts off and the battery powers all of the electrical components. When traffic moves again, the driver releases the brake and the battery seamlessly restarts the car. The start-stop battery is a low-cost solution achieving significant fuel savings because it only powers electrical functions and vehicle starting.

The challenge for today's standard lead acid battery is weight, life, and poor repetitive operation. In contrast, a lithium (Li)-ion based system would enable a smaller, lighter, longer life battery with superior operating characteristics. But it must demonstrate the ability to start a vehicle at very low temperatures, withstand high vehicle exposure temperatures, and be affordable. The challenge is that although Li-ion technology is the standard in today's consumer electronic devices, that specific class of battery is not the right design for the low temperature operation or fast charge required by start-stop systems.

Leyden Energy (Leyden) has developed a new Li-ion technology that is purpose-designed for start-stop applications. During its U.S. Department of Energy-sponsored U.S. Advanced Battery Consortium (USABC) program, Leyden became the first company to demonstrate the ability to repeatedly start a vehicle using Li-ion technology at the temperature of -30°C, as shown in Figure 1. This milestone was achieved through the use of Leyden's Li-Imide™ system together with proprietary electrolyte formulation and cell design. Together with surface-treated lithium titanium oxide for the anode in place of the graphite used in consumer Li-ion, cells achieved the high power required for multiple, cold temperature engine starts per day, an attribute regular Li-ion cells are incapable of achieving.

Leyden also showed progress in addressing long cycle life and calendar life targets, as of today achieving >500k shallow cycles at 30°C and >200k shallow cycles at 50°C. Leyden is planning to further expand the applicability of its start-stop battery technology for both in-cabin and under hood applications in future USABC programs, which will build on the work accomplished through its current program.

With its progress in addressing both low temperature performance and long term life targets, Leyden has positioned Li-ion technology as a possible enabler for the widespread adoption of future high performance start-stop systems, which in turn will contribute to achieving national fuel-saving and emission-reduction goals.

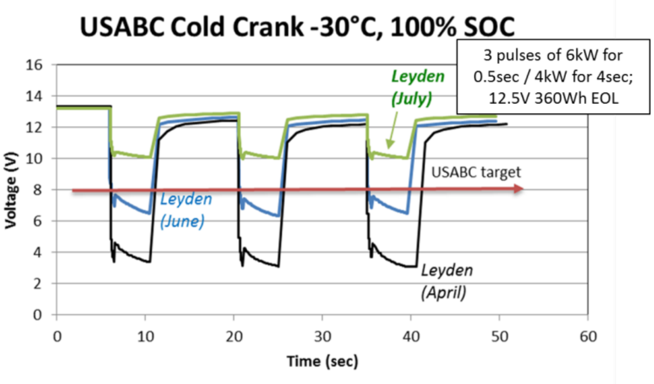


Figure 1. Development improvements in the ability to provide 3 consecutive vehicle starts at -30^{0}C.

Maxwell Delivers System Six Times Smaller than Predecessor

The new capacitor pack is six times smaller and five times lighter than existing ultra-capacitor packs with the same energy, an important step toward integrating them into vehicles or other products.

Maxwell Technologies Inc. and U.S. Advanced Battery Consortium

The research and development (R&D) team at Maxwell Technologies has built a capacitive energy storage system that holds over six times as much energy per liter and five times more energy per kilogram than current capacitor products while retaining the same high power capacity per volume and mass. This is the end result of a disciplined R&D effort in materials and pack design leveraging the wide knowledge of U.S. Advanced Battery Consortium (USABC) members. Dozens of alternative material and design permutations were evaluated for the new asymmetric ultracapacitor cells. The development demonstrated substantial performance and lifecycle improvements.

Overall, the project has delivered significant advancements over its course. Between the current capacitor product and the fourth generation now in R&D, the mass of the system decreased by 18kg and the volume diminished by 33L, as shown in Figure 1. At the same time, through a combination of continuously improved design, careful material selection and work with key suppliers, system cost has dropped more than $220, and by 15% this year alone.

Among the contributing features of the new system are cells built using Maxwell's proprietary low cost dry-electrode manufacturing process. This method significantly reduces the number of manufacturing steps and eliminates all solvents typically used in the typical commercial wet coating of electrodes.

Recent progress in electrode manufacturing techniques allowed the team to reduce electrode thickness by 20%, significantly improving the usage of the active material and decreasing the number of cells that will be required to meet USABC power and energy goals. Further, ongoing improvements indicate the future product will be close to meeting the USABC goals for mass and volume in low energy electrochemical storage systems.

This year Maxwell modeled and validated manufacturing techniques and processes, a crucial step toward commercial viability. While the pack does not yet meet all USABC goals simultaneously, the developers are actively studying early markets for the system and what has been learned here will contribute to Maxwell's ongoing development of automotive products.

Figure 1. The new asymmetric ultracapacitor pack, on the right, contains almost three times the energy yet it is less than half as large as the current product, shown on the left for comparison.

Advanced Monoblock Battery for 12-Volt Start/Stop Vehicles

Dramatically different approach to the way lithium-ion cells are fabricated and assembled into a system is being developed for a significant reduction in the cost of automotive 12 volt start/stop batteries.

Saft America and U.S. Advanced Battery Consortium

Cost is the most challenging requirement and is generally acknowledged as the critical path to widespread deployment of the lithium (Li)-ion battery in the automotive industry. About 20% of the cost of a robust cell design in volume-production today is in the cell hardware. Cell hardware means anything other than electrodes, including the foils, separator, and electrolyte. Another 50% cost burden is added as cells are integrated into a turnkey battery pack. Thus, the hardware in a Li-ion battery pack is responsible for a combined 70% of the cost before indirect costs, and it is the most significant part of the total cost.

The common use of a metal housing in the Li-ion battery industry today is mostly due to the fact that metals are easy to form and they possess good structural strength and thermal conductivity. These advantages come at a price, in the form of weight, volume, and added cost. Injection-molded thermoplastic polymers (IMTP) offer an exciting alternative to dramatically reduce the total system assembly and hardware costs.

A key innovation in this project, primarily focused on reducing hardware cost by >50%, is combining the cell and module packaging in a single IMTP monoblock (see Figure 1). Further efforts of this project include optimizing the electrolyte as well as the nickel-manganese-cobalt (NMC) positive conductor chemistry to meet the U.S. Advanced Battery Consortium's (USABC) cold-cranking requirements and reduce cost by >15%. Lithium-titanium-oxide (LTO) is a negative conductor chemistry particularly well suited to this optimization. LTO enables Saft America to use very low cost, low temperature electrolytes for enhanced performance. In order to reduce the electrode material costs, the LTO manufacturing process is being addressed by large volume manufacturers of titanium-dioxide for the paint industry. This could result in extremely low cost LTO, giving a significant cost advantage over traditional graphite-based Li-ion batteries. LTO is also well known for its excellent abuse tolerance.

With the cost reduction advantages offered by LTO chemistry and the monoblock module design in combination with low-cost electronics, the proposed NMC-LTO monoblock battery system is expected to approach USABC cost targets and meet that cost at identified volumes.

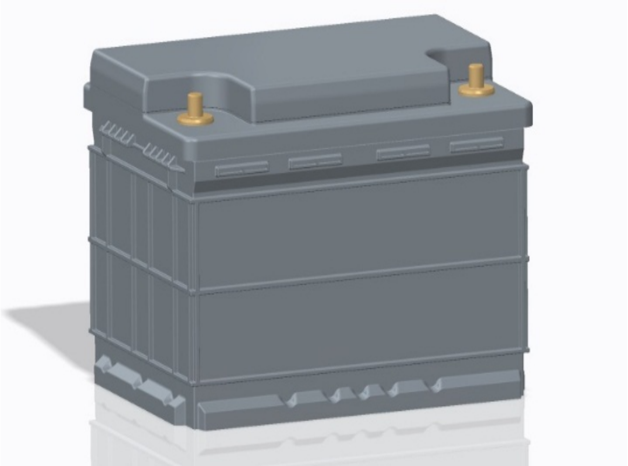


Figure 1. 12-volt Li-ion start/stop monoblock battery concept.

2013 U.S. DRIVE Highlight

High-performance Lithium-ion Battery for Electric Vehicles

High-energy battery cell shows surface-modified cathode can deliver long life at elevated temperatures.

SK Innovation and U.S. Advanced Battery Consortium

As requirements for electric vehicle (EV) batteries become more aggressive in terms of energy density and life for longer driving distance, SK Innovation (SKI) has developed and introduced a lithium manganese oxide (LMO) free high-energy cell for U.S. Advanced Battery Consortium's (USABC) EV technology assessment program.

SKI developed 40Ah cells with no manganese (Mn)-spinel at the positive electrode and named it LMO free cell. LMO free cell can avoid significant Mn-dissolution, which leads to crucial battery deterioration at high temperatures, thus LMO free cell is expected to have improved calendar life. SKI applied pure high nickel content nickel cobalt manganese oxide (NCM) as a positive active material to achieve high energy density and avoid crucial deterioration at high temperature. However, high nickel content NCM is unfavorable to abuse tolerance and cycle life. To obtain structural stability for better abuse tolerance and life, SKI has adapted a surface-coated NCM material for its cells to use in the SKI battery system.

Performance and calendar life testing shows satisfactory energy density of approximately 200Wh/kg at the unit cell. Figure 1 shows 3-hour discharge rate ($C_3/3$) capacity retention, and the results show 91.3% of retention at 800 USABC cycles. Calendar life tests are ongoing at temperatures of 25°C, 35°C, 45°C, and 55°C. Each battery is charged to state of charge (SOC) 100% at the $C_3/3$ rate and allowed to rest in an open circuit condition at the desired temperature for four weeks. After four weeks, the batteries undergo USABC reference performance test at 30°C. Figure 2 shows $C_3/3$ capacity retention at four temperatures after 24 weeks and results show 94.4%, 91.5% 87.4% and 81.0%, respectively.

Based on capacity retention of 80%, cycle life is expected to proceed more than 2,000 cycles and calendar life is regarded to last more than 70 weeks at 45°C and SOC 100% condition—, superior life performance exceeding USABC's life goal. SKI will continue to develop and modify cell design, including electrolyte optimization and adjusting cathode formulation, to further improve calendar and cycle life performance.

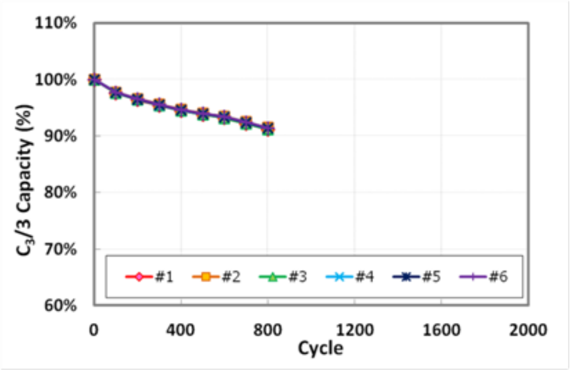


Figure 1. Reliable cycle life performance in LMO free battery.

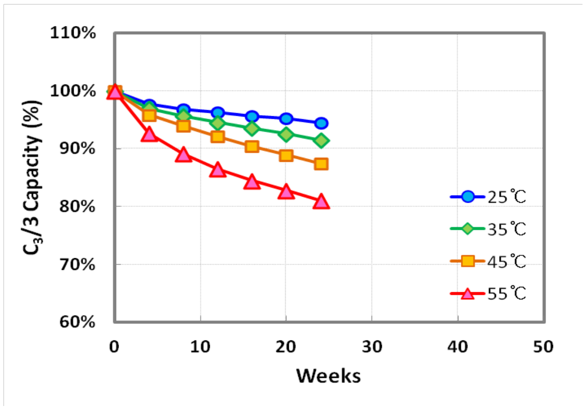


Figure 2. Stable calendar life performance in LMO free battery.

Fuel Cells

2013 U.S. DRIVE Highlight

Lower-cost High-activity Thin Film Electrocatalysts

A method to increase the activity of thin film catalysts 20 times more per surface platinum atom than that of traditional fuel cell cathode electrocatalysts.

Argonne National Laboratory

The platinum (Pt)-based cathode catalyst is one of the main contributors to fuel cell system cost. Finding more active catalysts can lead to reduced Pt content in the fuel cell, reduced cost, and improved commercial viability. Single crystals of a Pt alloy – Pt$_3$Ni – with a particular crystal orientation (111) have the highest known activity per unit surface area, due to a unique nano-segregated concentration profile (see Figure 1). However, bulk single crystals have low specific surface area and mass activity due to the thickness of material needed to obtain the bulk properties. Prior efforts to mimic the high specific activity of the ordered single crystal in structures with higher surface area, such as extended thin films, nanostructured thin film or nanoscale catalysts, have not led to the improvements expected from single crystal work.

Argonne National Laboratory (ANL) has developed a method that transfers the nano-structured surface morphology of individual randomly oriented nanoscale grains into a more single-crystal like mesostructured surface of large, interconnected (111) facets. This mesostructured material (PtNi Meso-TF in Figure 2) approaches the superior catalytic activity of the Pt$_3$Ni (111) single crystal without the low surface area of a single crystal. The specific activity of the mesostructured catalyst is twenty times that of a traditional Pt/carbon (Pt/C) catalyst.

Studies of membrane electrode assemblies (MEAs) have demonstrated that a surface energy treatment that transforms surface morphology of a nanostructured thin film (PtNi NSTF) towards a mesostructured thin film enhanced kinetics by 20 mV in hydrogen air.

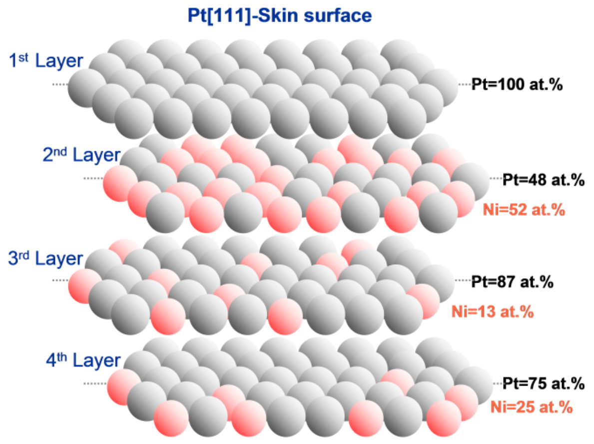


Figure 1. Highly active single crystal Pt$_3$Ni (111) showing nanosegregated structure with Pt segregated at the surface.

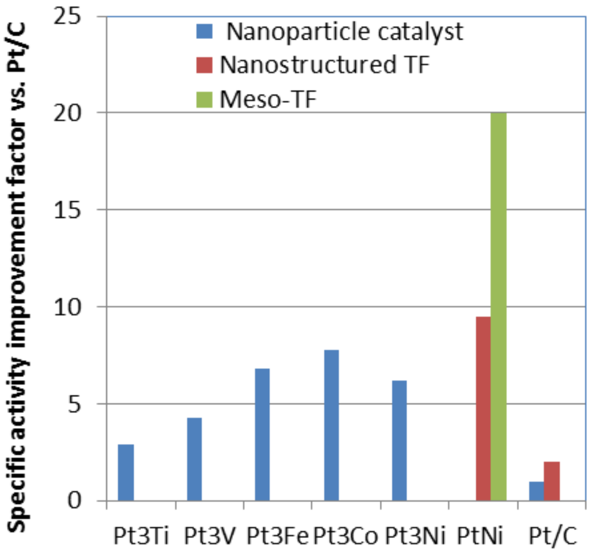


Figure 2. Activity per unit of surface area of ANL's mesostructured thin film PtNi material (PtNi Meso-TF) compared to nanostructured thin film (PtNi NSTF), and nanoparticle catalysts (Pt/C, Pt$_3$Co, Pt$_3$Ni).

2013 U.S. DRIVE Highlight

Roll-processed Durable Supports for Fuel Cell Membranes

Increased durable support porosity from 15% to 50% using a scalable means of production.

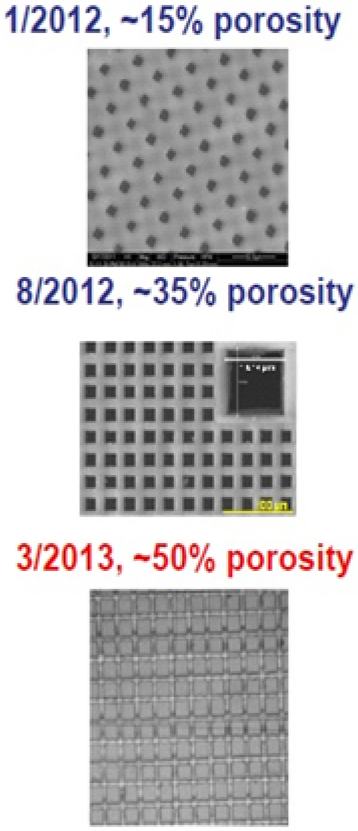
Giner, Inc.

Cost and durability are the two major vehicle-related barriers towards commercialization of automotive fuel cells. One of the known failure modes that can limit fuel cell lifetime is the mechanical failure of the membrane. Membrane failures often occur with cycling between wet and dry states that expand and contract the membrane. The expansion and contraction produce high tensile stresses, especially near flow channel walls, or at the edge of a cell.

To address membrane tensile stresses, manufacturers have added mechanical supports to reinforce the membrane. Supports are usually thin, porous layers filled and surrounded by the proton-conducting material that comprise the bulk of the membrane. Supports need to be strong enough to prevent expansion and contraction of the membrane within the plane of the membrane, but still thin and porous enough to not occupy space that is needed for the conduction of protons from anode to cathode.

Giner has sought to produce membrane mechanical supports through many techniques, one of which is through the mechanical shaping of thermoplastics using molds with microscopic features. The mechanical deformation technique has been considered to be the most promising due to the ease with which it could be adapted to high volume manufacturing. However, difficulty in mold release led to relatively thick supports with low porosity (20 µm and 15%, respectively) as late as early 2012.

Development of a new hot embossing method has enabled Giner to dramatically decrease support thickness while greatly increasing porosity (7 micron and 50%, respectively). Improvement is shown in Figure 1. Future work will focus on scaling up the manufacturing process and demonstrating fuel cell results using the membrane supports.


1/2012, ~15% porosity

8/2012, ~35% porosity

3/2013, ~50% porosity

Figure 1. Using a hot embossing method with polysulfone, Giner has shown quick progress in advancing its supports from 15% porosity to 50% porosity.

2013 U.S. DRIVE Highlight

High-activity De-alloyed Platinum Catalysts

Durable high-activity catalysts show reduced cost by using various de-alloying techniques and mass activity that meets U.S. Department of Energy targets after 30,000 voltage cycles.

General Motors

Cost of the fuel cell system is one of the biggest challenges to the commercialization of fuel cell electric vehicles. A significant portion of a fuel cell system's cost in mass-scale production is the cost of the precious metal catalyst used. De-alloying base metals from a platinum (Pt)–metal alloy provides a way to control the particle structure to optimize for both high activity and durability.

General Motors, in partnership with Johnson Matthey, Technical University of Berlin, and other institutions, has developed methods to de-alloy base metals like nickel (Ni) and cobalt from a Pt alloy precursor to control the structure of the resultant catalyst. The team had synthesized large batches of Pt-copper and Pt-Ni catalysts that met initial activity in oxygen and hydrogen-air performance. However, these initial catalysts were not durable.

The team worked on methods to alter the conditions during the preparation of precursors and acid leaching to slow down the rate of the base metal dissolution. The slower rate of base metal dissolution enables the formation of a uniform Pt shell and better particle size distribution. Figure 1 shows a comparison of microscopic images of catalyst prepared under the new and old preparation techniques. The catalyst prepared using the new methods shows more uniformly sized Pt particles and a smaller mean particle size diameter.

Most institutions synthesize new catalysts in milligram scale batches to test for performance and durability. However, scaling up these catalysts is neither straightforward nor commercially viable. This project was set up to enable a seamless transfer of technology to a catalyst manufacturer. The team made catalysts in 100-gram batches using the most promising techniques for further testing at 50cm^2 levels of both oxygen mass activity and hydrogen-air performance. Figure 2 shows the mass activity of Pt-Ni catalysts prepared using various techniques before and after voltage cycling durability. All catalysts show mass activity higher than 0.44 A/mgPt at the end of voltage cycling durability test; this could enable up to a 40% cost reduction compared to the current state of the art catalysts.

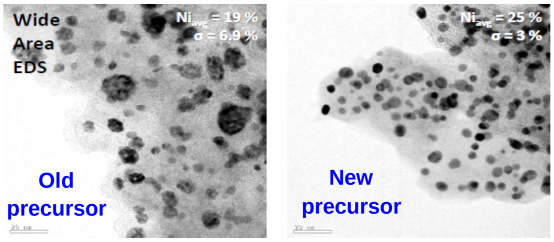


Figure 1. Transmission electron microscope image of de-alloyed Pt-Ni catalyst comparison of old and new method for preparation.

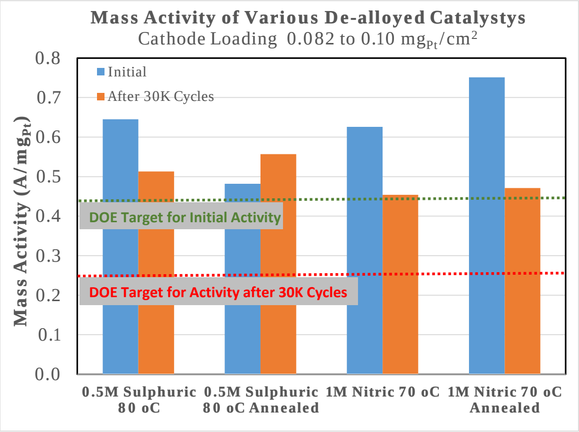


Figure 2. Mass activity measurement of de-alloyed Pt-Ni catalyst for various de-alloying techniques

2013 U.S. DRIVE Highlight

Improved Understanding of Mechanism for Non-precious Metal Fuel Cell Catalysts

Possible replacement of expensive platinum catalysts to reduce overall fuel cell cost.

Northeastern University

A major impediment to commercializing fuel cell systems is cost. Platinum (Pt) catalysts are the most expensive portion of the fuel cell stack, accounting for approximately half of the stack cost. Recent work to replace Pt, which costs over $1,000/ounce, with catalysts based on non-Pt group metals (non-PGM) that cost dollars/ounce or less has shown promise. However, efforts to improve the activity of these non-PGM catalysts have been hampered by our poor understanding of how oxygen (O_2) reacts with these catalysts and what the active catalyst site is.

Using a combination of characterization techniques including X-ray absorption spectroscopy, electrochemical measurements, and modeling, Northeastern University and its collaborators have identified a dual site mechanism for the O_2 reaction on non-PGM catalysts (Figure 1). In acidic media, one site is responsible for the initial adsorption of O_2 and reduction to peroxide (H_2O_2) and a second closely surrounding site is responsible for further reduction of the H_2O_2 to water (H_2O). The first site has been identified as a metal-nitrogen complex (M-N), the second as a metal/metal oxide particle (M/MO_x) (M=Iron (Fe) is one example). By judicious use of reactants that selectively poison the M-N sites or leach the M/MO_x sites, Northeastern University has shown that both sites are necessary for the O_2 reduction reaction in acidic media.

The new insight this work has provided into the dual site mechanism will allow for more directed synthetic approaches to optimize the concentration and distribution of the two sites, which should lead to significant gains in non-PGM catalyst activity. Additional effort in this project has resulted in scale-up of Fe-based catalysts by Pajarito Powder to a more than 30-gram batch, with the goal that the developed methods can be applied towards 100-200 gram batches in the near future, while further demonstrating a technology trajectory to 1,000 gram batches.

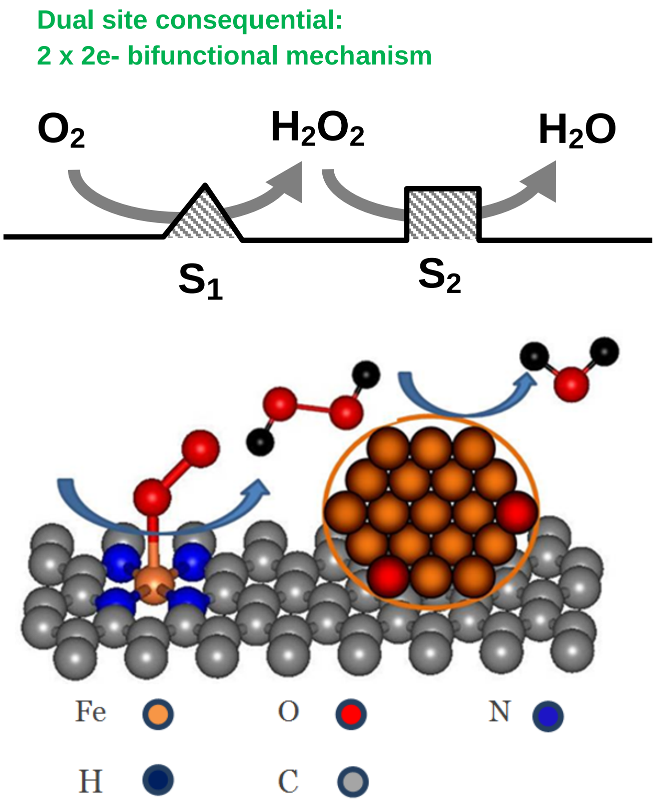


Figure 1. Dual site mechanism showing conversion of O_2 to H_2O_2 on Fe-N site (S1) and subsequent conversion to H_2O on the Fe/FeO_x site (S2).

Enhanced Understanding of Durability and Performance Trade-offs Using Advanced Microscopy

New methods show how different carbons influence platinum catalyst deposition, particularly in the context of graphitization of carbon.

Oak Ridge National Laboratory

The major technical challenges that proton exchange membrane fuel cells (PEMFCs) for automotive applications face are cost and durability. In particular, the platinum (Pt) cathode catalyst significantly affects cost, because it is responsible for the highest fraction of the fuel cell material cost. State-of-the-art cathode catalysts consist of Pt nanoparticles dispersed on a carbon support material. A higher performance catalyst can reduce the total amount of Pt; however, catalysts that demonstrate high performance at beginning-of-life are generally less durable. Fundamental understanding to elucidate materials degradation mechanisms in the fuel cell is imperative to improve performance and durability simultaneously.

Oak Ridge National Laboratory (ORNL) has established analytical methodologies for characterizing PEMFC membrane electrode assembles (MEA) utilizing state-of-the-art high-resolution transmission electron microscopy (TEM) and scanning transmission electron microscopy that incorporate multiple detectors and spectrometers. Recently, ORNL contributed to understanding the mechanism of carbon corrosion, which is a significant cause of performance loss for the cathode catalyst. ORNL also elucidated how carbon support structures are correlated with the initial catalyst dispersion and catalyst performance and stability. The degree of carbon corrosion relies on the graphitization level of the carbon support. High surface area carbon (HSAC) is highly disordered with a defective meso-graphitic outer shell and an amorphous core, which make it highly susceptible to oxidation (Figure 1a). Cathode degradation at high potential holds is due to carbon corrosion and concomitant loss of Pt as a result of Pt encapsulation in the densified cathode, as well as Pt dissolution and subsequent migration into the membrane. On the other hand, low surface area carbon (LSAC) comprises a highly ordered/faceted graphitic shell with a hollow core (Figure 1b). It exhibits significantly greater stability at high voltages and resists carbon corrosion due to higher graphitization of the surface. Electrochemical surface area loss of Pt is dictated by Pt coalescence due to poor initial Pt dispersion. The most critical structural factor affecting MEA performance and durability is defect density (surface area of defects), which shows better correlation with corrosion rate than the physical surface area, of the carbon.

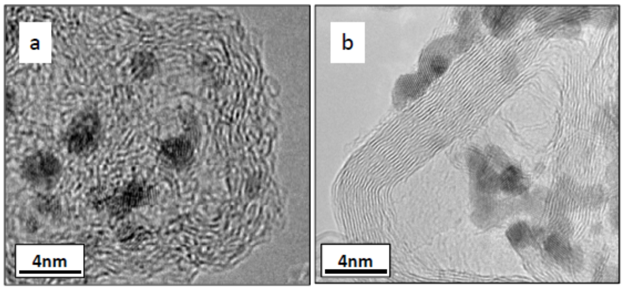


Figure 1. TEM images of cathode catalyst materials, Pt particles dispersed on HSAC (a) and LSAC (b).

2013 U.S. DRIVE Highlight

Low Platinum Carbon Composite Catalyst

Newly developed carbon composite platinum catalysts show high activity at both low and high current densities.

University of South Carolina

The cost of platinum (Pt) used in fuel cell stacks is expected to be a significant hurdle to commercializing fuel cell electric vehicles. High current density performance typically defines the total Pt requirement in a stack. Therefore, these catalysts need to show good performance at high current densities and good mass activity. Pt catalysts made with pyrolyzed carbon composite catalyst (CCC) support provide a pathway to enhance hydrogen (H_2)-air performance.

The University of South Carolina has developed methods to synthesize CCC and activated CCC (A-CCC) supports and deposit Pt uniformly on these to make highly active Pt particles. These particles provide a pathway to obtain both high mass activity and good H_2-air performance.

The team developed methods to improve the physical surface area of the CCC supports through surface modifications of the carbon black and various process conditions. The team has also developed methods to create hybrid cathode catalysts by depositing Pt on CCC supports impregnated with transition metals. Figure 1 shows the transmission electron microscope (TEM) images of the Pt catalyst using two different heat treatment approaches; the catalyst prepared with the modified heat-treatment method shows particle size around 3.4 nm and more uniform distribution. Some of these catalysts showed mass activities meeting U.S. Department of Energy targets.

One of the issues with typical Pt-alloy catalysts is relatively poor performance in H_2-air polarizations curves. The hybrid cathode catalysts developed under this project show relatively good performance under H2-air conditions. The 35% and 40% Pt/CCC catalysts show roughly 1.25 A/cm^2 (1.5/1.8 and 1.5/2.0 stoic.) at 0.58 volt (V), and the 35% Pt-M/A-CCC catalyst shows 1.45 A/cm^2 (2/2 stoic.) at 0.58V under operating conditions closer to automotive applications (see Figure 2).

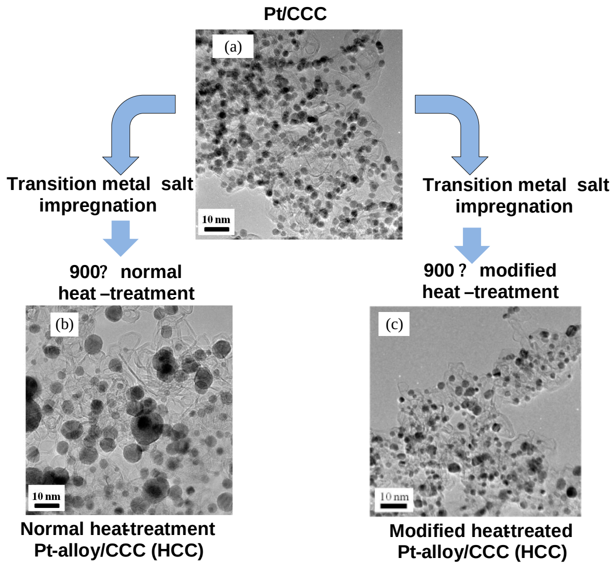


Figure 1. TEM image of Pt catalyst using two different heat treatment processes.

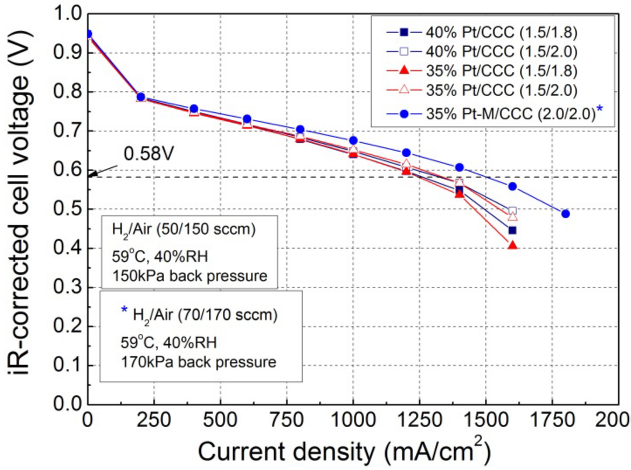


Figure 2. Polarization curves under H_2-air for various Pt/CCC.

Materials

2013 U.S. DRIVE Highlight

Integrated Computational Materials Engineering Approach to Development of Lightweight 3GAHSS

Demonstrating integrated computational materials engineering for the development and deployment of third generation advanced high-strength steels for improved vehicle lightweighting.

United States Automotive Materials Partnership LLC

The United States Automotive Materials Partnership LLC, working with partners Michigan State University and Brown University, has developed an initial three dimensional (3D) representative volume element (RVE) that is statistically equivalent to the actual microstructure of a third generation advanced high-strength steel (3GAHSS) based on a commercial QP980 steel. Figure 1 is a highly detailed computer representation of this microstructure, which consists of multiple dispersed microstructural phases such as soft ferritic, metastable austenite, and hard martensitic.

Accurate representation of the size, shape, distribution, and volume of the individual phases will enable computer modelers to assess the response of individual phases to mechanical strain. For instance, when sufficiently strained, such as during the forming of a sheet metal component, the austenitic phase in the QP980 transforms to a harder, less ductile martensitic phase. This transformation significantly changes the material properties of the steel. Additionally, the mechanical properties of sheet steels are anisotropic where the mechanical properties along the rolling direction are different from that perpendicular to the rolling direction. 3D RVEs have the advantage over two dimensional (2D) RVEs because 3D RVEs can better assess material response to strain while accounting for material anisotropy.

3D RVEs will enable improved computer simulations to determine the possible shapes that can be formed from 3GAHSS and subsequent component performance in a vehicle. This work is beneficial for producing lighter weight 3GAHSS structures that have similar or better performance than other (e.g., more costly) steels.

This development is the first known implementation of 3D RVEs in a metals integrated computational materials engineering (ICME) program, where less accurate 2D images have been used previously to model nonferrous alloys. 3D RVEs are a fundamental improvement, not only to the 3GAHSS ICME project, but to ICME modeling in general. It is expected that future enhancements to 3D RVEs will reduce requisite testing for generating constitutive material parameters necessary for ICME models and improved accuracy in ICME model simulations. Future work in the 3GAHSS ICME project includes validating 3D RVEs, and once validated, integrating them into an ICME model.

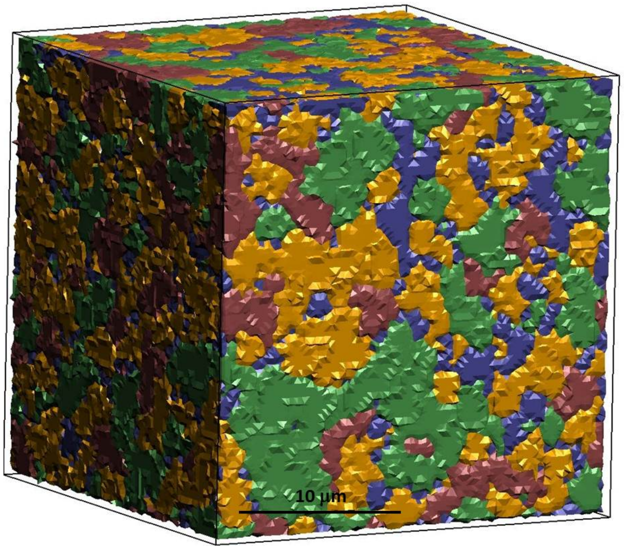


Figure 1. Three Dimensional Representative Volume Element of commercial QP980 Steel - (Green = Martensite, Blue = Austenite and Red + Yellow = Ferrite).

2013 U.S. DRIVE Highlight

Vehicle Mass: Road Load & Energy Consumption Impact

Energy consumption decrease of 4% to 5% for a 10% vehicle mass reduction was quantified for three vehicle powertrain architectures: hybrid electric, battery electric, and internal combustion engine.

Idaho National Laboratory, Argonne National Laboratory, and ECOtality North America

Idaho National Laboratory (INL), Argonne National Laboratory (ANL), and ECOtality North America tested various advanced technology vehicles in on-road fleets, on test tracks, and in laboratory settings to determine real-world fuel economy improvement.

The impact of vehicle mass (road load force) and energy consumption for three vehicle powertrain architectures was measured through test-track coastdown testing and chassis dynamometer testing. Testing was conducted on a Ford Fusion hybrid electric vehicle (HEV), a Nissan LEAF battery electric vehicle (BEV), and a Ford Fusion V6 internal combustion engine vehicle (ICE) and at multiple 250 pound test weights for each vehicle. This study provides results for further research, development, and modeling efforts.

Coastdown testing indicated a non-linear trend between changes in mass and road load force. For a 5% increase in mass, the road load force increases ~3% but for a 5% decrease in mass, the road load force decreases ~5%. This trend appears to be consistent across the three powertrain architectures (HEV, BEV, or ICE).

Chassis dynamometer testing quantified the impact of vehicle mass on energy consumption. The largest impact of vehicle mass reduction is observed during city and aggressive driving. For a 10% reduction in mass, there is up to ~5% decrease in energy consumption, as shown in Table 1. However, the conventional vehicle (ICE) has the largest decrease in net energy consumption (up to ~0.4 L/100km) during aggressive driving as compared to an HEV or BEV.

Figure 1. Photo of the vehicles tested (HEV, BEV, and ICE).

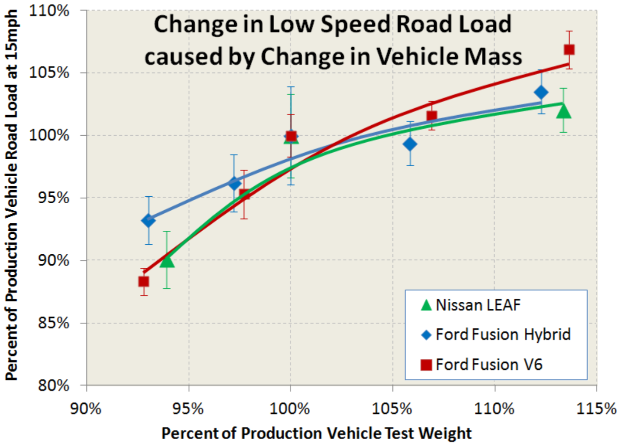


Figure 2. Vehicle road load vs. vehicle weight with respect to base vehicle.

	Percent consumption reduction **[%]**			Energy consumption reduction **[Lge/100km]**		
Driving type	*City*	*Highway*	*Aggressive*	*City*	*Highway*	*Aggressive*
ICE	~3.5 %	~3.0%	~4.5 %	~0.35	~0.19	~0.40
HEV	~2.5 %	~1.5 %	~4.0 %	~0.12	~0.06	~0.19
BEV	~5.0 %	~0.1 %	~2.5 %	~0.08	~0.01	~0.10

Table 1. Effects of a 10% reduction in vehicle mass.

2013 U.S. DRIVE Highlight

Carbon Fiber Technology Facility

The fully operational Carbon Fiber Technology Facility is a key resource for scaling and transferring lower cost carbon fiber technologies from the laboratory to the carbon fiber industry.

Oak Ridge National Laboratory

Oak Ridge National Laboratory (ORNL) is leading research and development efforts in lightweight materials for transportation with a focus on lower-cost carbon fiber (CF), which would be available at a target price of $5-7 per pound. ORNL has demonstrated at a laboratory scale that CF can be produced using alternative precursors, such as textile grade polyacrylonitriles, polyolefins, and lignins. ORNL is also developing lower-cost methods for converting precursors into CF including atmospheric plasma oxidation and microwave-assisted plasma carbonization. In order to commercialize these technologies, their viability must be proven on a continuous basis at near industrial scale.

The Carbon Fiber Technology Facility (CFTF), funded through the American Recovery and Reinvestment Act of 2009 by the U.S. Department of Energy's (DOE) Vehicle Technologies Office (VTO), is designed to scale up low-cost CF technologies and move them into the marketplace. In 2013 the CFTF (see Figure 1), was commissioned and is now fully operational with operating funds provided jointly by the DOE Advanced Manufacturing Office (AMO) and VTO.

The CFTF offers a flexible, highly-instrumented CF line for demonstrating advanced technology scale-up and producing market-development volumes of prototypical CFs made from alternative precursors. The CFTF is intended to bridge the gap between laboratory research and commercial-scale deployment of low-cost CF technologies. The CFTF is capable of producing up to 25 tons of CF a year. In addition to a conventional conversion line, CFTF has a melt-spun precursor fiber production line with a rated capacity of 65 tons per year. The 42,000 square foot facility has the capacity for expansion, including adding an advanced technology conversion line based off of technologies currently being developed at ORNL.

Recently the CFTF has:

- Successfully determined a conversion process for a textile based PAN precursor.
- Produced a melt blown lignin mat precursor at large scale.
- Processed industrial grade CF precursor with strengths as high as 550 ksi.
- Filed two invention disclosures.
- Implemented a worker training program to develop a future workforce for the carbon fiber industry.
- Began working with industrial partners to supply carbon fiber as part of the AMO Manufacturing Demonstration Facility.

Figure 1. Inside the Carbon Fiber Technology Facility.

2013 U.S. DRIVE Highlight

Magnesium Front End Research and Development

Enabling use of magnesium as a lightweighting material through development of advanced alloys, manufacturing and assembly processes, and mitigation of galvanic corrosion in dissimilar-metal joints.

United States Automotive Materials Partnership LLC

United States Automotive Materials Partnership LLC (USAMP) achievements in developing large, integrated all-magnesium alloy subassemblies comprised of high-integrity die castings and wrought forms have been reported previously. Such large-scale, lightweight substructures are capable of advancing the 50% vehicle weight reduction goal of the U.S. DRIVE's Materials Technical Team. This undertaking, collectively known as Magnesium Front End Research and Development, has also included an international partnership with magnesium researchers in Canada and China.

In the course of this broad effort, a number of key technical challenges have arisen and constitute major thrusts of the current work.

Challenge 1: For widespread application, magnesium-intensive substructures will ultimately need to incorporate and interface with dissimilar materials such as steel and aluminum.

Researchers initiated tasks to provide and assess joining of such dissimilar metals, as well as protecting against galvanic corrosion. In fiscal year (FY) 2013, these tasks demonstrated successful aluminum-magnesium joints using both friction stir welding (upper rail) and self-piercing rivets (lower rail). Figure 1 portrays the dissimilar-metal joints in the current embodiment of the demonstration structures. Adaptation of both technologies was enabled by fundamental advances in the metallurgy of the weld zone and deformation characteristics of magnesium in selected material stack-ups. Additionally, testing has begun on approaches developed for mitigating localized galvanic attack of magnesium adjacent to coated steel self-piercing rivets.

Challenge 2: Improving deformation properties of magnesium alloys for purposes of component fabrication and performance.

In FY 2013, a novel ZE20 magnesium extrusion grade was selected for evaluation, cast into billets and extruded into prototype lower rail profiles, as shown in Figure 1. These profiles will be used to evaluate crashworthiness, corrosion and fatigue properties of both the alloy and structure.

Challenge 3: Durability of magnesium-to-magnesium and magnesium-to-dissimilar metal joints.

In 2013, several improvements were made to computer-aided engineering tools used to predict joint failure in large structures through application of algorithms assessing localized structural stresses, which, in turn, can then be employed in conventional estimates of fatigue durability.

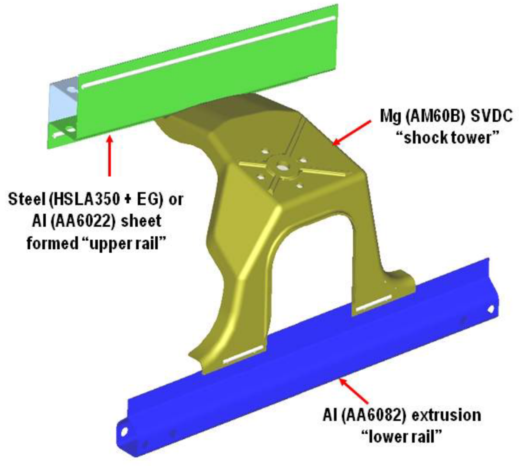


Figure 1. Demonstration "front-end" structure employing dissimilar metals as indicated.

2013 U.S. DRIVE Highlight

Implementation of Structural Composite Underbody Technologies

The learnings from the Automotive Composites Consortium Structural Composite Underbody project were used for the rapid commercialization of the Chevrolet Spark electric vehicle battery enclosure.

USAMP Automotive Composites Consortium

The United States Automotive Materials Partnership Automotive Composites Consortium (ACC) Underbody Project designed, built, analyzed, and tested an automotive underbody capable of carrying the crash loads of a vehicle, while saving about 13 kg of mass compared to the optimized high strength steel underbody in the donor vehicle. Minimizing the mass of this structure required a number of thickness zones in the part, ranging from 1.8 mm to 5.4 mm.

The underbody was made from a coarse weave glass fabric coated with a vinyl ester resin in a sheet molding compound (SMC)-like process. The prepreg was cut on an automated cutting table with patterns designed for minimal overlap to accommodate the complex thickness zones. These pieces were assembled into a preform and transferred to the compression molding tool. The part was assembled into a mock body-in-white, using composite-to-steel weld bonding (United States Council for Automotive Research patents). The weld bonding used laser-cut holes in the composite for the welding. Adhesive was applied to the steel structure and to doubler strips with divots matching the hole pattern. These were placed on either side of the composite, and double welded to the steel structure, providing peel stoppers, and acting as fixturing during the adhesive cure. The composite/steel structure was then tested simulating the underbody loads that would have been seen in a 40 mph offset deformable barrier. Results showed that while the molded part was slightly thicker than design, our models predicted the behavior within tolerance.

When the Chevrolet Spark electric vehicle team needed a new material for the two-piece structural battery enclosure with only a short time before production started, they saw an answer in the underbody. They used the coarse weave glass fabric/vinyl ester prepreg, further developing the resin system to virtually eliminate solvent emissions. The prepreg was then cut and placed on the tool with a laser-assist system, and the preform robotically placed in the mold.

After part cure and post processing, the battery tray was assembled to a lower steel structure, with the structural plates on the inside acting as the doublers. This used rivet bonding, similar to weld bonding (see Figure 1). The change to this material was very rapid because of the extensive research and development done by the ACC Underbody project.

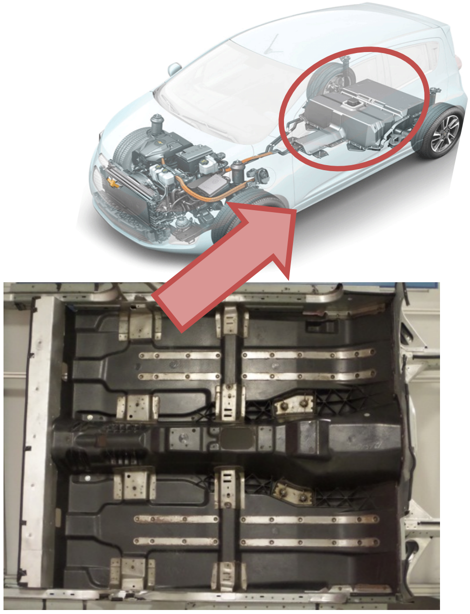


Figure 1. The materials, part fabrication, modeling, and assembly methodologies used in the Structural Composite Underbody were refined and utilized in the Chevrolet Spark EV battery enclosure.

2013 U.S. DRIVE Highlight

High-speed Joining of Dissimilar Alloy Aluminum Tailor-welded Blanks

Bridging the technology gaps for high speed joining of aluminum welded blanks to enable high volume stampings.

Pacific Northwest National Laboratory, General Motors, TWB Company, and Alcoa, Inc.

Pacific Northwest National Laboratory (PNNL) is leading efforts in joining lightweight materials for transportation by infusing the automotive supply chain with the technology needed to enable welding aluminum blanks for high volume applications. By delivering the technology expertise to the automotive supply chain, PNNL has brought together an integrated team including Alcoa, Inc., TWB Company LLC, and General Motors (GM). This team is working to hone the technology, ensure high volume quality, and develop the design and modeling tools necessary to rapidly implement new aluminum welding technology.

The project is funded by DOE's Vehicle Technologies Office and the investments of each of the team members. It aims to overcome technology barriers preventing implementation of enabling and efficient joining technologies.

PNNL's role is to bridge the technology gaps that remain between enabling technology and commercialization. When combined with the efforts of the entire supply chain, this role entails not only the development of the welding parameters, tooling, and modeling tools, but also the equipment, quality control methodologies, cost models, and process limitations that enable full commercialization of the joining technologies employed.

Recent accomplishments include the following:

- Transferred welding setup for full-size demonstrations parts at GM's research and development center.
- Completed stamping trials of dissimilar thickness AA5182 welded blanks with TWB Company LLC (Figure 1).
- TWB procured a high-speed friction stir welding (FSW) machine for setup at their facility in Monroe, Michigan (Figure 2).
- Submitted two technical papers one on a comparison of welding processes, and another on successful FSW properties and parameters.

Figure 1. Formability tests on dissimilar thickness welded panels demonstrating weld parameter variation on quality and post-weld formability.

Figure 2. Setup of a high-speed FSW machine at TWB Company LLC in Monroe, Michigan.

2013 U.S. DRIVE Highlight

Aluminum Formability Extension through Superior Blank Processing

50% improvement in aluminum sheet edge stretchability at room temperature enables increased application of aluminum and delivers cost and quality improvement.

Pacific Northwest National Laboratory, Ford Motor Company, Oakland University

The formability of the aluminum sheet in conventional automotive stamping is typically limited by the processes that prepare the blank for the stamping operation. Past research has shown that the room temperature formability of aluminum sheet can be reduced by as much as 50% as a result of inadequate blanking, piercing, and trimming operations. On the other hand, the automotive original equipment manufacturers (OEMs) and their Tier 1 suppliers have an extraordinary high capital investment in sheet metal forming facilities, equipment, and associated infrastructure. The ability to redirect these capitally-intensive facilities from steel to aluminum component manufacturing would dramatically increase the widespread commercialization of aluminum sheet into vehicles. This project's purpose is to enhance the overall room temperature edge stretchability of aluminum sheet with existing OEM infrastructure by developing enhanced processes for the blanking, piercing, and trimming operations to extend aluminum formability in the subsequent forming operations.

In this work, a combined experimental and numerical approach is used to develop processing windows and parameters for preparation of stamping blanks that achieve robust, extended ductility compared to conventionally trimmed blanks. The project has developed an integrated manufacturing process simulation tool suite that considers trimming induced edge damage in the subsequent stretchability predictions, and validated the trimming module and the subsequent stretchability module with controlled experiments at different trimming clearances. The trimming simulation has achieved greater than 90% accuracy by comparing the predicted and measured burr size at different trimming clearances (see Figure 1).

By integrating the trimming-induced burr geometry, initial plastic strain, internal stresses and damages at the shear affected zone into the stretchability module, both failure modes and subsequent tensile stretchability have been accurately predicted (see Figure 2).

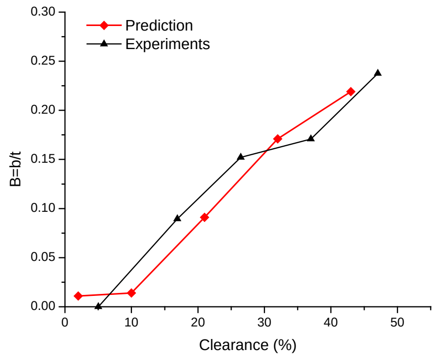


Figure 1. Comparison of predicted and measured burr height.

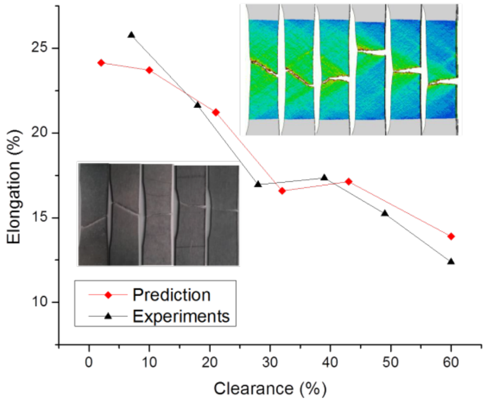


Figure 2. Comparison of predicted and measured stretchability for trimming processes.

2013 U.S. DRIVE Highlight

Validation of Crash Models for Carbon Composites

Enabling vehicle weight reduction through the high-volume use of lightweight carbon fiber composites in primary structural automotive crash and energy management applications by increasing the design confidence in material models.

United States Automotive Materials Partnership LLC

This four-year project, titled Validation of Crash Material Models for Automotive Carbon-Fiber Composite Structures Via Crash Testing (VMM), has completed the first year of an extensive collaborative industry program. VMM is validating four commercial constitutive models implemented in crash codes (i.e., ABAQUS, LS-DYNA, PAM-CRASH and RADIOSS), and two newer crash models – a meso-scale representative unit cell (RUC) model[1] and a micro-plane RUC model[2], developed by partners the University of Michigan, and Northwestern University, respectively.

The VMM project goal is to validate crash models for structural automotive carbon fiber composites. The project team chose a front bumper beam and crush-can (FBCC) application to validate the crash models, by developing a composite FBCC that can demonstrably absorb impact energy equivalent to a baseline steel FBCC under various crash-loading modes.

The project team includes automotive original equipment manufacturer researchers, academic researchers, automotive design/engineering service suppliers, composite manufacturers, material suppliers, test laboratories, and crash test vendors. In its first year, the project crashed a production steel FBCC assembly to provide the targets for the composite FBCC. The steel FBCC (Figure 1) is being tested under high- and low-speed crash conditions and is simultaneously being modeled to determine a baseline range of crash parameters, which composite FBCC crash models are expected to meet.

A composite FBCC is presently being designed and will be modeled using the six selected computer crash models. Initial materials have been selected, and testing of these materials is underway to determine the necessary input parameters for the crash models. The composite FBCC will be fabricated, and the structures tested in high-speed and low-speed crash, with variances assigned to gaps in the material models.

The VMM project will advance the application of critical carbon-fiber polymeric composite crash models and identify gaps in composite material modeling and crash-characterization, so as to establish their readiness for greatly reducing vehicle weight in automotive structures.

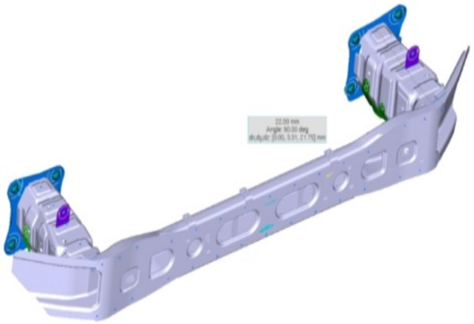


Figure 1. A representative FBCC assembly used for baseline crash testing and computer aided engineering.

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[1] Song S, Waas AM, et al., Composites Science and Technology, 67 (15-16), 3059-3070, 2007.

[2] Caner, F.C., et al., Journal of Engineering Materials and Technology, 133, 021024-1-12, 2011.

Vehicle Systems and Analysis

2013 U.S. DRIVE Highlight

Advanced Transmission Impact on Fuel Displacement

New models and controls of advanced transmissions can evaluate their impact on fuel displacement for several powertrain technologies.

Argonne National Laboratory

As a result of more stringent regulations and increased customer expectations, automobile manufacturers have considered numerous technology options to improve vehicle fuel economy.

Due to their cost effectiveness, transmissions have rapidly evolved in recent years. To properly assess the benefits of U.S. DRIVE-developed technologies, it is essential to understand the impact of transmissions on both component operating conditions and fuel displacement.

In the past, Argonne National Laboratory has characterized and developed models for five-speed automatic transmissions. The study objective was to develop and validate advanced transmission models (e.g., 6+ speeds automatic as well as dual clutch transmissions) and their shifting control in a vehicle systems context, using Autonomie (see Figure 1).

The main accomplishments are listed below.

- Integrated and analyzed more than a dozen sets of vehicle test data from Argonne Advanced Powertrain Research Facility.
- Developed and validated a shifting initializer to create new sets of calibration for multiple vehicles.
- Developed a model of a dual clutch transmission along with its controller.

Future work will focus on:

- Evaluating the fuel displacement potential of advanced engines when combined with advanced transmissions.
- Evaluating the impact of advanced transmissions on current engine targets (i.e., operating conditions).
- Automating the shifting map calibration process from vehicle test data.
- Developing and validating additional advanced transmission models.

Preliminary simulations have demonstrated a fuel consumption reduction of up to 10% for conventional powertrains. The new advanced transmission models and shifting algorithm will enable an accurate evaluation of the fuel displacement potential of advanced powertrain and component technologies.

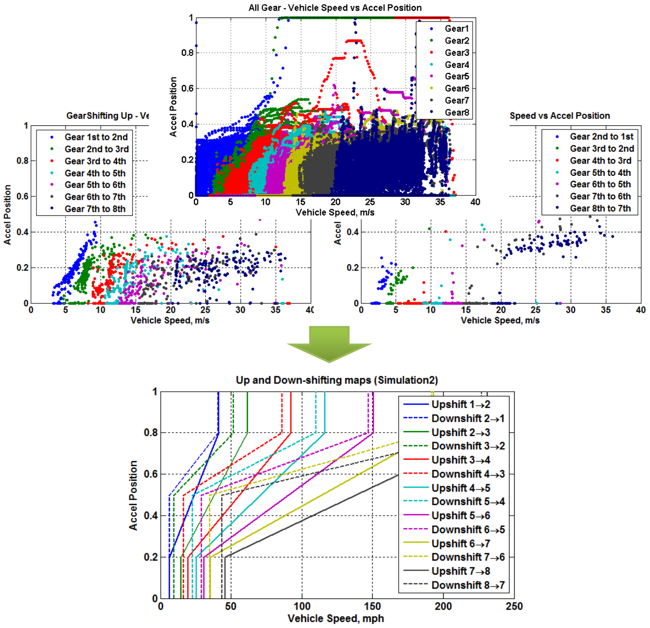


Figure 1. Shifting Algorithm Development for an 8-speed automatic transmission.

2013 U.S. DRIVE Highlight

Reducing Climate Control Loads in Electric Vehicles

Testing demonstrates zonal climate control can reduce air conditioning power and improve range while maintaining driver thermal sensation.

National Renewable Energy Laboratory

When the climate control system in an electric drive vehicle (EDV) is operating, the energy consumed has a significant impact on range. This project's objective is to increase in-use EDV range by minimizing climate control energy requirements. The goal is to increase EDV range by 10% during operation of the climate control system through improved thermal management while maintaining or improving occupant thermal comfort.

Currently, conventional vehicles heat cabins with engine waste heat, but because EDVs do not have an engine, automobile manufacturers are presented with new climate control challenges. Using the battery for cabin electrical resistance heating takes valuable energy away from propulsion. Therefore, it is critical to minimize climate control loads in EDVs to maximize vehicle range.

The National Renewable Energy Laboratory (NREL) worked with the automotive industry to develop strategies to reduce climate control loads and evaluate their effectiveness. This project leverages the zonal climate control approach developed under the U.S. Department of Energy's thermoelectric heating, ventilation, and air conditioning (HVAC) projects.

As part of a cooperative research and development agreement project with Ford Motor Company, NREL researchers completed summer thermal load reduction testing on two Ford Focus electric vehicles (EVs). Using a combination of temperature and power measurements as well as a thermal manikin (Figure 1), researchers assessed three zonal climate control configurations and six thermal load reduction configurations. At the same flow rate as the established baseline, the zonal vent configurations demonstrated up to a 16.7% reduction in climate control energy compared to the baseline HVAC system. Reducing the total air-flow rate increased the energy savings up to 50%. The results indicated the opportunity to reduce energy consumption and improve thermal sensation with a zonal climate control approach. A computational fluid dynamics /RadTherm/human model was used to assess a zonal climate concept. Using Autonomie, vehicle simulations over the SCO3, city, and highway drive cycles showed that a zonal A/C system has the potential to increase vehicle range 7% to 15% during operation of the air conditioning.

Figure 1. HVAC manikin test in the Ford Focus EV.

2013 U.S. DRIVE Highlight

DC Fast Charge Effects on Electric Vehicle Battery Performance

The effects of charge rate on electric vehicle battery performance were investigated through prescribed on-road mileage accumulation and laboratory testing at 10,000 mile intervals for two groups of electric vehicles.

Idaho National Laboratory

Limited range is frequently noted as a barrier to the large-scale adoption of electric vehicles (EVs). However, fast charging infrastructure can increase the practical driving range of an EV through rapid battery charging (charging to ~80% in about 30 minutes). Though convenient, there are concerns that fast charging may compromise the life of the battery pack. On the 2012 Nissan LEAF, alternating current (AC) Level 2 charging provides up to 3.3 kW to the battery, while direct current (DC) Level 2 "fast charging" provides up to 50 kW. Idaho National Laboratory is conducting research to quantify the effects of DC fast charging on EV performance and battery life for a 2012 Nissan LEAF.

Six identical 2012 Nissan LEAFs were baseline track-tested to quantify their overall performance characteristics when new. Four were driven daily on a prescribed on-road route, while the other two had their battery packs removed for laboratory cycling. Two cars from the on-road group were designated to be charged only by AC Level 2, while the other two on-road vehicles were designated DC fast-charge only. Each on-road test vehicle was driven on a fixed route until five miles of indicated range remained. The vehicles were driven in pairs, one from each group, to duplicate the ambient conditions between the test groups. Data were collected from each vehicle in real-time during each driving and charging event.

At 10,000-mile intervals, the battery packs were removed and underwent a series of reference performance tests to quantify energy capacity, power capability, and internal resistance growth. The tests are based on U.S. Advanced Battery Consortium vehicle battery test manuals. The on-road test vehicles have completed the 40,000 mile laboratory testing, and are approaching the 50,000 mile test, at which point they will be track-tested again to quantify whole system performance. Testing results to date are shown in Figure 1 below.

At the conclusion of testing, differences in range and performance will be reported. While most EV drivers will likely charge their vehicle with a mix of the two charging levels, study results will provide bookends for the extreme usage cases, and the differences encountered between the two cases. A quantitative measure of the tradeoff between convenience of fast charging and battery degradation will empower EV drivers to maximize the utility of their EV.

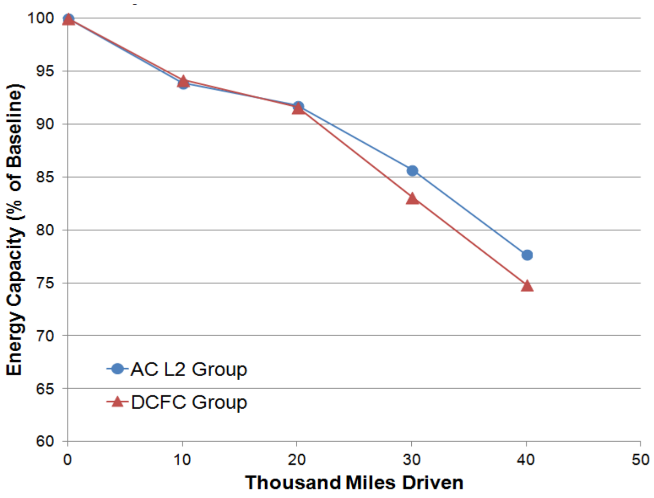


Figure 1. C_3 energy capacity at 10,000 mile test intervals.

2013 U.S. DRIVE Highlight

Providing Public Access to Advanced Vehicle Test Data

Web-based portal provides access to dynamometer data to enhance understanding of system-level interactions of advanced vehicle technologies and help researchers, students, and professionals engaged in energy efficient vehicle research, development, and education.

Argonne National Laboratory

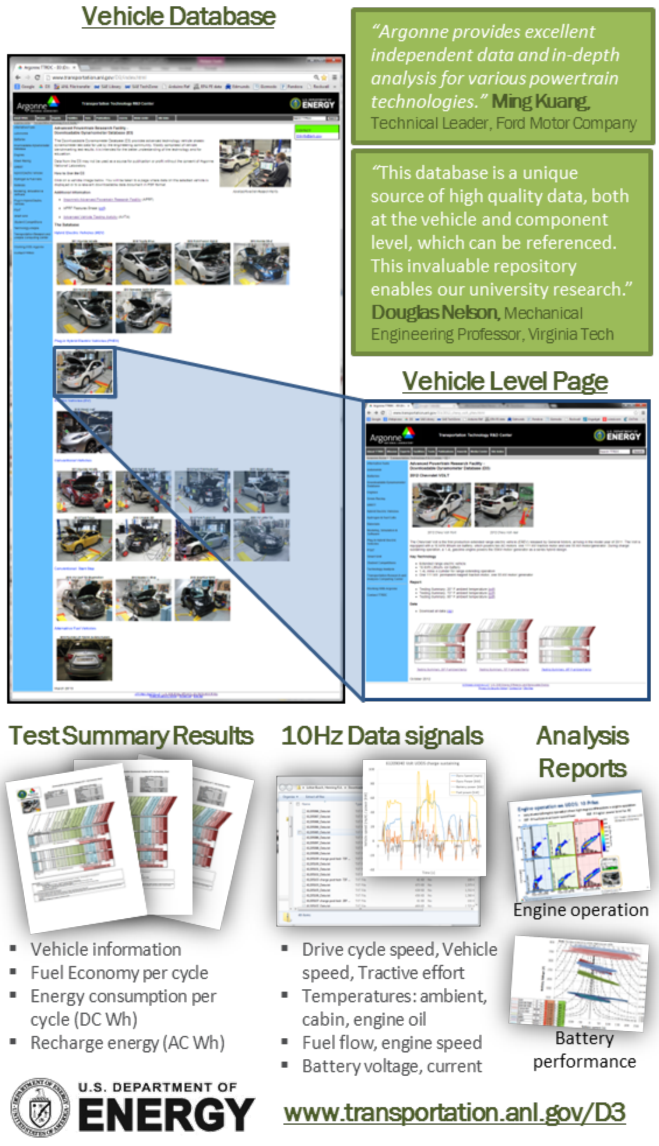
The Advanced Powertrain Research Facility was purpose-built with U.S. Department of Energy funds to benchmark advanced technology vehicles (ATVs). Experienced researchers test extensively instrumented ATVs on two or four wheel drive chassis dynamometers.

The Downloadable Dynamometer Database (D^3) is a public repository of independent vehicle test data that provides high-level detail useful to the research community.

Test vehicles range from conventional vehicles, hybrid electric vehicles, plug-in hybrid vehicles, and battery electric vehicles, as well as alternative fuel vehicles (e.g., hydrogen, natural gas, and ethanol). Typically, vehicle- and component-level data are generated from standard transient test cycles in temperature conditions of 20°F, 72°F and 95°F with 850 W/m^2 of radiant sun energy.

Openly-shared vehicle data is rare outside of the largest industry labs, as it is normally too expensive for most research institutions to generate. The prime users of the database include:

- *Academia*: D^3 is the source of public ATV data for research conducted at universities and graduate level studies.
- *Government*: D^3 serves model data population and validation, research and development target-setting, identifies and quantifies challenges to and opportunities for ATVs, and supports codes and standards development.
- *Manufacturers and suppliers*: D^3 data are used to calibrate models and provide deeper understanding of new technologies across the competitive automotive landscape.
- *Startup companies*: D^3 enables exploratory feasibility studies and model calibration.



"Argonne provides excellent independent data and in-depth analysis for various powertrain technologies." **Ming Kuang**, Technical Leader, Ford Motor Company

"This database is a unique source of high quality data, both at the vehicle and component level, which can be referenced. This invaluable repository enables our university research." **Douglas Nelson**, Mechanical Engineering Professor, Virginia Tech

- Vehicle information
- Fuel Economy per cycle
- Energy consumption per cycle (DC Wh)
- Recharge energy (AC Wh)

- Drive cycle speed, Vehicle speed, Tractive effort
- Temperatures: ambient, cabin, engine oil
- Fuel flow, engine speed
- Battery voltage, current

www.transportation.anl.gov/D3

Figure 1. Illustration of the D^3 content available for all vehicles, spanning a wide range of vehicle architectures.

CROSSCUTTING TECHNOLOGIES

Codes and Standards

2013 U.S. DRIVE Highlight

First International Regulation Governing Fuel Cell Electric Vehicles Facilitates Global Commercialization

Global Technical Regulation on hydrogen and fuel cell vehicles is completed, which will harmonize safety requirements across key markets and support commercialization.

U. S. Department of Transportation, National Highway Transportation Safety Administration

In June 2013, the United Nations Economic Commission for Europe (UNECE) World Forum for Harmonization of Vehicle Regulations Working Party 29 accepted the Global Technical Regulation (GTR) governing the safety of fuel cell electric vehicles (FCEVs). As the first international legislation in this field, the United Nations' acceptance enables the GTR to establish a global standard for certifying and commercializing FCEVs. The support, expertise, and involvement of the U.S. DRIVE Partnership's Hydrogen Codes and Standards Tech Team and the U.S. Department of Energy (DOE) were an integral part of this key milestone.

The GTR contains the minimum safety requirements for FCEVs and covers the on-board storage and fuel cell system (including the fuel cell stack and high voltage components). As shown in Figure 1, the GTR was developed based on system-focused performance criteria from sources such as Society of Automotive Engineers J2579 standard rather than prescriptive requirements. The GTR effort was co-sponsored by the United States, Germany, and Japan, but the content was a global collaboration taking into account existing industry standards and regulations from Canada, China, the European Union, Japan, Korea, and the United States.

The U.S. Department of Transportation's National Highway Transportation Safety Administration was instrumental in the adoption of the GTR. DOE provided a key support role by funding the participation of U.S. experts in the GTR process and by sponsoring work at the U.S. national labs that is directly reflected in the GTR language. This global standard facilitates commercialization by having a single requirement for multiple markets. The final step for the United States is the adoption of the GTR by the Federal Motor Vehicle Safety Standard within the next three years.

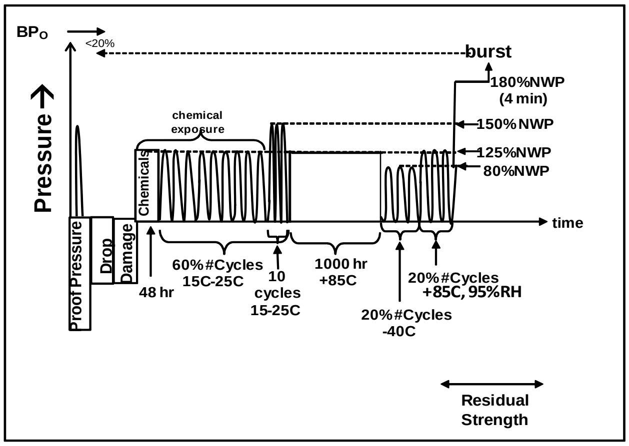


Figure 1. Verification test for durability (hydraulic) performance. Source: UN Global Technical Regulation on Hydrogen and Fuel Cell Vehicles, [http://www.unece.org/fileadmin/DAM/trans/doc/2013/wp29/ECE-TRANS-WP29-2013-041e.pdf.](http://www.unece.org/fileadmin/DAM/trans/doc/2013/wp29/ECE-TRANS-WP29-2013-041e.pdf)

On-board Hydrogen Storage

2013 U.S. DRIVE Highlight

Material Requirements for Viable Vehicular Hydrogen Storage via Chemical Hydrogen Storage

Engineering analyses and testing have established new guidelines that fill critical knowledge gaps to guide research on new chemical hydrogen storage materials for on-board storage in light-duty vehicles.

Hydrogen Storage Engineering Center of Excellence

The Hydrogen Storage Engineering Center of Excellence (HSECoE) has developed integrated system models able to provide rational guidelines concerning the material properties necessary for a chemical hydrogen (H_2) storage material to meet the U.S. Department of Energy's (DOE) 2017 hydrogen storage system targets. DOE's on-board H_2 storage targets are for the complete system, as opposed to material-specific targets, so there has been a critical knowledge gap concerning H_2 storage material properties required for automotive applications.

The unique approach taken by the HSECoE to combine chemical H_2 storage system and vehicle models allowed the team to identify and size all storage components (e.g., reactors, heat exchangers, tanks, valves, purifiers, etc.) necessary for a fully functional H_2 storage system able to meet numerous drive cycles. The required material properties needed to meet DOE's 2017 H_2 storage system targets (e.g., gravimetric and volumetric density of H_2 as well as the imposed limits for the kinetics and thermodynamics of H_2 release) were then calculated as function of system mass and volume.

These new models, based on a realistic H_2 storage system, offer a higher fidelity to provide a rational baseline for specific material properties necessary for newly developed materials.

For example, while current chemical H_2 storage materials show promise to meet volumetric system storage targets, gravimetric targets are a greater challenge. As illustrated in Figure 1, modeling shows that an idealized chemical H_2 storage system with a minimum mass of 31 kg would require a chemical H_2 storage material with a minimum gravimetric density of 7.8 weight percent (wt.%) H_2 to meet DOE's 2017 gravimetric capacity system target of 5.5 wt.% H_2.

While no current chemical H_2 storage materials can meet all performance targets for light-duty vehicles, new promising materials can be evaluated using the requirements established by the HSECoE *Chemical Hydrogen Storage System Models*.

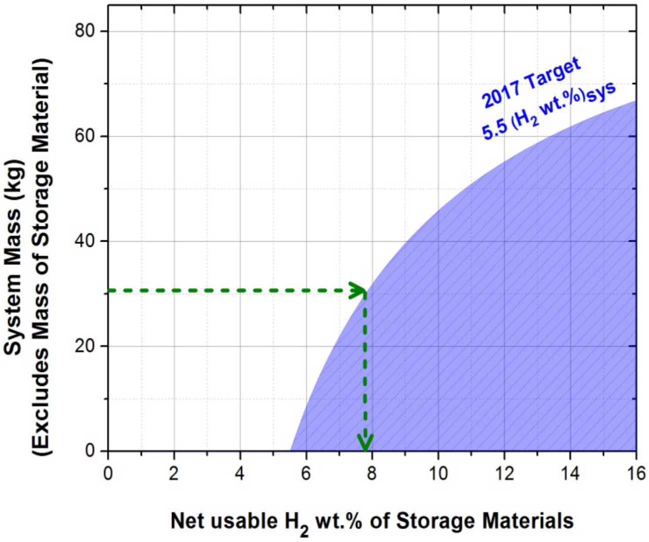


Figure 1. Plot of Available System Mass as a Function of Net Usable H_2 wt.%. For a given H_2 storage system mass obtained from the mass of all the system components (e.g., heat exchangers, pumps, purifiers, etc.) a materials developer can calculate the required gravimetric H_2 density for a new material. Alternately, for a given material, systems engineers can calculate the required size of the system.

2013 U.S. DRIVE Highlight

Advanced Models Reveal Optimal Hydrogen Storage System Design from Millions of Potential Configurations

Optimized adsorbent system designs were identified using models that compare a large number of system design variables in a high throughput fashion.

Hydrogen Storage Engineering Center of Excellence

The Hydrogen Storage Engineering Center of Excellence[1] (HSECoE) has identified a few highly promising adsorbent-based system designs for hydrogen storage from more than 62 million potential system configurations using a customized, high throughput screening tool it developed. System variables used in the model include internal heat exchanger configurations, tank designs, various materials, as well as operating pressure and temperature ranges. A multitude of these combinations were analyzed using a high throughput approach to project the adsorbent system performance and thereby down-select the optimal designs.

HSECoE partners conducted comprehensive analytical and experimental assessments of critical sub-components needed for efficient adsorbent storage systems. The goals of these efforts were to enable efficient system designs and to refine models that could accurately project performance. As a result of these efforts, the adsorbent system Go/No-Go milestones were met in the summer of 2013 and the work will continue into the third and final phase of the project.

The HSECoE modeling team used the Simulink framework to evaluate the impact on vehicle attributes arising from modifications to several storage system parameters. This analysis provided a normalized ranking of candidate systems, which is shown in Figure 1 for several hundred systems from the millions of combinations. The system ranking revealed the effects of configuration trade-offs between system designs and allowed for the selection of optimal parameters. As a result, the highest-ranked combinations of heat exchange subsystem design and media packing options were identified to be (i) the hex-cell heat exchanger with powder media, and (ii) the Modular Adsorption Tank Insert with densified "puck" media. These optimized configurations also book-end the space of design options and provide the HSECoE with the opportunity to explore variations in system cooling efficiency, media density, cost, and design complexity during the design and testing of these prototype systems.

Progression to Phase 3 will allow the HSECoE to construct and test the two configurations noted above, validate predictions made by the HSECoE's many models, and confirm that the sub-scale systems deliver optimal combinations of cost and performance under realistic operating conditions.

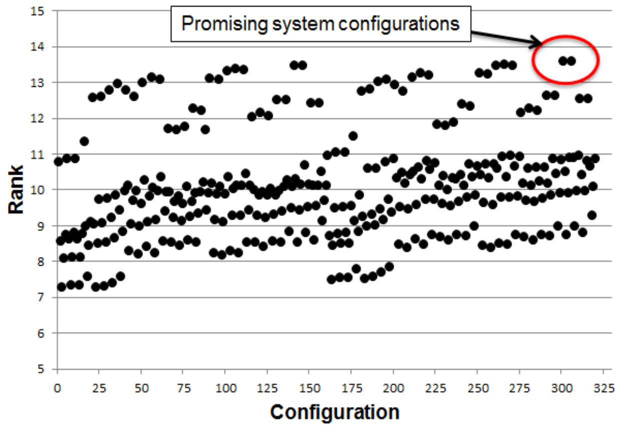


Figure 1. Results from high throughput screening of several hundred candidate systems from millions of possible configurations. The normalized system "Rank" measures system performance with respect to a combination of volumetric density, gravimetric density, and cost.

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[1] HSECoE is led by Savannah River National Laboratory with ten industry, university, and national lab partners.

2013 U.S. DRIVE Highlight

Enhanced Materials and Designs Reduce the Cost of On-board Hydrogen Storage Tanks by 15%

Advancements in composite materials and manufacturing design were shown to have potential in reducing the cost of 700 bar compressed hydrogen storage tanks toward the U.S. DRIVE target.

Pacific Northwest National Laboratory, AOC, Toray Carbon Fibers America, Hexagon Lincoln, and Ford Motor Company

The team lead by Pacific Northwest National Laboratory (PNNL) identified a feasible pathway to reduce the cost of Type IV, 700 bar pressure tanks by 15%, as shown in Figure 1. This would lower the projected cost of a system containing 5.6kg hydrogen (H_2) from $3,170 ($17/kilowatt hour (kWh)) to $2,700 ($14.5/kWh). Cost reductions for the pressure tank were achieved by:

- Using a low-cost resin (4% cost reduction),
- Incorporating nano-additives to increase matrix strength (5% cost reduction), and
- Improving winding designs to enhance composite fiber material usage (6% cost reduction).

Type IV, lightweight pressure tanks with a carbon fiber (CF) composite overwrap are considered the most likely near-term H_2 storage solution for fuel cell electric vehicles using 700 bar. The current cost for a Type IV tank system, manufactured at high volume (500,000 units/year), is projected to be $3,170. More than 60% of the cost is attributed to the CF composite overwrap, which consists mainly of CF and resin.

Therefore, the team's efforts have focused on optimizing materials for and design of the composite portion of the tank. The resin is a critical component of the CF composite because the interfacial adhesion between the resin and fiber must be optimized in order to use the strength of the CF reinforcement efficiently. Use of a low-cost vinyl ester (VE) resin combined with optimized CF surface treatments resulted in a 4% cost savings and better performance. Modification of the low-cost VE resin matrix with nano-additives increased the strength of the composite, allowing an additional reduction in amount of CF (cost savings = 5%). As a final cost saving step, the team used advanced modeling techniques to evaluate alternative fiber winding angle combinations and composite designs using the VE modified resin with respect to cost and mass. The alternative fiber angle tailoring approach evenly distributes the stress through the thickness, delivering an additional 6% cost savings. Cumulatively, these measures can lower the cost of Type IV, 700 bar pressure tanks by 15% down to $14.5/kWh. The ultimate goal of the project is a 30-40% cost reduction, which would meet the 2020 U.S. DRIVE target of $10/kWh.

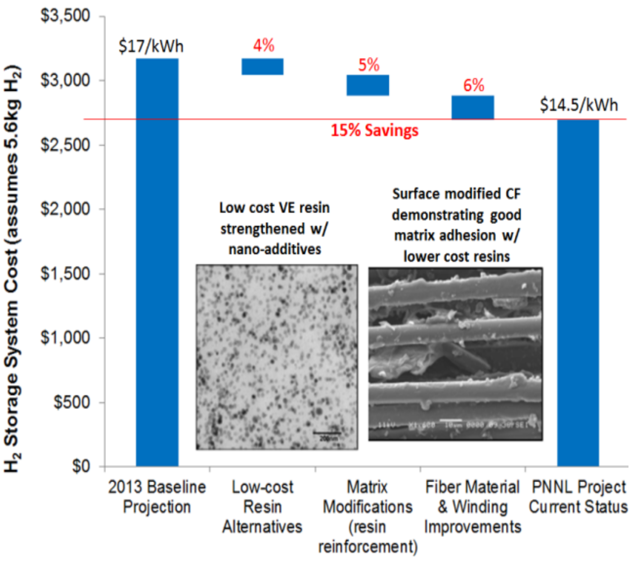

Figure 1. Waterfall plot showing pathway to achieving 15% cost savings for Type IV composite tanks as a result of composite optimization.

Grid Interaction

2013 U.S. DRIVE Highlight

Independent Testing of Wireless Power Transfer System

Results from the first independent test of a commercially-available wireless power transfer system for plug-in electric vehicles will help to refine test procedures and measure the effectiveness of today's wireless power transfer technology in the real world and the laboratory.

Idaho National Laboratory

Idaho National Laboratory (INL) has built and implemented a laboratory setup to test wireless power transfer (WPT) systems that charge a plug-in electric vehicle (PEV) via resonant electromagnetic coupling across a large air gap between the PEV and a power supply on or below the road surface.

WPT systems for PEV charging are beginning to enter the commercial marketplace. Because these technologies are new, testing is needed to measure WPT efficiency, or the percentage of energy that is successfully transmitted from the power supply to the PEV battery. The electric and magnetic field (EMF) strengths in the vicinity of the WPT system during PEV charging also need to be measured to ensure that they do not exceed safety limits. The impact on the electrical grid of plugging in and charging increasing numbers of PEVs also needs to be understood. Finally, testing WPT systems supports the Society of Automotive Engineers' J2954TM standards committee and is conducted in conjunction with its guidelines.

INL's test fixture for WPT systems can identify the EMF strengths at 2,600 testing positions. The setup uses a multi-axis positioning system to move the WPT system's primary coil (connected to the power supply) and secondary coil (ordinarily mounted underneath the PEV) relative to each other.

In 2013, INL conducted the first independent test of the PLUGLESSTM Wireless Charging System from Evatran Group, Inc., a WPT system now commercially available in the United States (see Figure 1).

Evatran's system is a Level 2 (208-volt alternating current) charger with 3.3 kW output. INL measured the EMF and system efficiency, which achieved a maximum of 88.8% at a 100 mm gap between coils (almost four inches) and 89.2% at a 110 mm gap. The efficiency is the fraction of energy going into the PLUGLESSTM control panel that eventually came out of the PLUGLESSTM vehicle adapter.

The results show that the system efficiency varies depending on the horizontal alignment between the primary and secondary coils. The vertical gap also has a strong impact on the system efficiency and the EMF measured in the vicinity. INL's report is available at http://avt.inel.gov/evse.shtml.

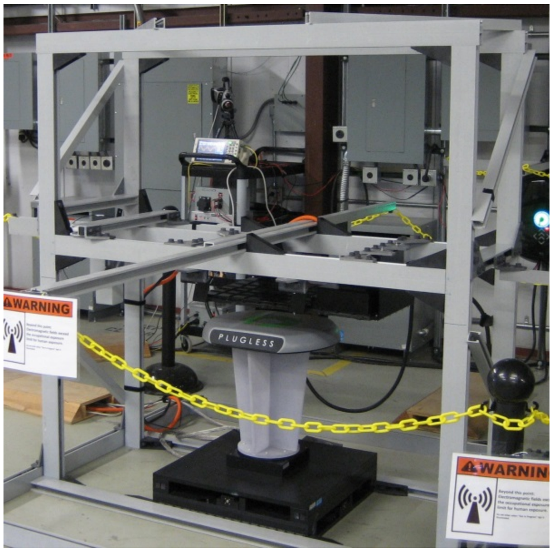

Figure 1. Wireless PEV charger coil positioning measurement setup testing the Evatran PLUGLESSTM wireless charging system at INL. Horizontal alignment occurs through moving the secondary coil mounted in the center of the metal frame relative to the primary coil mounted on the pedestal on the black base. The coil-to-coil gap is the vertical distance between these two parts.

FUEL INFRASTRUCTURE TECHNOLOGIES

Fuel Pathway Integration

2013 U.S. DRIVE Highlight

Updated Hydrogen Fuel Pathway Analysis Reveals Improvements in Cost and Emissions

Improved technology modeled scenarios show hydrogen produced via natural gas reformation – either on-site or centrally with pipeline or truck delivery – offers lower fuel costs and low greenhouse gas emissions.

Fuel Pathway Integration Technical Team

U.S. DRIVE's Fuel Pathway Integration Technical Team (FPITT) provided feedback to the U.S. Department of Energy's (DOE) preliminary evaluation of the lifecycle cost (including the cost of hydrogen (H_2) infrastructure), energy use, and greenhouse gas (GHG) emissions of eight advanced-technology H_2 production, delivery, and distribution pathways. DOE's 2013 H_2 pathways assessment complements DOE's previous evaluation of currently available H_2 technologies, investigating the changes in cost, energy use, and GHG emissions predicted to result from advanced H_2 technologies anticipated to be available in 2025. As with the previous assessment, FPITT members reviewed DOE's analysis methods, assumptions, and data.

The previous analysis of current-technology H_2 pathways found that all studied pathways except distributed production of H_2 via water electrolysis resulted in well-to-wheels (WTW) GHG emissions for fuel cell electric vehicles of less than 400 grams (g)/mile, measured on a gram carbon dioxide-equivalent per mile driven basis.[1] The 2013 analysis of advanced-technology H_2 pathways found that technology improvements are expected to reduce WTW GHG emissions to below 300 g/mile (25% decrease compared to the previous study) for all studied pathways, except distributed electrolysis using the U.S. grid mix.

The advanced-technology pathways evaluation is being conducted using DOE's publicly available models, based on an on-board fuel cell electric vehicle storage pressure of 10,000 psi, with cost reported in 2007 U.S. dollars.[2] The study, expected to be published in 2014 following further review by DOE and industry stakeholders, evaluates both WTW fuel-cycle emissions and vehicle-cycle emissions. Figure 1 shows preliminary levelized costs and GHG emissions for the eight pathways analyzed. The lowest-cost pathways are distributed reforming of natural gas and central natural gas reformation with gaseous H_2 truck delivery. These pathways result in lower WTW GHG emissions than those achieved with conventional gasoline or hybrid electric vehicles.

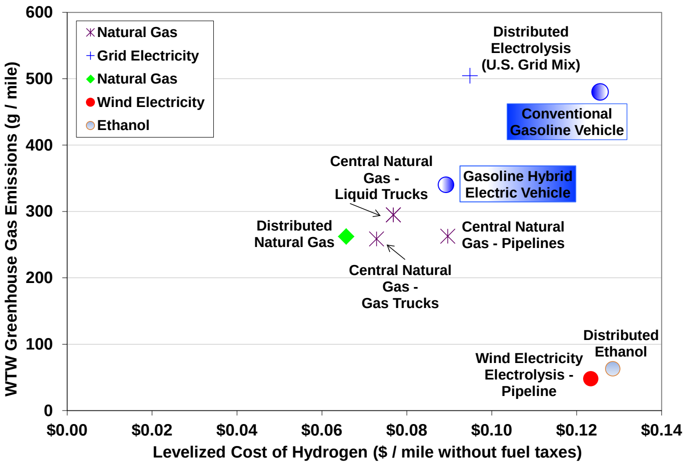

Figure 1. Preliminary WTW results comparing H_2 levelized cost (including cost of infrastructure) and GHG emissions for eight advanced-technology hydrogen pathways (based on a 58 miles per kilogram H_2 fuel economy).

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[1] See Ramsden, T.; Ruth, M.; Diakov, V.; Laffen, M.; Timbario, T. A. (2013). Hydrogen Pathways: Updated Cost, Well-to-Wheels Energy Use, and Emissions for the Current Technology Status of Ten Hydrogen Production, Delivery, and Distribution Scenarios. National Renewable Energy Laboratory, Golden, CO.

[2] The analysis uses a version of DOE's Hydrogen Macro-System Model that incorporates the latest component models as of September 2013: H2A Version 3 (2012), HDSAM Version 2.3 (2012), GREET 1 (2012) and GREET 2 (2012).

2013 U.S. DRIVE Highlight

Hydrogen Station Dispensing Pressure Analysis

Assessment of potential customer future interest in intermediate fueling pressure between 350 bar and 700 bar.

Fuel Pathway Integration Technical Team

Vehicle manufacturers are adopting 700 bar (70 megapascal/10,000 pounds per square inch (psi)) compressed hydrogen (H_2) storage tank technology to achieve greater than 300 mile range in a fuel cell electric vehicle (FCEV). The U.S. Department of Energy's (DOE) activities, such as tank cost reduction, are consistent with enabling FCEV rollout with 700 bar tanks. DOE is assessing long term options, such as materials that could store H_2 at lower pressures than 700 bar. Dispensing H_2 at 700 bar incurs higher station compression, storage, energy, and operations and maintenance costs compared to lower pressures, which increases the fuel cost to the consumer. A methodology was developed to evaluate the tradeoffs between consumer refueling convenience (i.e., fewer trips to the station) and H_2 cost.

Argonne National Laboratory calculated H_2 station cost information by using the Hydrogen Delivery Scenario Analysis Model. The methodology was applied to H_2 refueling station pressures of 350, 500, and 700 bar to determine the trade-offs between H_2 cost at the pump and consumer convenience based on travel time and number of trips to the station. While higher H_2 storage pressures result in longer vehicle ranges, they also result in higher cost. Therefore, an intermediate fueling pressure of 500 bar could simultaneously satisfy the criteria of drive range and affordability.

The preliminary analysis resulted in the following side-by-side comparisons of the three fueling pressures of interest: 1) 700 versus 350: a 700 bar dispensing pressure is more valuable than 350 bar to consumers with trip times (to a station) exceeding 10 minutes and when consumers value their time greater than \$20 per hour; 2) 350 versus 500: there is minimal incentive or value for the consumer to fuel at the lower 350 bar pressure; 3) 500 versus 700: a 500 bar dispensing pressure is more favorable than 700 bar when trip times to the station are less than 10 minutes and consumers value their time at less than \$30 per hour, as illustrated in Figure 1.

Future analysis will include the cost of pre-cooling for the various fueling pressure levels.

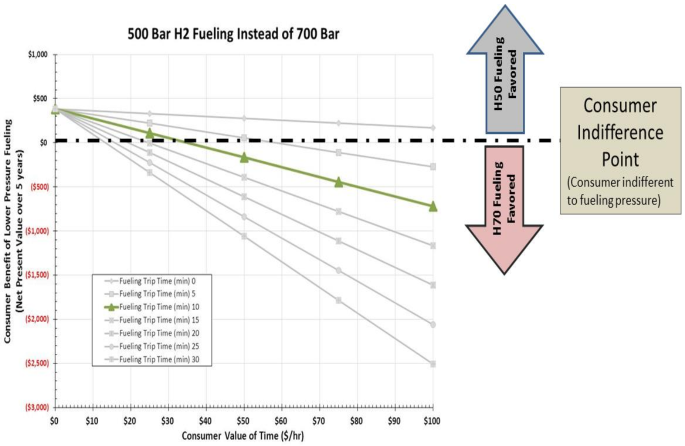

Figure 1. Preliminary analysis suggests that 700 bar fueling is favored over 500 bar fueling when time to the station exceeds 10 minutes and the consumers value their time greater than \$30 per hour.

Hydrogen Delivery

2013 U.S. DRIVE Highlight

World's First Oil-free Centrifugal Hydrogen Compressor

Successful single-stage prototype operation at 60,000 revolutions per minute proves feasibility.

Mohawk Innovative Technologies, Inc.

Mohawk Innovative Technologies, Inc. successfully completed the initial validation testing of a single-stage prototype compressor operating at 60,000 revolutions per minute (RPM) (see Figure 1). This technology is critical to enabling hydrogen (H_2) pipeline delivery for high-volume markets.

Pipeline delivery of H_2 for fuel cell electric vehicles presents particular challenges, including concerns regarding leakage and embrittlement because of the small size of the hydrogen molecule. Another challenge is that oil, which is commonly used to lubricate the high speed centrifugal compressors used for pipeline compression, can leak into the H_2 gas stream and contaminate it.

Natural gas centrifugal compressors typically operate at less than 2,000 RPM. Increasing the operating speed to 60,000 RPM required the use of two 100 kilowatt motors coupled together in order to achieve the desired speed, as well as detailed engineering of the compressor blades and dynamic seals to withstand the speed at which they would operate. The engineering of the blade took into careful consideration material choice. A beta titanium alloy was chosen to provide the strength needed to perform at tip speeds of 488 meters per second and resistance to hydrogen embrittlement.

Mohawk Innovative Technologies, Inc. developed a coupling technology that enabled the synchronized operation of the two motors – both proven thermally and dynamically stable in independent evaluations – in order to drive the compressor blades at speeds 30 times greater than what is typical for this type of compressor. The compressor includes a dual-entry design that significantly decreases differential pressure the seals must contain. The design is flexible, allowing 6-9 stages of compression to provide a range of delivery flow rates from 240,000-500,000 kilograms per day (kg/day) at compression ratios of 2.4 to 3.3. The compressor is designed for inlet pressures of 300-500 pounds per square inch gage (psig) and outlet pressures of 1,200–1,500 psig.

The completed fabrication and validation stage demonstrates notable progress in developing a domestically-manufactured compression technology that is up to four times smaller and twice as efficient as existing, single-entry gas compression technology. In addition to the great promise embodied by this development, this gearless single-stage H_2 compressor is also the world's first oil-free, internally gas-cooled, direct-drive compressor with no transmission or gearbox. Overall, this technology has significant potential to achieve cost reduction and reliability improvement in H_2 pipeline transport technology.

Figure 1. The operation of the single-stage centrifugal compressor in the new test chamber at 60,000 rpm.

Hydrogen Production

2013 U.S. DRIVE Highlight

Hydrogen Cost from Polymer Electrolyte Membrane Electrolysis Updated

New analysis highlights potential for forecourt and centralized hydrogen production via polymer electrolyte membrane electrolysis.

Strategic Analysis, Inc.

Improved cost projections ranging from $4-$5/kilogram (kg) of hydrogen (H_2) are now available for H_2 production from polymer electrolyte membrane (PEM) electrolysis. Using the newly-updated Hydrogen Production Analysis Model Version 3, researchers prepared case studies[1] of costs for H_2 production through PEM water splitting based on well-vetted assumptions and input from electrolyzer manufacturers. PEM electrolysis technologies have made significant recent progress, resulting in commercially-available products. These new case study results will guide research and development efforts to further the goals[2] of low-cost H_2 production.

Strategic Analysis, Inc. and the National Renewable Energy Laboratory prepared the studies with four electrolyzer manufacturers providing input and vetting the results. Analysis evaluated four cases: current (~2012) and future (2025) for both forecourt (1-5 metric tons H_2 per day) and centralized (100-500 metric tons H_2 per day) plants. Stack, balance-of-plant, indirect, replacement, decommissioning, operating and maintenance, and feedstock costs were evaluated.

Sensitivity analysis around the ~$5.10/kg base-line for the current forecourt case is shown in Figure 1; similar trends were found for the central production cases. The price of electricity is the major driver of production cost. A ~50% increase from $0.061 to $0.092 per kilowatt hour (kWh) results in an increase of over $1.50/kg of H_2. Tied closely to electricity price is electricity usage, which is driven by electrolyzer efficiency. This highlights the importance of achieving the U.S. Department of Energy's (DOE) electrolyzer system efficiency target of 75%, as higher efficiency requires less electricity.

Reductions in capital cost, electricity usage, and site preparation cost as well as increases in replacement interval were assumed for the future cases. These effects, combined, show the potential to reduce forecourt H_2 production cost from ~$5.10/kg to ~$4.20/kg (untaxed production cost only without compression, storage, and delivery costs). Further improvements in efficiency, capital cost decreases, and significant reductions in electricity price will be needed to reach DOE's long-term targets of <$2/kg H_2 produced. Still, in regions with electricity prices low, PEM electrolysis could be a viable regional solution for low cost H_2 production in the near term.

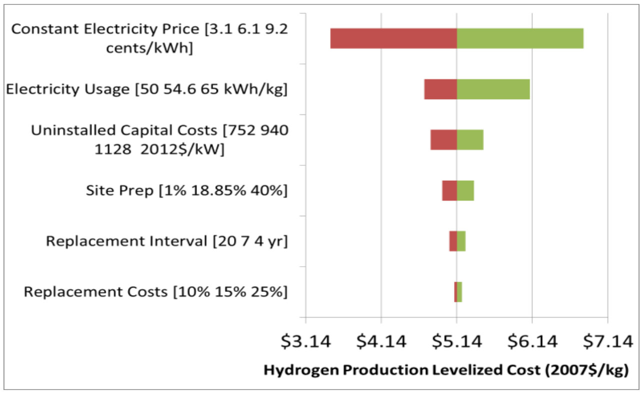

Figure 1. Sensitivity analysis for the current forecourt case, with a baseline H_2 cost of ~$5.10/kg, showed the dominant factor in H_2 cost is the price of electricity, followed by electricity usage.

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[1] http://www.hydrogen.energy.gov/h2a_prod_studies.html

[2] U.S. DOE, Fuel Cell Technologies Office. (2013). Multi-Year Research, Development, and Demonstration Plan. (Tables 3.1.4 and 3.1.5). http://www1.eere.energy.gov/hydrogenandfuelcells/mypp/pdfs/production.pdf

2013 U.S. DRIVE Highlight

Efficient Hydrogen Production through Isothermal Hercynite Cycle Water Splitting

Novel approach shows potential for significant increases in hydrogen production relative to state-of-the-art temperature swing processes.

University of Colorado-Boulder

Laboratory results have demonstrated a new process with the potential to increase direct solar-driven hydrogen (H_2) production from water. Solar-thermochemical hydrogen (STCH) production offers a long-term pathway (2025 or beyond) to high volume H_2 from water and sunlight.

Two-step, metal oxide-based STCH cycles typically generate H_2 through sequential high-temperature (~1300–1600°C) chemical reduction and lower-temperature (~1000-1200°C) water re-oxidation of a metal oxide, with oxygen (O_2) produced during the reduction step and H_2 during the oxidation step. The temperature swings between the reduction and oxidation steps have an efficiency penalty due to radiative heat losses, and the need to repeatedly heat and cool the active material and transfer heat between solids. This also raises a concern about thermal fatigue of the active materials and the reactor itself.

Researchers at the University of Colorado-Boulder have demonstrated that isothermal operation of the hercynite STCH cycle at 1350°C exhibits H_2 production capacity more than three times that of the temperature swing operation of the hercynite cycle and more than 12 times that of the temperature swing operation of the ceria cycle (see Table 1). Isothermal operation can be optimized through control of the partial pressure of the oxidizing gas, rather than temperature swings, to produce the chemical potential differences which drive the reactions.

Isothermal operation has additional advantages, such as reduced irreversible heat loss and decreased thermal shock, both of which limit efficiency and operations of traditional temperature swing water splitting cycles. In addition, isothermal operation has the potential for faster cycle times and increased system lifetimes due to reduced thermal fatigue.

The hercynite cycle chemistry occurs via a reaction between and within spinel phases of $FeAl_2O_4$ (hercynite). During the O_2 production step, Fe_3+ reduces to Fe_2+, and during re-oxidation by H_2O (water), Fe_3+ re-forms, and H_2 is produced.

The team is designing a solar receiver and solids flow reactor process along with a lower-cost and compatible feed preparation system, which may lead to industrial scale-up.

Future work will also focus on evaluating the active material at higher temperatures, improving the reaction stoichiometry, developing reaction kinetics models, updating the solar reactor model, and completing a discounted cash flow analysis for H_2 cost from an isothermal plant.

Process Conditions	**H_2 Production (μmol H_2/g of active material)**
Hercynite Isothermal (1350°C)	217 ± 38
Hercynite Temperature Swing (1350/1000°C)	66.8 ± 4.9
Ceria Temperature Swing (1350/1000°C)	16.4 ± 3.6

Table 1. Laboratory test results showing the increased H_2 production from hercynite under isothermal water splitting conditions, relative to temperature swing water splitting of both hercynite and ceria.