

# FreedomCAR & Fuel Partnership



DAIMLERCHRYSLER



GM General Motors



DEPARTMENT OF ENERGY

USCAR  
UNITED STATES COUNCIL FOR AUTOMOTIVE RESEARCH



ConocoPhillips

ExxonMobil



Shell Hydrogen

## FreedomCAR and Fuel Partnership

2006

## Highlights of Technical Accomplishments

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## Preface

This report contains brief summaries of key technical accomplishments of the FreedomCAR and Fuel Partnership program for 2006. This program was initiated in 2002 as the FreedomCAR Partnership between the United States Department of Energy (DOE) and the United States Council for Automotive Research (USCAR), the latter being a legal partnership comprising DaimlerChrysler Corporation, Ford Motor Company and General Motors Corporation. In his 2003 State of the Union address, President George W. Bush announced a national Hydrogen Initiative. In response to this, the FreedomCAR Partnership was expanded in September 2003 to include five energy companies (BP America, Chevron Corporation, ConocoPhillips, ExxonMobil Corporation and Shell Hydrogen LLC (US)) and became the FreedomCAR and Fuel Partnership.

The accomplishments described in this report support the overall FreedomCAR and Fuel Partnership goals and the progress being made. These goals are the “Freedoms” originally embraced by the FreedomCAR Partnership:

- Freedom from dependence on imported oil;
- Freedom from pollutant emissions;
- Freedom for Americans to choose the kind of vehicle they want to drive, and to drive where they want, when they want; and
- Freedom to obtain fuel affordably and conveniently.

Previous annual reports are available on the FreedomCAR and Fuel Partnership page on the USCAR website at [www.uscar.org](http://www.uscar.org).

The material for the 2006 Highlights of Technical Accomplishments Report was selected from the many hundreds of projects now active and put into the form of single page accounts, arranged by subject matter corresponding to the various technical teams formed by the partnership. The various Technical Teams are listed below:

### Vehicle Technical Teams (Members from the USCAR partners and DOE)

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

### Joint Technical Teams (Members from the USCAR partners, the energy partners and DOE)

- Codes and Standards
- Onboard Hydrogen Storage

Energy Technical Teams (Members from the energy partners and DOE)

- Hydrogen Production
- Hydrogen Delivery
- Fuel Pathway Integration

An accomplishment from the DOE Hydrogen Analysis Resource Center (HyARC) has also been included in this report because the data generated by this project are used by several of the technical teams to prioritize their research endeavors.

Each of the accomplishments summarized in this report was selected by the relevant technical team as representing a significant milestone reached, or breakthrough made, in 2006. It represents achievements in work that may well have begun in previous years but does not necessarily indicate that the final goals of a particular project have yet been met.

## *2006 FreedomCAR and Fuel Partnership Highlight*

### *Model of 3D Diesel Particulate Filter Shows Location Where Soot Collects*

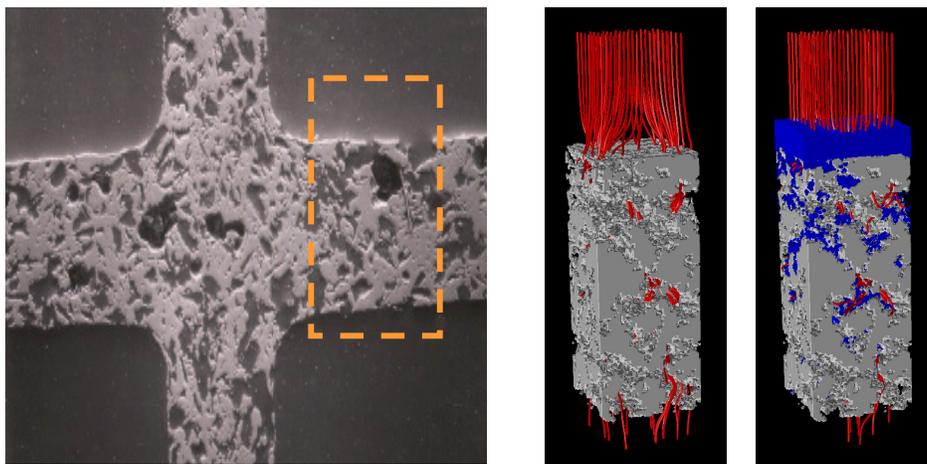
**Pacific Northwest National Lab**

Diesel engines produce particulate material which can be removed by a diesel particulate filter (DPF). A computer model was developed for exhaust gas flow and soot collection in a DPF. The model focuses on the porous microstructure of the DPF and how exhaust gas and soot flow through it.

The three-dimensional model of the wall was constructed from two-dimensional images of the porous wall obtained by scanning electron microscopy. Different wall materials have different porosities and microstructures. Calculated exhaust flow through the wall matched experimental data for pressure drop. Pore size and connectivity affected the pressure drop.

Soot collection was modeled with a discrete particle simulation through the porous structure. The location and thickness of the collected soot as a function of time was calculated. The model indicates that initially most soot collected in the porous wall structure at a depth of 0.1 to 0.2 mm depending on porosity. For longer filtering times, most soot collected on the surface of the wall as a layer with increasing thickness.

These results predict where soot collects in the DPF as a function of design parameters (porosity, wall thickness) and filtering time. Knowing where soot collects for different wall porosity enables better location of the catalyst.



Electron microscope image of porous wall separating flow channels in a DPF. Exhaust gas flows through one channel, through the wall, and into the adjacent channel (left). Calculated flow streamlines (red) in a clean wall section (center). Calculated flow streamlines and collected soot (blue) in a wall section with soot loading.

## *2006 FreedomCAR and Fuel Partnership Highlight*

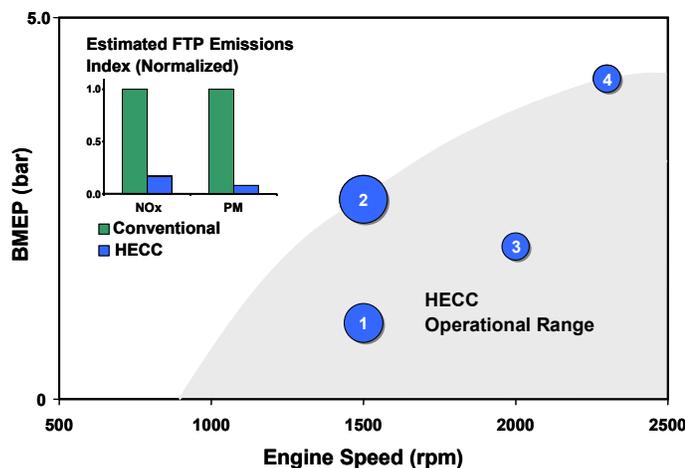
# *High-Efficiency, Low-Emission Combustion Achieved at Modal Test Conditions Relevant for Small-Car FTP*

**Oak Ridge National Lab**

An objective of combustion R&D is to achieve high-efficiency clean combustion (HECC) over a wide engine-operating range. A modified four-cylinder, direct-injection diesel engine was operated in HECC modes over four of the key steady-state points identified as representative of the light-duty Federal Test Procedure (FTP) for a small car. Engine adjustments included increased EGR, higher fuel-rail pressure, and optimized fuel injection timing. A weighted sum of the engine emissions at the steady-state evaluation conditions was used to estimate the FTP emissions. This procedure does not include transient and cold-start effects included in an actual FTP cycle.

The experimental results indicate that in this combustion mode both NO<sub>x</sub> and PM emissions are reduced by over 85%. The researchers constrained the HECC combustion mode to have no less efficiency than conventional combustion, so no impact on the fuel consumption was observed. However, CO and hydrocarbon emissions increased because of the use of elevated levels of EGR, but not enough to affect fuel consumption.

These results demonstrate that improvements in the combustion process reduce the NO<sub>x</sub> and PM emissions. Lower engine-out emissions reduce the aftertreatment performance requirements and regeneration frequency.



Four non-idle test conditions used in FTP simulation of a small car and normalized cycle-weighted emissions for NO<sub>x</sub> and PM for both conventional and high-efficiency modes.

HECC= High-Efficiency Clean Combustion

## *2006 FreedomCAR and Fuel Partnership Highlight*

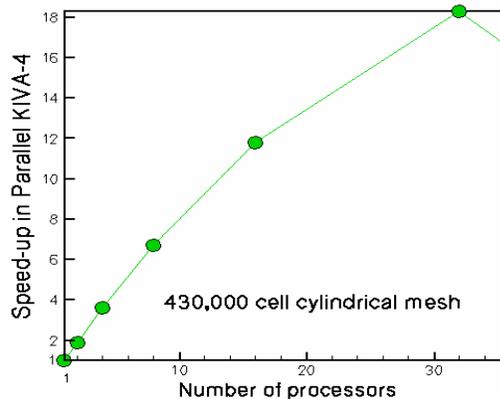
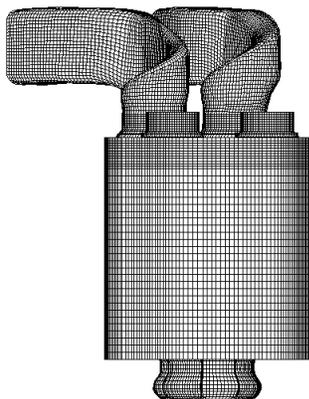
### *KIVA Enhanced for Faster Computations and HCCI Combustion*

**Los Alamos and Lawrence Livermore National Labs**

Combustion modeling is an important tool for understanding and improving the efficiency of gasoline and diesel engines. KIVA is a computer code used for high-resolution calculation of three-dimensional gas flow and combustion in engines with realistic geometry. The code consists of a grid structure that represents the geometry, solution algorithms for the gas flow through the grid elements, and models for fuel injection and combustion. Significant improvements in the code were made in 2006. The geometry representation improved by accommodating not only structured meshes but also unstructured meshes (which are easier to construct). Air-flow modeling improved by validating algebraic stress turbulence models against experimental laser velocity data. A fuel spray model based on x-ray analysis of fuel sprays improved combustion. Finally, conversion of the code to a parallel-processor version reduced execution time by up to a factor of 18 (assuming 32 processors for a 430,000 cell grid).

Modeling of HCCI (homogeneous charge compression ignition) combustion further increases the complexity and time requirement for calculations since now both air flow and chemical kinetics must be simulated. A model for ignition and combustion of complex fuels was developed that only increased the computational time by only 10%. This model calculates the ignition in each cell from the local temperature, pressure, fuel-to-air ratio, and amount of exhaust gas recirculation.

Due to improved and validated sub-models and faster execution, KIVA has become a standard code for engine simulation. The code is used by automobile companies, national labs, and universities.



Three-dimensional representation of engine geometry used in KIVA calculations (left). A parallel-processor version of KIVA reduced calculation time by a factor of 1 to 18 depending on the number of processors used (right).

## *2006 FreedomCAR and Fuel Partnership Highlight*

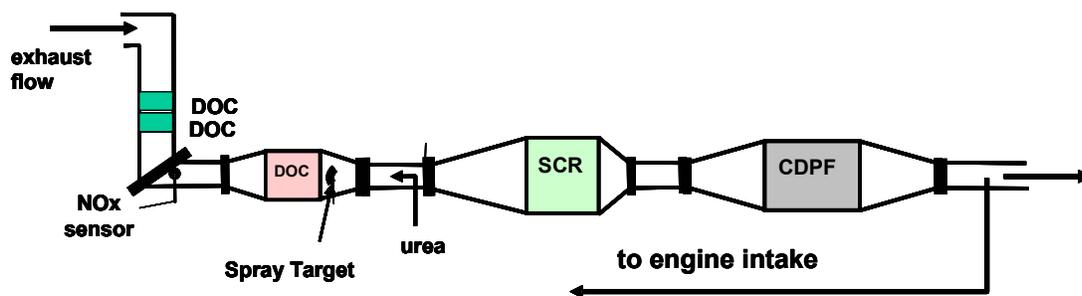
# *Durability of a DOC-Urea SCR-DPF System for a Light-Duty Truck Studied for 120,000 Miles*

**Ford Motor Company, ExxonMobil, FEV**

Aftertreatment may be necessary to comply with exhaust emission regulations. An experimental aftertreatment system for a 6,000-pound light-duty truck with a diesel engine was studied on the cold-start Federal Test Procedure (FTP-75) for light-duty vehicles. To obtain more information about performance for extended operations, a total of 120,000 miles were accumulated on an engine dynamometer using a transient durability cycle that incorporated both city and highway driving modes. The aftertreatment system consisted of a diesel oxidation catalyst (DOC), a urea selective catalytic reduction (SCR) converter to reduce NO<sub>x</sub>, and a catalyzed diesel particulate filter (CDPF). Engine-out NO<sub>x</sub> was reduced by approximately 40% through increased exhaust gas recirculation. The aftertreatment system further reduced the engine-out NO<sub>x</sub> by approximately 80-90%. The control strategy included a rapid warm-up of the aftertreatment system following the engine start, transient urea injection control, and automated CDPF regenerations. Aqueous urea injection was optimized using an air-assisted injection system in conjunction with a spray target.

A total of 643 CDPF regenerations occurred during the 120,000 mile testing. The system achieved Tier 2 Bin 5 emission standards for all components except NO<sub>x</sub> (0.128 g/mi vs. 0.07 g/mi standard). NO<sub>x</sub> conversion was affected mainly by lack of a reliable warm-up strategy during cold-start due to issues with the prototype nature of the engine. Also noted was some deactivation of the DOC and SCR catalysts as predicted by laboratory aging. The CDPF performance did not noticeably change. A new SCR catalyst material was lab aged and tested on the vehicle with the engine-aged DOC. Results were favorable for meeting Tier 2 Bin 5 without a warm-up strategy (0.08 g/mi).

These tests show that the tested aftertreatment system has the potential to achieve the Tier 2 emission requirements for light-duty trucks. Issues for future improvement of the aftertreatment system were identified.



Schematic of aftertreatment system tested

# 2006 FreedomCAR and Fuel Partnership Highlight

## DC/DC Converter for Fuel Cell and Hybrid Vehicles

Ballard Power Systems / Oak Ridge National Laboratory

Fuel cell and hybrid vehicles have onboard high voltage, 200-400 Volts (V), power available from fuel cells and/or batteries. In order to supply power to low voltage vehicle auxiliary loads a DC/DC converter is needed to convert high voltages to low voltages (typically 10-16V).

This project demonstrated the functionality of a 5 kW DC/DC converter which meets FreedomCAR and Fuel Partnership goals of 92% efficiency, 5L volume and 6kg weight. Ballard has identified a plan for further cost reduction. The converter used new planar magnetics which integrated the windings into the Double Bonded Copper, which was then soldered to the base plate. This resulted in enhancing the converter cooling and power density. Figure 1 shows the design of the novel interleaved DC/DC converter topology providing low power loss, smaller magnetics and low EMI. A converter with 92% efficiency (higher than that of a conventional converter, typically 90% efficient) having 60% reduced package size and weight was built, Figure 2, and successfully tested at 105°C coolant inlet temperature.

Figure 1: The interleaved DC/DC converter topology

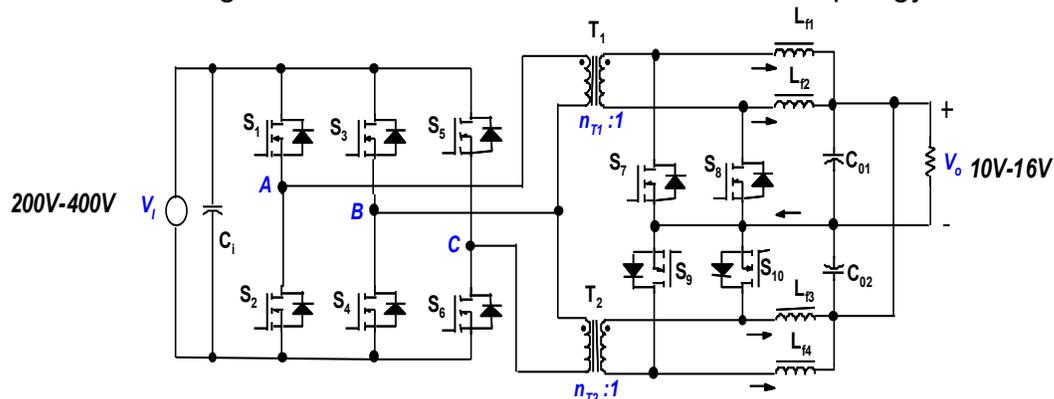
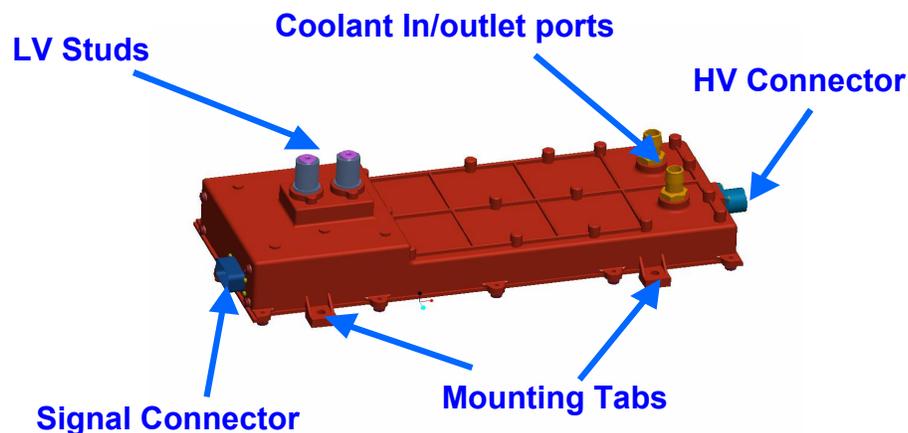


Figure 2: DC/DC converter



# 2006 FreedomCAR and Fuel Partnership Highlight

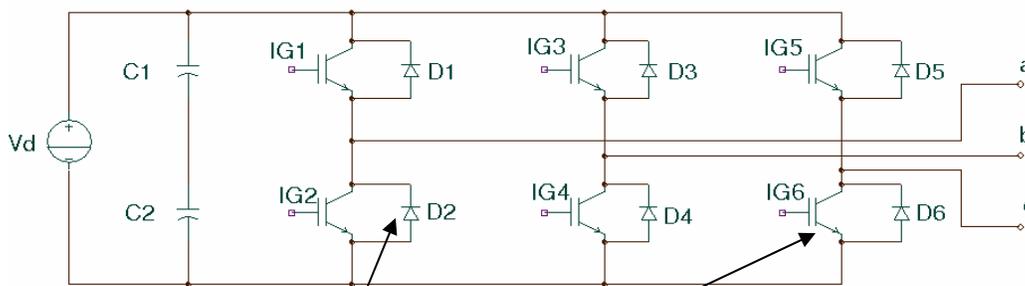
## Silicon-Silicon Carbide Hybrid Inverter

Oak Ridge National Laboratory

Inverters are used to convert DC to AC to drive AC motors in hybrid and fuel cell electric vehicles. To meet FreedomCAR and Fuel Partnership goals, inverters with higher efficiency, power density and operational temperatures are needed. Presently inverters use silicon(Si) transistors(IGBTs) and Si diodes. The efficiency of these inverters can be improved by using Silicon Carbide(SiC) devices, such as SiC Schottky diodes. These diodes can operate at higher temperatures and can reduce reverse recovery losses in the inverter.

This project demonstrated the feasibility of hybrid inverter (using conventional Si IGBTs and SiC Schottky diodes) with higher efficiency. A 30kW (continuous) hybrid inverter was built and tested. The schematic representation of a hybrid inverter is shown in Figure 1. Figure 2 shows a comparison of typical peak power output versus efficiency curves of an all Si (conventional) with the hybrid inverter. The hybrid inverter showed a 20% decrease in inverter losses. This confirms the directional progress toward the goal to increase power density and operating temperatures.

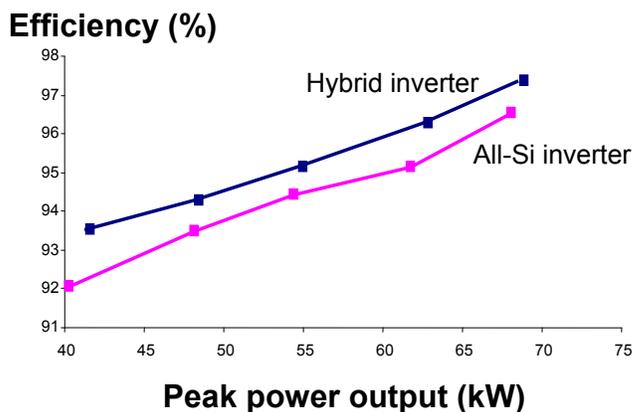
Figure 1: Inverter topology



SiC Schottky Diodes (D1, D2, D3, D4, D5, D6)

Si Switches (IG1, IG2, IG3, IG4, IG5, IG6)

Figure 2: Comparison of peak-power vs. efficiency of hybrid and Si inverter



## 2006 FreedomCAR and Fuel Partnership Highlight

### New High-Power Cell Chemistry Identified

Argonne National Laboratory

As part of DOE's Advanced Technology Development activity, Argonne National Laboratory evaluates low-cost advanced cell materials and components that offer enhanced stability in lithium-ion (Li-Ion) batteries. The enhanced stability of these materials should aid in simultaneously achieving longer life and enhanced inherent abuse tolerance, which are two key barriers for Li-Ion batteries to become commercially viable for HEV applications.

During the last year, Argonne studied the use of nano-phase lithium titanate ( $\text{Li}_4\text{Ti}_5\text{O}_{12}$ ) as a replacement for carbonaceous anode materials. Argonne coupled the titanate anode with a lithium manganese spinel ( $\text{LiMn}_2\text{O}_4$ ) cathode, which possesses excellent high-rate capabilities, due to its 3-dimensional structure. However, when used with conventional graphite or carbon anodes, cells suffer rather rapid power loss when operated at elevated temperatures, due to  $\text{Mn}^{2+}$  dissolution from the cathode, which reduces at the anode to form metallic manganese. The metallic manganese is believed to play a catalytic role in the formation of a resistive film on the graphite anode. Use of the titanate anode circumvents this problem, because it is poised at 1.5 volts above metallic lithium, where the  $\text{Mn}^{2+}$  is not reduced to  $\text{Mn}^0$ . Argonne evaluated several commercially-available lithium titanate materials and then developed a process for making a more optimal nano-phase material (shown below). Cells employing these materials exhibit extremely high rate capabilities. They can be completely discharged in about 1 minute, as shown below. This titanate cell also possesses many other attractive characteristics for the HEV application:

- Low cost relative to synthetic graphite
- Limited surface reactivity with the electrolyte for extended life & enhanced inherent abuse tolerance
- No structural or volume changes during cycling (no structural stress)
- No plating of lithium during high-rate regenerative braking at low temperature

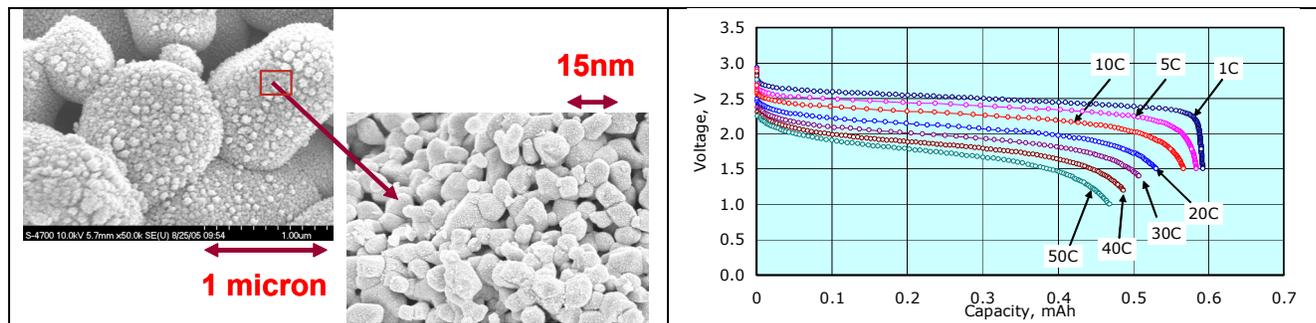


Figure 1: Cells incorporating Argonne's nano-phase lithium titanate material exhibit extremely high rate capability when coupled with lithium manganese spinel cathode.

# 2006 FreedomCAR and Fuel Partnership Highlight

## Gap Analysis Software Developed Battery Design Studio<sup>®</sup>

Software was developed that quickly evaluates how well a battery technology meets United States Advanced Battery Consortium (USABC) goals and generates a detailed analysis of the performance. This software standardizes the Gap Analysis reporting procedures for USABC battery developers. The software uses physics-based models to make performance estimates of next-generation systems. The standardized interface developed under this program provides a means for battery developers to collaborate more easily with researchers in national labs and universities. The software has been provided to the battery developers with USABC contracts.

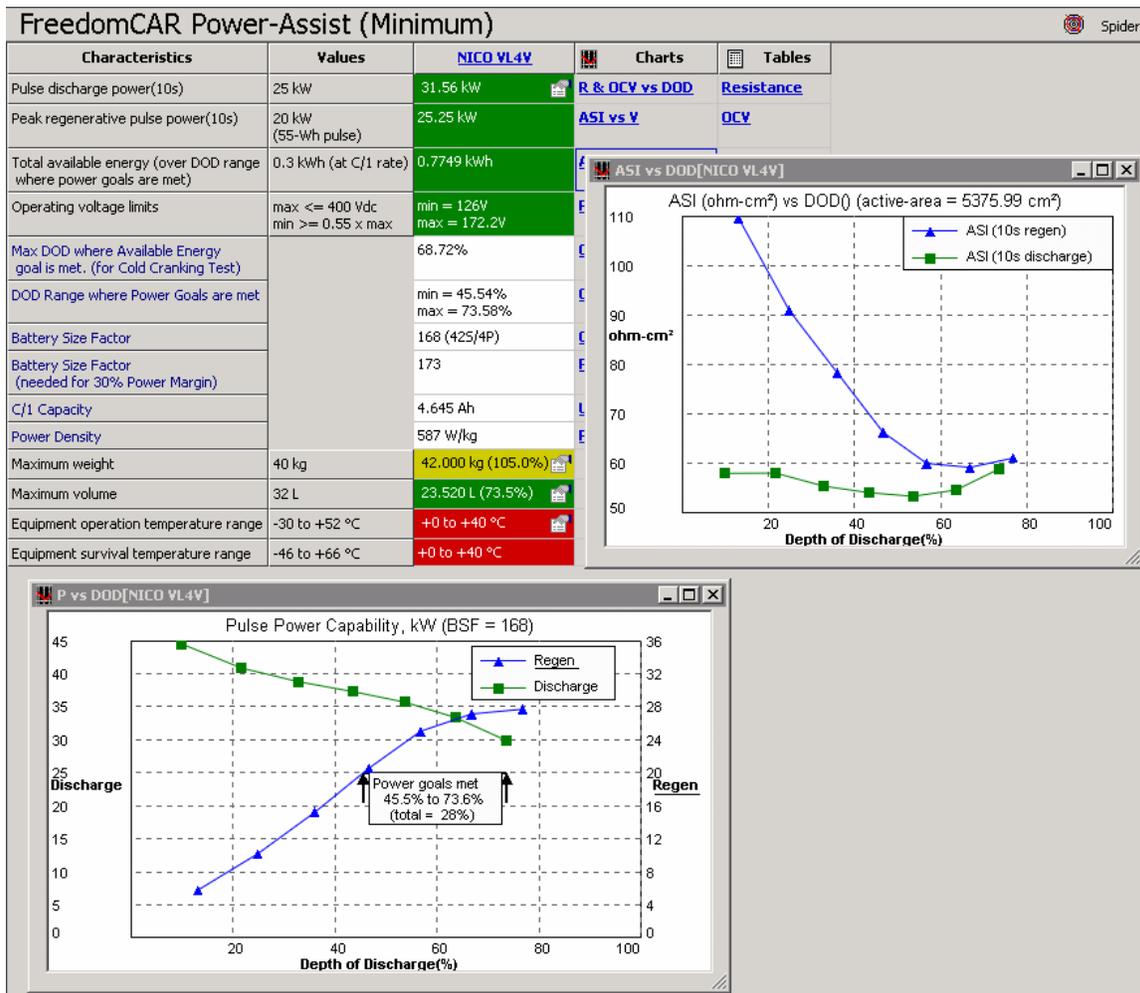


Figure 1: Example of Report from Gap Analysis Software

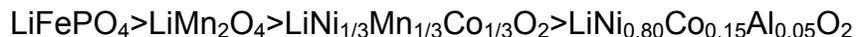
# 2006 FreedomCAR and Fuel Partnership Highlight

## Li-Ion Cells with Enhanced Abuse Tolerance

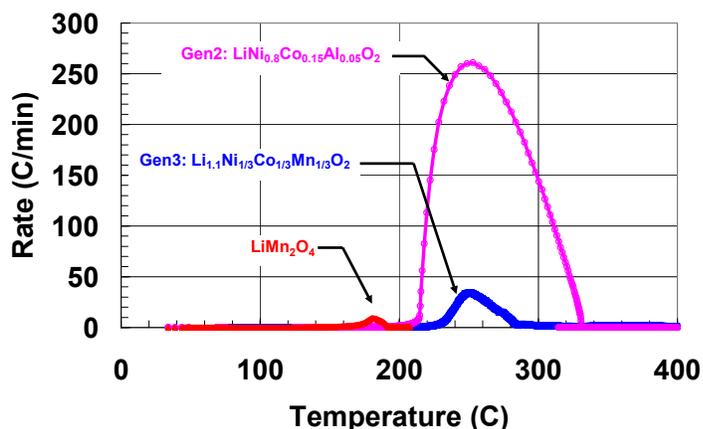
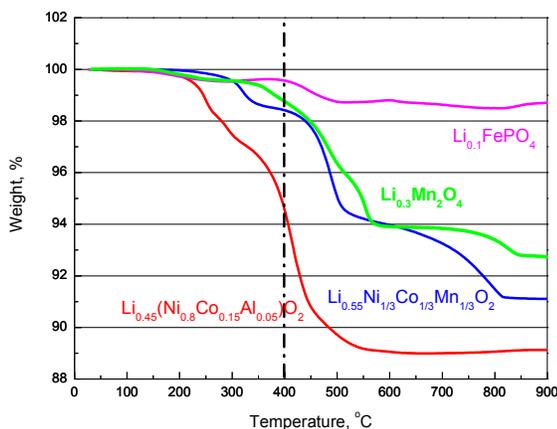
Argonne National Laboratory & Sandia National Laboratory

As part of DOE's Advanced Technology Development activity, Argonne National Laboratory and Sandia National Laboratory are working together to improve the abuse tolerance of high-power Li-Ion cells. They are collaborating to understand the factors that limit the inherent abuse tolerance of high-power Li-Ion cells and then identifying/developing more stable cell materials and components that enhance the inherent abuse tolerance characteristics of these cells. Argonne identifies and develops more stable cell materials and component, while Sandia verifies and quantifies the effect of these materials at the cell level, using 18650 cells.

During the last year, Argonne demonstrated that the release of oxygen, due the thermal decomposition of the cathode active material, is proportional to the quantity of heat generated by reactions between these delithiated cathode materials and the electrolyte (via differential scanning calorimetry) and that this was the dominant heat generating reaction during a thermal event. This result was validated at the cell level by accelerated rate calorimetry (ARC) and thermal block tests that were conducted by Sandia on 18650 cells. Shown below are the comparative weight loss data obtained by Argonne (via thermal gravimetric analysis) on different types of delithiated cathode materials, as well as Sandia's ARC data on 18650 cells that incorporate three of these different cathode materials. It can be seen that the quantity of oxygen released by the different cathode materials (below 400°C) directly correlates to the quantity of internal heat generation in cells that employ these cathode materials. The relative thermal stability of delithiated cathode materials is:



The conclusion of this work is that the inherent thermal abuse tolerance of Li-Ion cells can be significantly enhanced by the use of a cathode material based on  $\text{LiFePO}_4$  that releases little or no oxygen during thermal excursions to temperatures  $>180^\circ\text{C}$ .



# *2006 FreedomCAR and Fuel Partnership Highlight*

## *Performance Enhancements and Cost Reduction*

**NessCap Co., Ltd.**

NessCap Co., Ltd. has made significant performance enhancements and cost reductions in ultracapacitors designed for the 42-V start-stop architecture specified by the United States Advanced Battery Consortium (USABC).

Ultracapacitors are electrochemical energy storage devices that bridge the gap between conventional capacitors and batteries. They can store much more charge than can the former and deliver (discharge) and absorbing (charge) energy in a short time; typically in seconds, as opposed to minutes or hours for batteries. Further, ultracapacitors exhibit far longer lifetimes than do batteries. However, the energy density is typically only 5% or less than that of a battery. Ultracapacitors are therefore often preferred over batteries for applications that require only high power (rather than high energy density) but more development is necessary for wide adoption in the automotive industry, especially in passenger cars.

NessCap Co., Ltd. has made significant improvement in energy density and cost reduction as shown in Table 1. Indeed, cost has been cut by two-thirds, which brings the cost of these ultracapacitors down to \$180 per 6kW pack, compared to the cost goal of \$80 per 6kW pack. These advancements were made possible by a new electrode formulation and packaging technology.

	<b>Change (Sept. 2005 to Sept. 2006)</b>
<b>Gravimetric Energy Density</b>	<b>37.7% improvement</b>
<b>Volumetric Energy Density</b>	<b>27.9% improvement</b>
<b>Cost</b>	<b>66.7% reduction</b>

**Table 1: NessCap Ultracapacitor Accomplishments**



# 2006 FreedomCAR and Fuel Partnership Highlight

## Calendar Life/Cell Performance Improved

### Compact Power/LG Chem

Battery life (both total cycles and calendar life), low temperature performance, and cost are major challenges for most Li-Ion based hybrid electric vehicle (HEV) batteries. Compact Power/LG Chem (CPI/LGC) delivered a cell design that exceeded the FreedomCAR goal of 300,000 cycles (presently the cell is at 400,000 cycles). CPI/LGC has also developed a patent-pending abuse tolerant separator that will further improve the performance of this cell design.

The CPI/LGC cell (Li Ion with a Mn – Spinel cathode material) has excellent cycle life, is abuse tolerant, and offers great potential for lower cost when compared to available alternatives. By suitably modifying the cell chemistry and incorporating a proprietary separator, the system has the potential to meet the calendar life and performance goals without sacrificing abuse tolerance.

The beneficial effects of the proposed cell chemistry on prolonging calendar-life continue to be proven in long-term storage tests. Based on the results from cells aged more than 1 year, CPI predicts an average calendar life of 10-years for G4.1 & G4.1.1 chemistries using a curve fitting method to explain power fade. Based on the G4.1 results and comparing them to the most recent data for the new chemistry (G4.1.1 below), CPI/LGC expects to meet the 15-year target with the new chemistry.

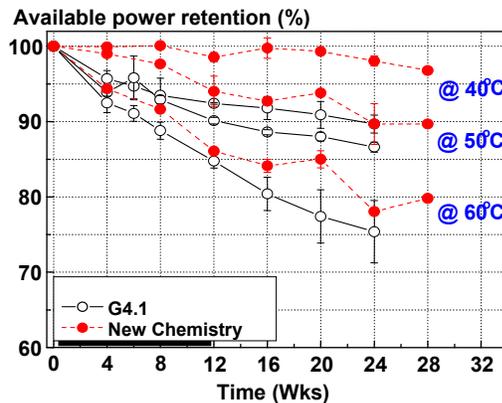


Figure 1: Calendar Life Improvement  
The new chemistry (G4.1.1) results in significant improvement @ 40°C in terms of available power retention.

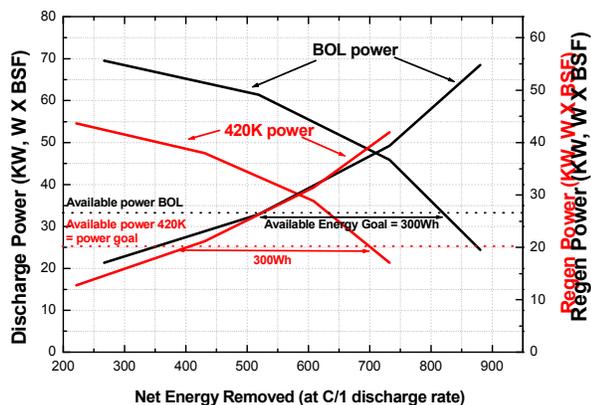


Figure 2: Energy vs. Power for G4.0 @ BOL & EOL (420,000 cycles). G4.1 & 4.1.1 tests in process are trending similarly or better than G4.0.

## 2006 FreedomCAR and Fuel Partnership Highlight

# Identified Method to Recover Fuel Cell Performance Loss Caused by Sulfur Poisoning

Los Alamos National Laboratory

Efficient fuel cell operation relies on the availability of both high-purity fuel and air. It has been shown that the activity of the electrode catalysts and the proton conductivity of the ionomer are very sensitive to the presence of certain impurities. Typical fuel impurities are carbon monoxide, ammonia, and hydrogen sulfide ( $H_2S$ ). On the cathode side, ambient air contains pollutants (e.g., nitrogen oxides and sulfur dioxide) that also degrade fuel cell power output. This project focuses on assessing the severity of the impurity effects, understanding the degradation mechanism(s) and finding ways to mitigate their negative effects on performance.

Prior work had shown that effects of sulfur poisoning are not reversed by subsequent exposure to clean reactants. The current work, however, indicates that fuel cell power output can be partially recovered from sulfur poisoning by cycling to open circuit voltage (OCV). Anode recovery is aided further by exposing the anode to air. The figure below shows almost complete recovery after exposure to 1 ppm  $H_2S$  from cycling to OCV and exposure to air. Further research is needed to verify these findings at the stack level. This valuable information can be used to help develop strategies to minimize and recover from performance loss due to sulfur present in the fuel, and can enable the use of fuels with higher sulfur levels.

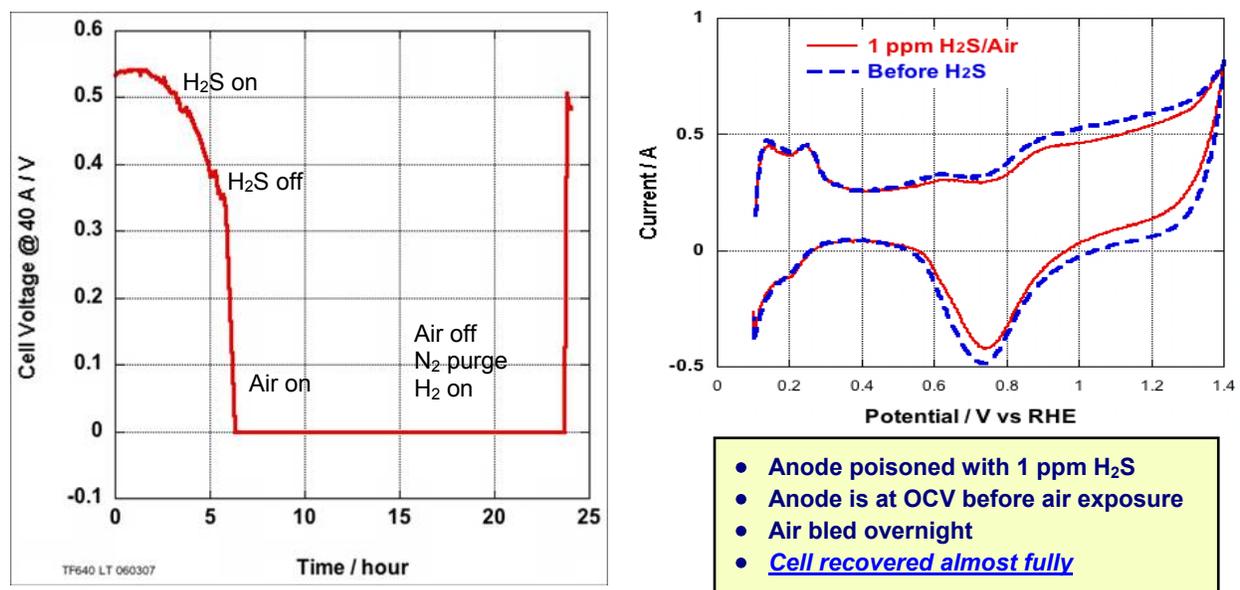


Figure 1: Air Effect on Anode Due To Shut-down

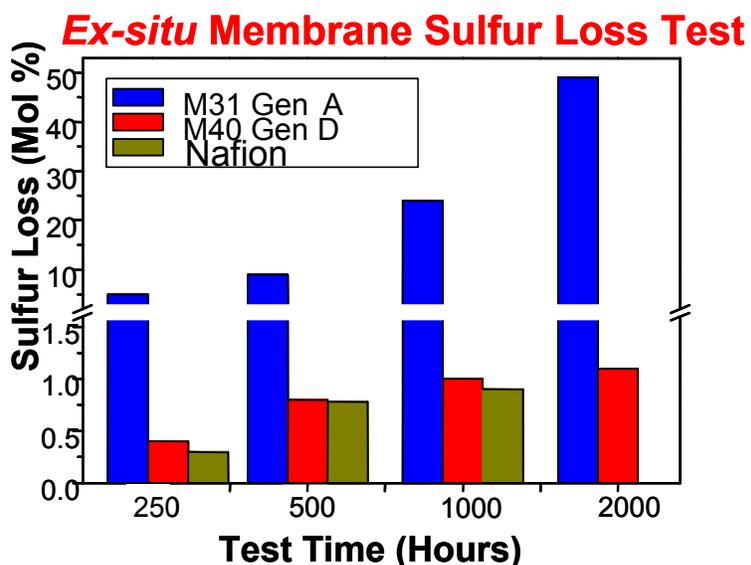
## 2006 FreedomCAR and Fuel Partnership Highlight

### Durability of Low Cost Membrane is Improved

Arkema

Although fuel cells have the potential to play a major role in future automobiles, cost and durability issues pose major challenges to widespread adoption. Perfluorinated, proton-conductive membranes have been the most widely used polymer membrane materials in low temperature fuel cells such as polymer electrolyte membrane fuel cells (PEMFCs). Substantial efforts have been made to reduce the high cost of PEMFCs. One methodology being explored to achieve this goal utilizes fluorinated polymers that are cost-effective, such as Kynar<sup>®</sup> PVDF. Arkema has sought to create a low-cost, proton-conductive, mechanically-stable membrane by combining a proprietary polyelectrolyte with Kynar<sup>®</sup>. They also have developed a flexible manufacturing process for fabricating this membrane. Arkema was able to show initial in-cell performance equivalent to that of conventional perfluorosulfonic acid (PFSA) membranes. Their durability, however, was poor. Although the membrane did not suffer from as much fluorine loss as observed for PFSA, it did suffer from loss of sulfonic acid groups as measured by a decrease in sulfur content in the membrane.

After identifying the degradation mechanism, Arkema successfully produced membranes that addressed the deficiency while maintaining conductivity. The vulnerable linkage to the sulfonic group in the polyelectrolyte was eliminated. A chemical stability test of the membrane showed that M31 (the membrane that demonstrated the original degradation) lost 50% of its sulfur over 2000 hours, while M40 (the improved membrane) lost only 1% over the same time. Unlike the M31 generation, subsequent single cell studies showed that M40 was able to maintain approximately the same voltage performance after 24 hours at 80°C and 100% RH. This performance remains even after a 2 hour excursion to higher temperatures (120°C). Although membrane-electrode assemblies (MEAs) with M40 have not yet been optimized for performance, their voltages were similar to those measured for MEAs containing the baseline Nafion 112. These preliminary results are encouraging but further research is needed: first, to establish MEA durability when operated under an automotive drive cycle and, then, to evaluate durability in a fuel cell stack.



## *2006 FreedomCAR and Fuel Partnership Highlight*

# *Improved Platinum Alloy Catalyst Activity Could Dramatically Reduce Fuel Cell Cost*

**Lawrence Berkeley National Laboratory**

A four-fold reduction of platinum (Pt) loading in the air electrodes of fuel cells constitutes a necessary step towards reducing fuel cell cost to the levels required for mass-produced vehicles. Pt alloys supported in the conventional manner as small metal particles on high surface carbon (C) have twice the activity of pure Pt similarly supported on carbon, only half of the needed improvement. In the past few years, it has been shown that a thin film of Pt has about 10-fold higher activity per surface atom than small particle Pt/C. LBNL has now shown that the hexagonally-closest packed (111) crystal face of the Pt-nickel alloy Pt<sub>3</sub>Ni gives about an additional 10-fold increase in activity, thereby demonstrating an overall 90-fold improvement per surface Pt atom vs. conventional Pt/C. With this extremely high specific activity, only a very small area of Pt<sub>3</sub>Ni (111) surfaces (<3 m<sup>2</sup>/g<sub>Pt</sub>) would be needed to exceed the target of a four-fold activity increase per gram of Pt. The lower surface area form of Pt alloy should be more durable against the effects of varying loads in stressful automotive operating cycles.

While these experiments were performed on idealized surfaces of large single crystals, the results point a way to the synthesis of durable, high-activity supported catalysts through the control of which faces of alloy particles are exposed. Further research is needed to demonstrate these results in a membrane electrode assembly. This new way of optimizing catalysts could deliver fuel cell oxygen reduction catalysts with costs low enough for automotive mass production.

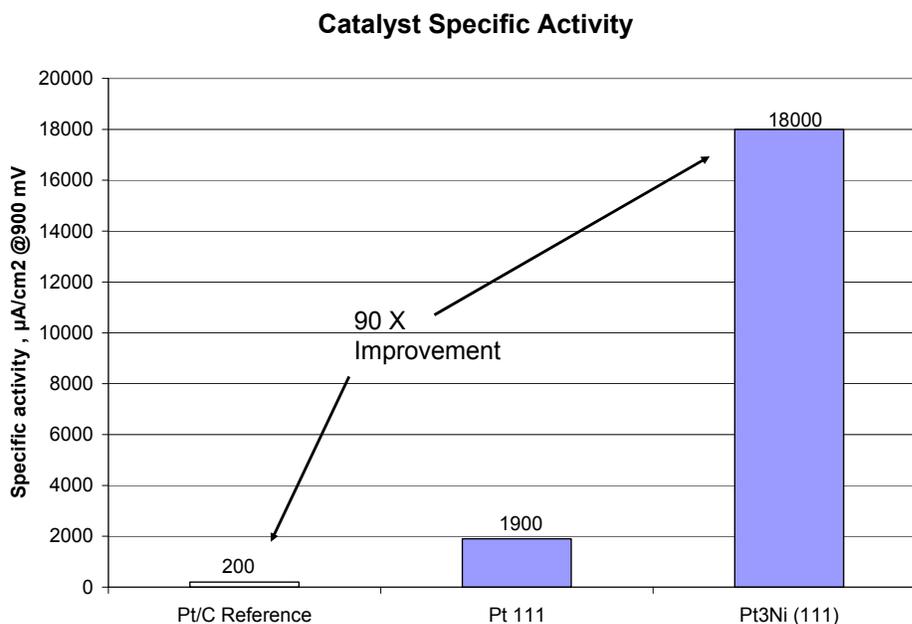


Figure 1: Platinum and Platinum Alloy Specific Activity

## 2006 FreedomCAR and Fuel Partnership Highlight

### *A Platinum Catalyst Degradation Mechanism is Identified*

Argonne National Laboratory

One of the challenges facing the development of polymer electrolyte membrane fuel cells (PEMFCs) is the durability of the fuel cell materials. PEMFC performance loss has been attributed in part to oxidation and dissolution of the platinum (Pt) cathode electrocatalyst. Dissolution may be prevalent during potential cycling typical of varying load conditions, and also during holds at high potentials typical of idling in the automotive application. This project seeks to determine the mechanisms and rates of loss of Pt and Pt alloy electrocatalysts under conditions relevant to the automotive application. The data from this study can be used to predict electrocatalyst lifetimes and to define conditions that accelerate or mitigate catalyst degradation.

Without cycling, the behavior of bulk platinum (Pt) and platinum/carbon (Pt/C) electrodes was consistent with Pt dissolution concurrent with oxide layer formation. At potentials of 1.1 V and 1.0 V, for Pt wire and Pt/C, respectively, the oxide formed a protective film, inhibiting further Pt dissolution. At potentials  $>1.2$  V, which can be encountered during start-up and shut-down procedures, the concentration of dissolved Pt increased further for the Pt/C electrode, most likely due to concurrent corrosion of the carbon support. Cycling accelerated dissolution of Pt at potentials of 1.0 V and higher. This indicates that formation and reduction of the oxide film are responsible for the increased degradation rates of fuel cell electrodes under potential cycling conditions. Cycling the PEMFC between potentials typical of open circuit conditions ( $\sim 1$  V) and potentials typical of load conditions should be minimized in order to mitigate cycling-related acceleration of Pt dissolution. This knowledge is a significant contribution to the understanding of catalyst performance loss. It will be used to develop catalysts that are tolerant to this type of degradation and also will be used by systems integrators to avoid conditions that produce these mechanisms.

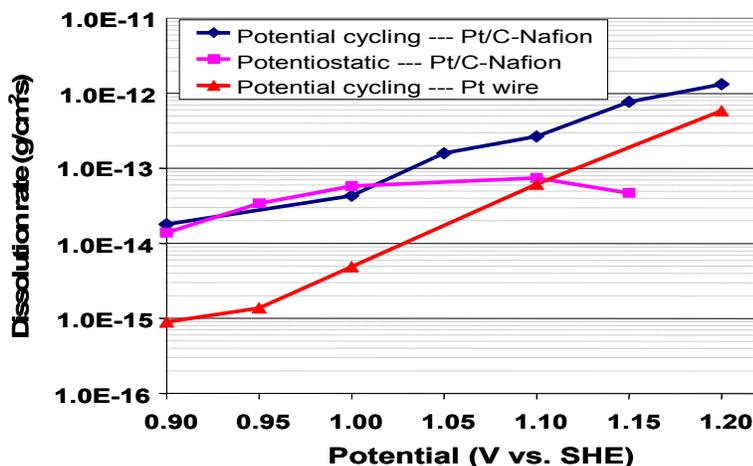


Figure 1: Effect of potential and potential cycling on Pt dissolution rate

## 2006 FreedomCAR and Fuel Partnership Highlight

### *New Membrane Demonstrates Improved Durability with No Loss in Performance*

**DuPont with University of Southern Mississippi**

DuPont has developed a new membrane that has demonstrated extended life under automotive fuel cell operating conditions. The new membrane, which has recently been marketed by DuPont as Nafion® XL™, combines advanced chemical stabilization to improve the membrane's oxidative stability in the presence of peroxide radicals and a mechanical reinforcement. As shown in Figure 1, the new membrane provides over a 10-fold increase in membrane life over the baseline 1 mil cast Nafion® NRE211 and at least a 5-fold improvement over a membrane with only mechanical reinforcement. Furthermore, there is dramatic improvement in lifetime over last year's version of a reinforced, chemically stabilized membrane.

The new chemical stabilization demonstrated a 30-fold lower fluoride emission rate (FER) in open circuit voltage (OCV) testing compared to the baseline Nafion® NRE211, and over a 10-fold improvement from the 2005 chemically stabilized membrane. The improved mechanical strength gained by the addition of the reinforcement is demonstrated by a 50% reduction in swelling compared to Nafion® NRE211 and a 50% increase in tensile strength. These results have been accomplished while maintaining the same voltage performance as the Nafion® NRE211 membrane.

The Nafion® XL™ membrane also lasted for 3500 hours in an automotive drive cycle test. Further testing is needed to validate the 3500 hour durability in a vehicle, and to explore the potential for the membrane to reach the 2015 durability target of 5000 hours at temperatures up to 120°C.

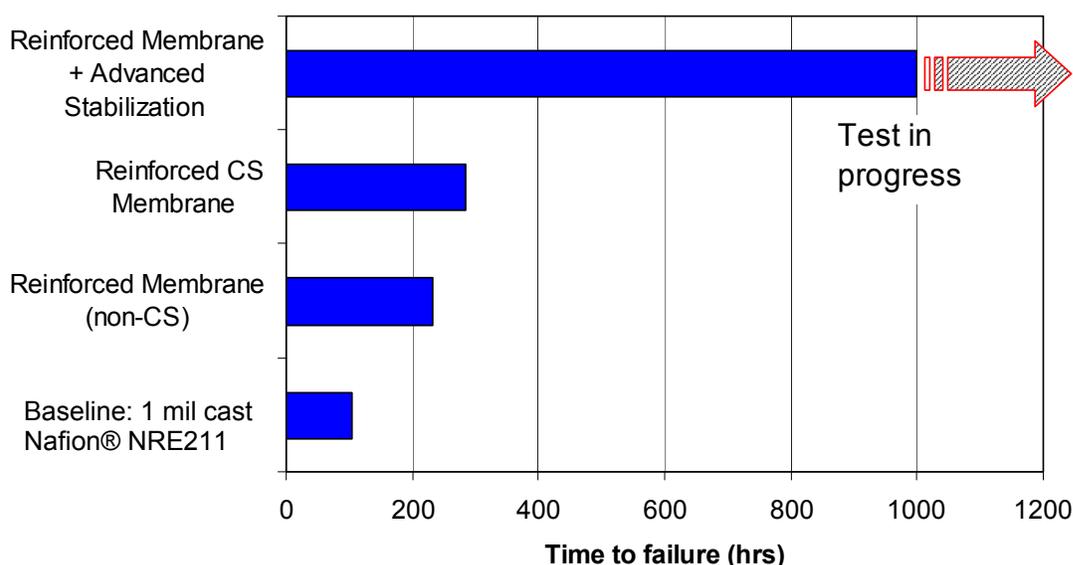


Figure 1: Accelerated durability test results: combined humidity cycling and load operation of DuPont membranes

## 2006 FreedomCAR and Fuel Partnership Highlight

# Increasing Hydrogen Storage in Metal Organic Frameworks

UCLA / University of Michigan / UC Berkeley

Storing hydrogen by physical adsorption is attractive because the uptake and release of hydrogen is fast, and the energy required to release hydrogen is relatively low - typically near 2.5kJ/g H<sub>2</sub>. Subsidiary benefits are a reduced heat transfer requirement, because less heat is being moved, and the potential to use low cost materials such as carbon. These advantages have been offset by the low amount of hydrogen stored on a mass or volume basis. Until now, typical physical adsorption methods held less than 4% by weight hydrogen in the storage media above 77°K, with estimates of roughly half that much storage for a complete tank.

Recently, many groups have explored hydrogen storage in a family of engineered materials called metal organic frameworks, or MOFs. MOFs have extraordinarily high surface areas, so at cryogenic temperatures they could adsorb a significant amount of hydrogen. There are two goals to storage work in this area, increasing the amount of hydrogen stored, and operation at less extreme temperatures.

In the last year several groups have reported improved hydrogen storage. A record achieved this year is more than 7 weight % at 77°K (on a material basis). The volumetric storage has also increased from less than 25 to near 35g/L. While neither value meets the current *system* targets, this is rapid progress in an area with room for much more discovery. MOFs with even higher surface area have been proposed, with the possibility of even higher hydrogen storage.

The heat of adsorption has been improved as well, increasing from ~2.5kJ/g hydrogen, to 6kJ/g of hydrogen. This has been accomplished by altering the chemistry of the materials used to construct the MOF. This higher binding energy is a required step toward room temperature operation.

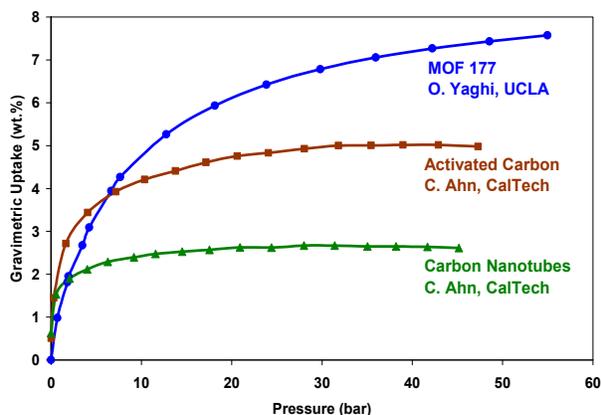


Figure 1: New engineered materials such as MOF177 by O. Yaghi (UCLA) adsorb significant amounts of hydrogen at 77°K.

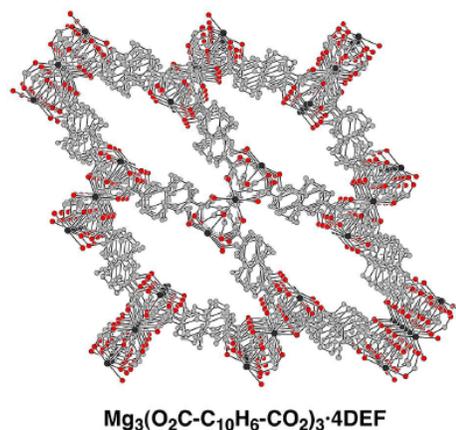


Figure 2: Example of material developed by J. Long, UC Berkeley

## 2006 FreedomCAR and Fuel Partnership Highlight

# Predicting the Thermodynamics of Complex Hydrogen Storage Mixtures via Atomistic Modeling

UCLA

The importance of modeling and simulation has grown dramatically in virtually all areas of science and engineering during the past several decades. Recent FreedomCAR & Fuel Partnership efforts aimed at developing high-density hydrogen storage materials for mobile applications have likewise benefited from a strong connection to computational modeling. Since the thermodynamics of hydrogen storage are governed by atomic-scale phenomena (e.g., bonding), state-of-the-art atomistic simulation methods are a valuable tool in screening for new materials with promising characteristics, thereby guiding subsequent experimental efforts.

By combining two computational techniques, researchers at UCLA have developed a new methodology for predicting the thermodynamics of complex, multi-component hydride systems. In the first phase of this approach, the free energies of all relevant solid and gaseous compounds are determined using highly-accurate first-principles calculations. The energies are then fed into a linear programming routine that determines phase fractions as a function of temperature and pressure. This work is noteworthy because it can predict the temperatures and compositions at which thermodynamically reversible hydrogen storage reactions will occur in complex multicomponent systems where experimental phase diagrams are not available. The method can therefore pinpoint the compositions which show the greatest promise for further experimental study. Initial testing on the quaternary Li-Mg-N-H system have shown good agreement with experiments (see Figure 1), and new work on the quinary Li-Mg-B-N-H system is in progress.

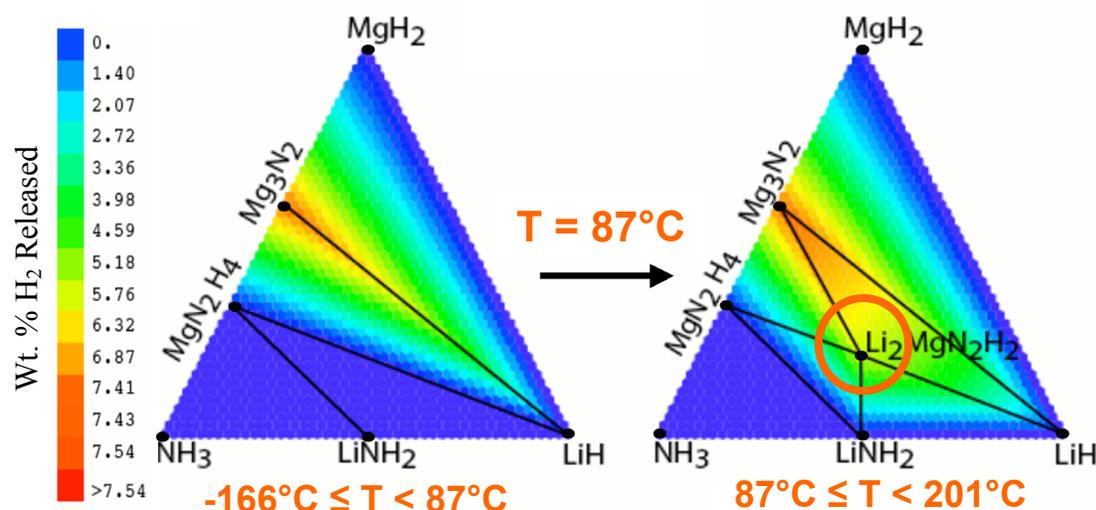


Figure 1: Calculated phase diagrams and weight percent hydrogen released for the reaction  $2 \text{LiH} + \text{Mg}(\text{NH}_2)_2 \rightarrow \text{Li}_2\text{Mg}(\text{NH})_2 + 2 \text{H}_2$  at  $T = 87^{\circ}\text{C}$  in the quaternary Li-Mg-N-H system. The appearance of the  $\text{Li}_2\text{Mg}(\text{NH})_2$  phase within the yellow-shaded region in the right diagram (circled) indicates that 5.6 wt.% hydrogen will be released at those compositions.

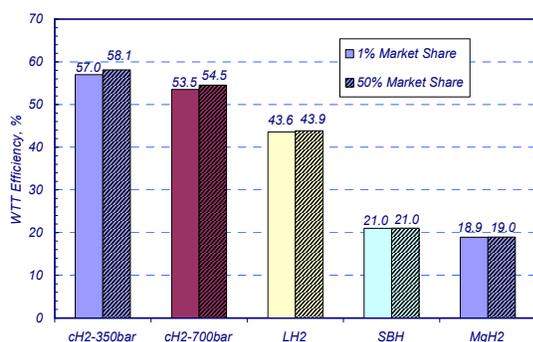
# 2006 FreedomCAR and Fuel Partnership Highlight

## Hydrogen Storage Systems Analysis Argonne National Laboratory and TIAX

Automobiles are commonly designed to have driving ranges of more than 300 miles whatever the fuel. In the case of hydrogen, finding suitable materials that can store sufficient hydrogen to provide such a range is a major challenge. Each different class of material will probably require its own unique system configuration when used in a vehicular fuel tank and it is necessary to understand these differences in order to design an optimal fuel storage system. A viable storage system will satisfy not only the targets for weight, volume and cost but also the constraints such as minimum delivery pressure of hydrogen, minimum full flow rate of hydrogen and refueling time. It is important to determine the performance of the overall storage system as opposed to the performance of the storage material alone.

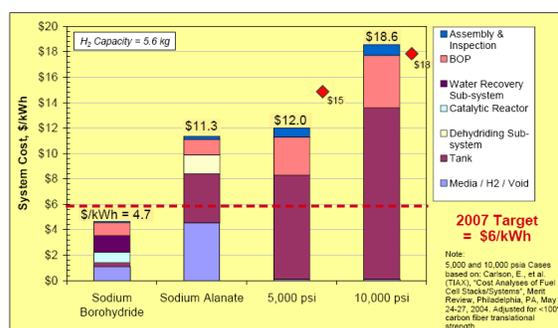
Argonne National Laboratory has developed a modeling tool to guide scientists in evaluating the performance of their materials at an early stage of development and in identifying specific properties with the largest impact on storage system performance. Argonne has used this approach to determine the material capacity and thermal conductivity that sorbents must have in order to satisfy 2010 and 2015 targets for volumetric and gravimetric capacity of the overall system. For materials that require off-board regeneration, Argonne has developed a modeling tool to estimate the effect of the energy consumed in regeneration on the overall hydrogen storage and fuel cycle efficiencies. To complement Argonne's systems analyses efforts, TIAX is focusing on cost analyses and has estimated the costs of sodium borohydride, sodium alanate and gaseous hydrogen storage systems.

These system analysis studies have provided important information on the performance expected from materials currently under study. They also have provided insight into subsystem and component characteristics needed to minimize system weight, volume and cost and help guide the down-selection of various materials and storage concepts.



Preliminary fuel cycle efficiencies (ANL)

Note: Fuel cycle efficiencies are slightly dependent on market penetration due to hydrogen delivery options.



Estimated costs of storage systems (TIAX)

# 2006 FreedomCAR and Fuel Partnership Highlight

## 2<sup>nd</sup> Generation Cryo Compressed H<sub>2</sub> Tank

Lawrence Livermore National Lab

Lawrence Livermore National lab has completed construction and has initiated testing of a second generation cryo compressed hydrogen storage vessel. This vessel provides the user with a “dual fuel” option of filling with either gaseous (5,000 psi) or liquid hydrogen depending on customer requirements for driving range. The second generation vessel has an improved gravimetric and volumetric hydrogen storage capacity due to design improvements such as insulation thickness and packaging.

A recent Argonne National Laboratory assessment of the new tank design determined that a hydrogen gravimetric capacity of 4.7 weight % and volumetric capacity of 0.030 kg/L is feasible using the LLNL approach.

Some other potential advantages that this technology offers include:

- Greatly extended dormancy ~5-10x longer than traditional liquid H<sub>2</sub> tanks
- Potentially lower pressure vessel cost (2-3x less fiber for given capacity)
- The approach is potentially adaptable for solid state storage materials (e.g., carbon)
- The hydrogen storage capacity of the second generation tank is clearly approaching the 2007 interim system targets of 4.5 weight % and 0.036 kg/L.

Future work will include performance testing on board a vehicle. A preliminary cost study is also underway.

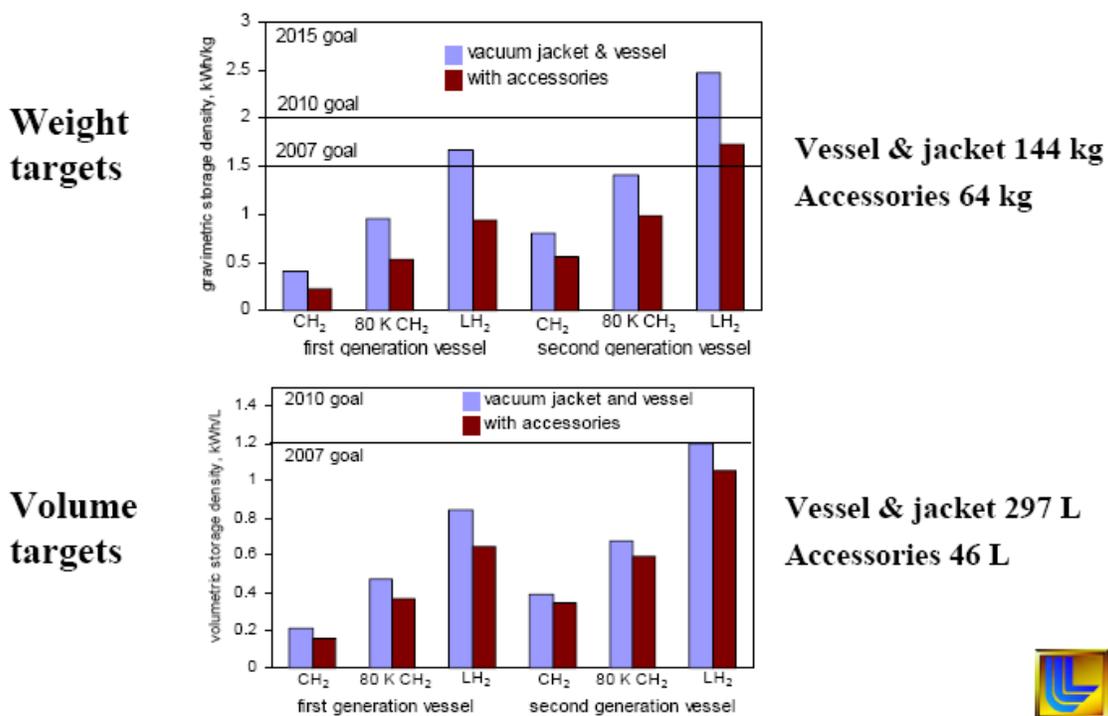


Figure 1: Weight and volume estimates for first and second generation tanks

## 2006 FreedomCAR and Fuel Partnership Highlight

### Improved Hydrogen Release from High-Density Chemical Hydride, $\text{NH}_3\text{BH}_3$

University of Pennsylvania

Efficient on-board storage of hydrogen ( $\text{H}_2$ ) requires a system that: a) provides hydrogen at high densities by volume and weight, b) allows removal of the  $\text{H}_2$  with modest or no energy input, and c) uses a simple, low-cost method to recharge the material back to its original state. Ammonia borane,  $\text{NH}_3\text{BH}_3$ , is one emerging hydrogen storage material candidate that has recently received a great deal of attention due to its high hydrogen content (approximately 18 weight % on a material basis). Unfortunately, it releases hydrogen slowly and it is very difficult to replace the hydrogen to re-form ammonia borane.

Researchers at the University of Pennsylvania (in conjunction with the DOE Chemical Hydrogen Storage Center of Excellence) have recently demonstrated several methods to improve the rate (or lower the temperatures) of  $\text{H}_2$  release from this material. Specifically, chemical additives, ionic liquids and/or metal catalysts were shown to increase the rate and extent of hydrogen release from ammonia borane and several systems have been identified that have the potential to meet system targets. The addition of lithium amide,  $\text{LiNH}_2$ , to ammonia borane yields a mixture that liberates 6.9 weight %- $\text{H}_2$  in 6 hours and 9.3 weight %- $\text{H}_2$  in 15 hours at  $85^\circ\text{C}$ , making this one of the best chemical hydrogen release systems that has been reported to date.

In order to utilize  $\text{NH}_3\text{BH}_3$  as an on-board storage technology, more research is still required. The highest priority is to develop a practical method to regenerate the spent material back into  $\text{NH}_3\text{BH}_3$ . Finally, the infrastructure implications of a solid-state hydride storage option, that is not rechargeable on-board the vehicle, need to be evaluated.

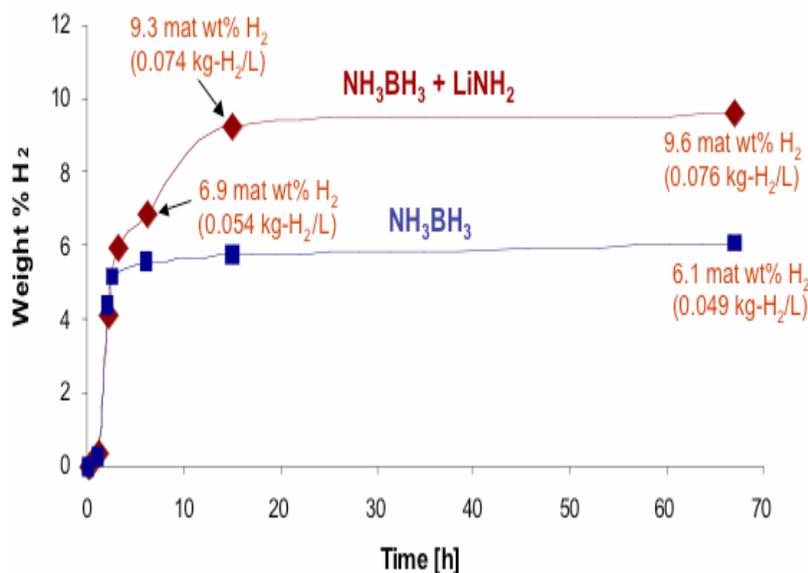


Figure 1: Dehydrogenation of ammonia borane at  $85^\circ\text{C}$  versus a reaction with added lithium amide. For the pure ammonia borane reactions, the hydrogen release is slow, and incomplete. In contrast, ammonia borane mixtures containing 10 mol% of  $\text{LiNH}_2$  showed both faster rates and more extensive hydrogen release.

# 2006 FreedomCAR and Fuel Partnership Highlight

## Auto/Steel Partnership Future Generation Passenger Compartment

### USAMP – ASP240

The Future Generation Passenger Compartment project demonstrated more than a 30 percent mass savings of the passenger compartment at cost parity relative to a typical 2005 baseline four-door five-passenger sedan. This was accomplished by the intensive use of Advanced High-Strength Steels (AHSS) combined with state-of-the-art design optimization and manufacturing approaches. The design solution improved performance for the new Insurance Institute for Highway Safety (IIHS) side impact test and proposed Federal Motor Vehicle Safety Standards (FMVSS) side pole impact and 2.5X roof strength requirements while maintaining performance in static and dynamic stiffness, durability, and front and rear crash. The design solution was determined to be robust to both the IIHS side impact bumper height variations and vehicle weight increases. Also, manufacturing feasibility evaluations assessed the solution to be acceptable for high volume manufacturing.

The project scope included additional objectives to expand learnings. The packaging study comprehended both conventional and fuel cell powertrain requirements. Crash analysis identified that the worst case loading scenario for the IIHS side impact test was controlled by the internal combustion engine variant and not the fuel cell variant. Project results indicate that if steel grades with tensile strengths of 1600 MPa can be developed that meet the manufacturing forming requirements, mass savings could improve by an additional six to eight percent. Mass compounding effects are expected to enable even further mass reduction.

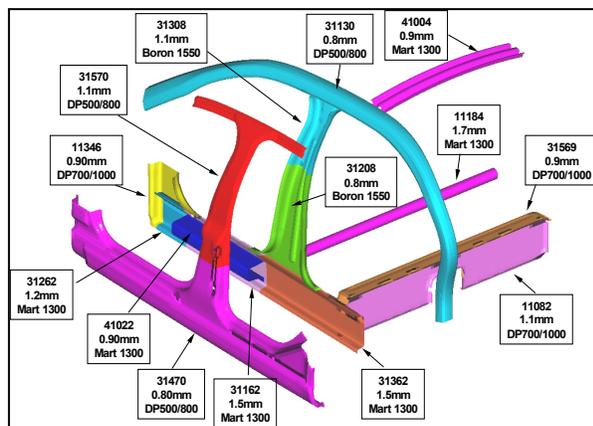


Figure 1: Optimized Advanced High Strength Steel Solution

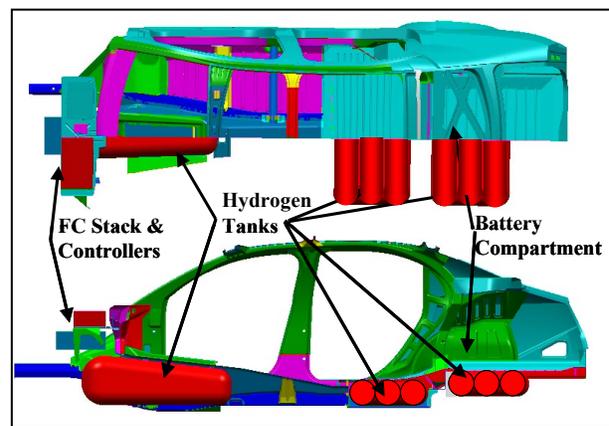


Figure 2: Fuel Cell Powertrain Components Comprehended

## *2006 FreedomCAR and Fuel Partnership Highlight*

### *Composite Intensive Body Structure (ACC Focal Project III)*

**USAMP - ACC-080**

Although carbon fiber composites offer light-weighting potential, current manufacturing processes use slow autoclave or resin infusion molding processes. Successful automotive implementation requires the development of a rapid, low cost fabrication technology, such as the liquid molding of dry fiber preforms. The process must be able to form the geometries required to provide the strength and stiffness necessary to achieve significant mass savings.

The Automotive Composites Consortium (ACC) FP3 team has successfully developed and demonstrated such a rapid molding process, the P4 preforming process, for carbon fiber composites. With this process, a robotically controlled chopper gun directs fiber and binder onto a forming tool to produce a preform in the shape of the part to be molded (Fig. 1). This preform is then placed into the composite molding tool.

The ACC optimized the SRIM process for molding these preforms into the final composite panels which were then bonded together (Fig. 2) into the final structure. This is an important enabler for a carbon fiber body-in-white design that could have 60% less mass than its equivalent steel structure



Figure 1: Carbon fiber preform for B-pillar outer panel.



Figure 2: Carbon fiber B-pillar inner and outer panel in bonding fixture.

# 2006 FreedomCAR and Fuel Partnership Highlight

## Ultra Large Castings for Lightweight Vehicle Structures

USAMP – AMD406

The Ultra Large Casting (ULC) project seeks to describe and substantiate the rationale for using light metal castings in place of conventional stamped and welded steel automotive body structures to reduce vehicle weight significantly. The ULC project is being executed in two concurrent phases. *Phase I* focuses on process issues and emerging casting processes aimed at improving the quality of cast components vs. conventional high pressure die-casting. *Phase II* focuses on designing, analyzing, producing and testing a demonstration component for a "real-world" vehicle application. The demonstration component chosen by the ULC team replaces the conventional multi-piece steel structure (Fig. 3) that forms the inner front fender - known in the industry as a "shotgun" - with a single thixomolded magnesium casting (Fig. 1). Ultimately, this "shotgun" will become part of an integrated front-end structure for a large body-on-frame pickup or SUV made entirely of magnesium castings (Fig. 4).

The thixomolded magnesium shotgun demonstrated a mass reduction of over 60% compared to conventional steel construction. It also was made with a first-of-its-kind multiple-drop direct injection hot runner system (Fig. 2), enabling fabrication of larger components than feasible with conventional thixomolding.



Figure 1: Thixomolded magnesium shotgun casting

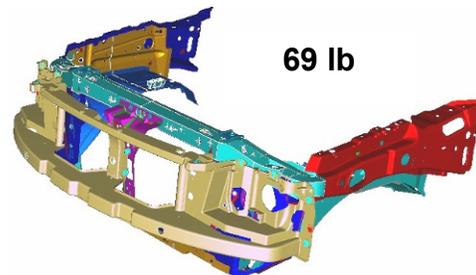


Figure 3: Conventional steel front-end structure (2006 Ford Expedition)

ELAPSED TIME = 0.02400

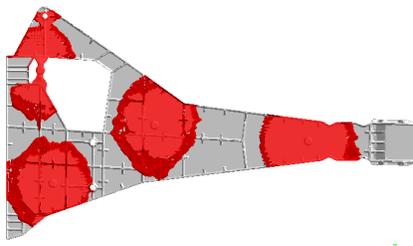


Figure 2: Flow simulation showing start of filling pattern for hot runners, as the part is filled simultaneously in four locations

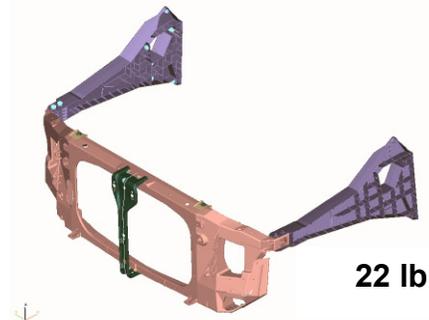


Figure 4: ULC cast magnesium front-end proposal (68% less weight)

## 2006 FreedomCAR and Fuel Partnership Highlight

# Friction Stir Spot Welding of Advanced High Strength Steels

### Direct-funded from Advanced Lightweight Materials

This project is a collaborative effort between ORNL and PNNL, guided by an industry steering committee. It addresses the questions of whether the friction stir spot welding (FSSW) process can be accomplished in Advanced High Strength Steels (AHSS) and, if so, whether FSSW has advantages over conventional processes like Resistance Spot Welding (RSW). Preliminary work on FSSW of AHSS suggests that several features of the process may produce cost and energy saving advantages over RSW. In addition, the process may be able to join lightweight materials (e.g., DP1000, Martensitic Steels, Hot Stamped Boron Steels) which present issues for conventional joining techniques. If this can be accomplished, the FSSW process could be an important enabler for more widespread use of these light-weight, advanced and ultra-high-strength materials.

Friction stir spot welds were made on two-high stack-ups of DP780 and Hot Stamped Boron steel using polycrystalline boron nitride tools. Initial mechanical testing demonstrated that FSSWs can achieve failure stress levels that exceed the minimum required by industry standards for RSWs. However, load carrying capability must still be improved if FSSW is to be competitive with RSW. This aspect of the process depends directly on stir tool considerations and process parameters. Key technology barriers associated with stir tooling include design, material, durability and cost. Redesigned tools indicate the potential to improve the load-carrying capability of welds produced at welding times of 4 seconds.

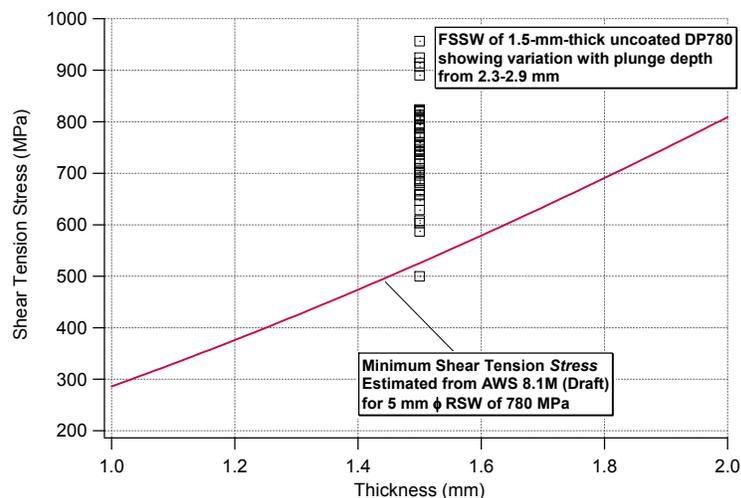


Figure 1: Variation of shear tension stress with DP780 sheet thickness. The data indicate that the intrinsic strength of FSSWs exceeds the minimum specified for RSWs.

## *2006 FreedomCAR and Fuel Partnership Highlight*

### *Warm Forming of Aluminum*

#### **USAMP – AMD 307**

The need to improve fuel economy has led automakers to explore lightweight materials like aluminum for automobile body and closure applications. However, there are challenges to the widespread use of aluminum including lower formability and higher cost compared to mild steel. A prior study into the warm forming of aluminum focused on the development of special alloys with improved formability. This approach increased material cost and the process cost differential with conventional stamping. However, this project developed and used a technical cost model to evaluate and optimize the warm forming process as well as to determine the potential cost advantages of the process. Results of the model indicated a significant cost advantage for the production of an aluminum door inner as compared to a multi-piece design fabricated with conventional stamping methods.

In the AMD 307 project the warm forming process was demonstrated on a production grade, commercially-available aluminum alloy AA5182-O. A new cleanable lubricant suitable for use at warm forming temperatures was developed and used in all of the forming trials. Two dies were utilized in the project: a production die for the stamping of steel door inners refitted with cartridge heaters and a purpose-built die for warm forming. The second of these two tools was designed and built using finite element simulation tools and the knowledge of thermal and distortion behavior gained during trials with the production door inner die. The temperature distribution in this new warm forming tool was shown to offer exceptional thermal control and minimal distortion as compared to the door inner die. Post-forming analyses are underway, but depth-of-draw and formability control differences can be seen in the AA5182-O panels yielded by the two dies. Figure 1 shows the typical panel produced with the refitted die and Figure 2 shows two typical panels formed using the purpose-built die. Specific accomplishments included demonstrating the viability of the technology and potential applicability through:

- Development and demonstration of key elements of warm forming technology with the forming of a door inner panel from a commodity aluminum alloy.
- Application of thermal and forming simulation tools for improved process control in warm forming.
- Design and construction of a new, optimized warm forming die for excellent forming and thermal control.



Figure 1: Inner door panel warm-formed using refitted steel-stamping die.



Figure 2: Deep-drawn panels warm-formed using a purpose-built warm-forming die.

## 2006 FreedomCAR and Fuel Partnership Highlight

### Control Strategy for Plug-In Hybrid Vehicles

National Renewable Energy Laboratory

Plug-In Hybrid Vehicles (PHEVs) have the potential to reduce petroleum consumption by utilizing electrical energy from a local grid. However, successful market introduction of PHEVs requires overcoming major barriers such as the currently prohibitive battery cost. Battery cost is directly related to battery size; which in turn is based on system requirements and control strategies. In 2006, National Renewable Energy Laboratory's (NREL) analysis provided results comparing different control strategies with respect to petroleum reduction and battery sizing. NREL concluded that control strategy can significantly affect battery sizing.

NREL analyzed two different control strategies for PHEVs: an All-Electric Range (AER) and a Blended Range. Both strategies require charging the battery from the electric grid. In charge depletion mode (CD), the energy for vehicle propulsion comes primarily from discharge of the battery, giving a net reduction in its state-of-charge (SOC). During CD mode, a vehicle utilizing the AER strategy runs as an electric vehicle only with no use of the combustion engine. A Blended Range strategy intermittently engages the combustion engine in time of large power demand. Both strategies will switch to a charge-sustaining mode once the vehicle completes the CD mode (battery discharged to a designated set point). Once in charge sustaining mode, the vehicle control strategy periodically charges / discharges the battery similar to currently available hybrid electric vehicles.

The simulation results (Figure 1) show how increasing battery power, as expected, offers the potential for greater reduction in petroleum use. By definition, an AER vehicle in the CD mode uses no petroleum but, for the driving range and conditions employed in the simulation, even a lightweight vehicle requires a battery rated at about 60 kW. Conversely, a Blended Range control strategy can reduce the battery power requirement by almost 50 percent and still maintain approximately 90% fuel consumption reduction in CD mode. The lower power requirement results in a smaller battery design thus lowering costs, and increasing the commercial viability.

Even with a Blended Range strategy, battery costs remain a significant barrier to commercialization and continue to stimulate extensive research at DOE.

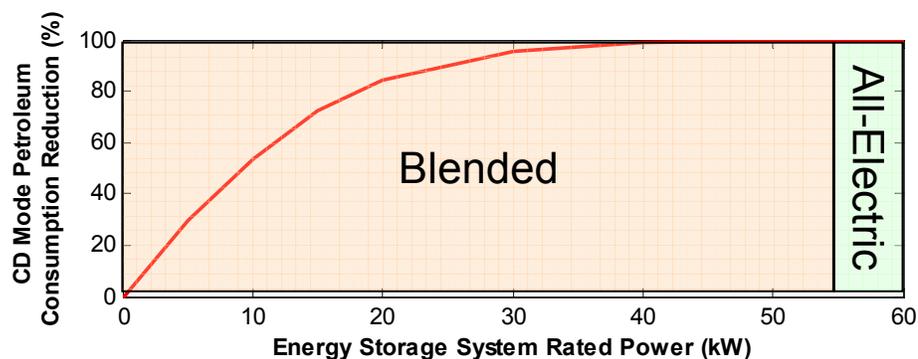


Figure 1: Petroleum Reduction vs. Battery Power during Charge Depleting Mode

## *2006 FreedomCAR and Fuel Partnership Highlight*

### *Hybrid Performance Testing Collaboration Reveals Consistent Performance over Life*

**Argonne National Laboratory**

As Hybrid Electric Vehicles (HEVs) continue to gain in popularity, so has the need to understand the vehicle characteristics throughout the life of the vehicle. Argonne's Advanced Powertrain Research Facility (APRF), in collaboration with Idaho National Laboratory's (INL) evaluation fleet, is performing Beginning Of Life (BOL) and End Of Life (EOL) testing on a dynamometer. INL fleet evaluation performs an accelerated reliability test by driving the vehicles 160,000 miles within 3 years.

ANL has performed BOL testing for the following vehicles in 2006: Toyota Highlander HEV, Lexus RX400h, H2 Silverado, H2 F-150; the test was also performed on a low-mileage (6,000 miles) 2001 Toyota Prius. The procedure consisted of city (UDDS) and highway (HWY) driving cycles along with other standard tests. The APRF has additionally performed to date an EOL test on a 2001 Honda Insight and a 2002 Toyota Prius.

The results for the 2002 Toyota Prius were compared to those obtained from the low mileage 2001 Toyota Prius: these vehicles have similar powertrain and energy storage devices. No significant change in performance was seen. As shown in Figure 1, it was determined that only a small decrease in fuel economy existed between the 2001 Prius with 6,000 miles and the 2002 Prius with 168,000 miles. The decrease in economy ranged from 0.5% to 2.3% depending on the test cycle. These results do not necessarily apply to all HEVs.

The importance of this work lies in the adoption of uniform test procedures that are now accepted as standards for such vehicle characterizations.

	2001 Low mileage Prius average fuel economy [mpg]			2002 End of Life Prius average fuel economy [mpg]			Decrease in fuel economy [%]
	Average fuel economy [mpg]	SOC Start to End [%]	Engine On Time [%]	Average fuel economy [mpg]	SOC Start to End [%]	Engine On Time [%]	
CS UDDS	52.1	56.0% - 55.8%	44.2%	51.5	56.8% - 56.5%	45.8%	1.1 %
HS UDDS	59.4	56.6% - 56.7%	35.2%	58.0	57.2% - 57.2%	36.7%	2.3 %
HWY	58.1	61.0% - 65.0%	91.7%	56.9	57.0% - 60.5%	94.5 %	2.1 %
NEDC	55.9	61.5% - 62.5%	34.3%	55.2	61.5% - 63.0%	33.5%	1.3 %
US06	39.9	64.0% - 62.5%	-	39.7	66.5% - 59.5%	-	0.5 %

Figure 1: Comparison of fuel economy between a low-mileage 2001 Toyota Prius and an end-of-life 2002 Toyota Prius.

# *2006 FreedomCAR and Fuel Partnership Highlight*

## *Pathway Components Model*

### **Fuel Pathways Integration Technical Team**

In 2006, the US Department of Energy (DOE) announced a new hydrogen cost goal of \$2.00 – 3.00/gge (delivered, untaxed, 2005\$). With the announcement of that goal, the Fuel Pathways Integration Technical Team (FPITT) recognized the need to develop a transparent process to determine how to divide the pathway target between the different components of the hydrogen pathway (production + delivery + storage). The component cost breakdowns are necessary to set hurdle targets for each component of the technology pathway.

The following pathways have been analyzed at a common point in time and initial hurdle targets have been estimated.

Central biomass with pipeline delivery	Central natural gas SMR with pipeline delivery
Central biomass with liquid truck delivery	Central natural gas SMR with liquid truck delivery
Central coal with no CO2 sequestration and pipeline delivery	Forecourt natural gas SMR
Central coal with no CO2 sequestration and liquid truck delivery	Forecourt Ethanol SMR
Central wind electrolysis with pipeline delivery	Forecourt Electrolysis
Central wind electrolysis with liquid truck delivery	

The Pathway Component Methodology was developed by FPITT and used to analyze several hydrogen pathways. The methodology adjusts the individual component costs (production, delivery and storage) in each pathway through a normalization process to meet the hydrogen cost goal of \$2.00 – 3.00/gge.

For pathways involving central production, the current Hydrogen Analysis (H2A) production cases were combined with key delivery technologies from the Hydrogen Delivery Scenario Model (HDSAM) to set base component costs. Forecourt cases used only the H2A production models because delivery is intrinsic to those models.

The Pathway Component Methodology and its results were reviewed by the Production, Delivery and Storage tech teams. The methodology with supporting documentation will be made available to all tech teams for target and goal assessment. The FPITT will consider how current DOE cost goals in the DOE Multi-Year Research, Development and Demonstration Plan correlate to the developed pathway components goals.

## *2006 FreedomCAR and Fuel Partnership Highlight*

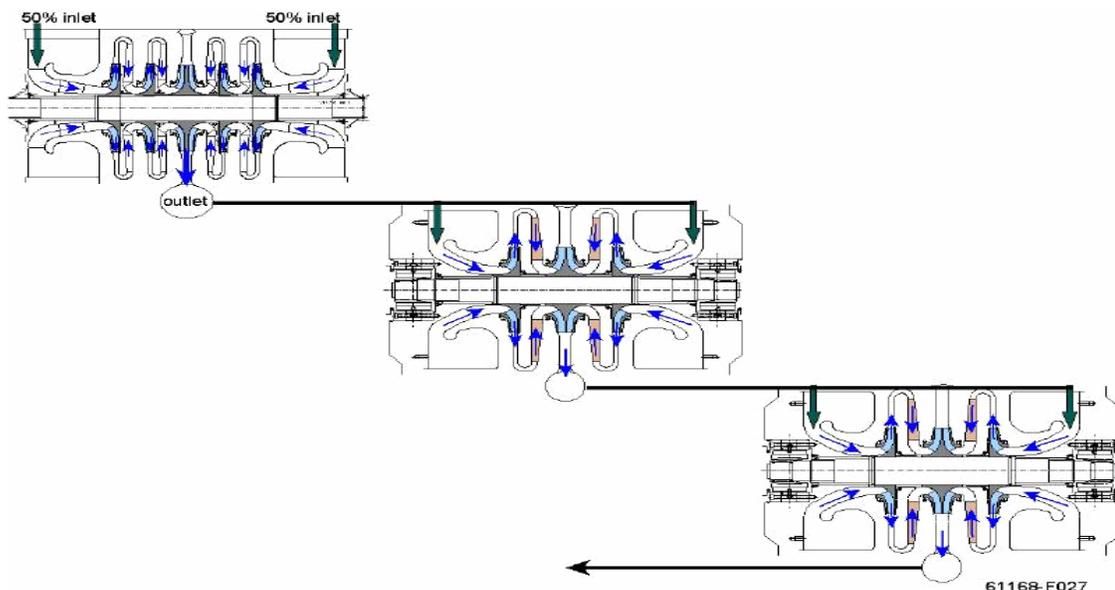
# *Hydrogen Compression R&D: Feasibility Design for a Hydrogen Centrifugal Compressor For Hydrogen Pipeline Delivery*

**Mohawk Innovative Technologies, Inc.**

Current technology for high volume throughput hydrogen compression applications such as for pipeline delivery, utilizes reciprocating compressors. Due to the frequent maintenance that is required, and less than desirable reliability, two or even three compressors are installed to ensure sufficient availability. This adds significantly to the cost. In contrast, natural gas pipelines are served by centrifugal compressors which are lower cost and highly reliable. Current centrifugal compression technology does not work with hydrogen due to its very low molecular weight and gas density.

Mohawk Innovative Technologies, Inc. has been able to develop a design for a centrifugal compressor for hydrogen pipeline delivery they believe will overcome the challenges of hydrogen centrifugal compression. The key to the concept is being able to operate at very high RPM compared to natural gas centrifugal compressors. They believe this will be possible through the use of their unique air foil seals and bearings as well as other aspects of their design. In addition, the air foil seals and bearings do not require oil lubrication and thus will avoid the chance of oil contamination of the hydrogen, a requirement for the use of hydrogen in PEM fuel cells.

The next step in this research effort will be to begin to test the air foil seals and bearings under the conditions they will encounter in this compressor design.



## *2006 FreedomCAR and Fuel Partnership Highlight*

### *Development of a Turnkey Hydrogen Fueling Station*

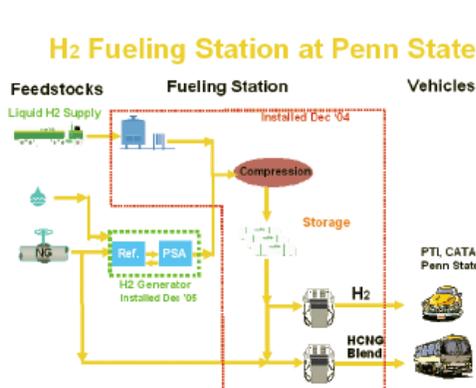
**Air Products and Chemicals, Inc.**

The Turnkey Hydrogen Fueling Station at Pennsylvania State University demonstrated a distributed hydrogen production system using natural gas reforming technology. The integrated design is based on steam methane reforming and features 5,000 psi hydrogen dispensing capability, as well as a hydrogen/natural gas blending dispenser. The 110 kg/day fueling system was commissioned in March 2006 and its design and operation were reviewed by the Hydrogen Production Tech Team. The project moved into the validation stage in April 2006. Over a 3 month period, the system operated for more than 2000 hours, resulting in 95% availability, and has achieved the performance specifications for hydrogen purity (>99%), system efficiency (65%) and hydrogen production rate (51 nm<sup>3</sup>/hr).

Several significant milestones were achieved:

- A cost-effective route for production and delivery of hydrogen at a commercial fueling station was validated.
- Fueling station operational costs were minimized by developing a turn-key system that could be continuously monitored and operated remotely.
- An advanced PSA hydrogen separation system was developed and demonstrated that met the DOE targets for efficiency and hydrogen recovery.
- The integrated design resulted in individual component and overall system efficiencies that met or slightly exceeded the DOE technical targets.

H<sub>2</sub>A analysis shows that when scaled up to a 1,500 kg/day H<sub>2</sub> fueling station and deployed in volumes of 500 per year, the \$3.00/kg H<sub>2</sub> DOE 2006 target is potentially achievable.



# 2006 FreedomCAR and Fuel Partnership Highlight

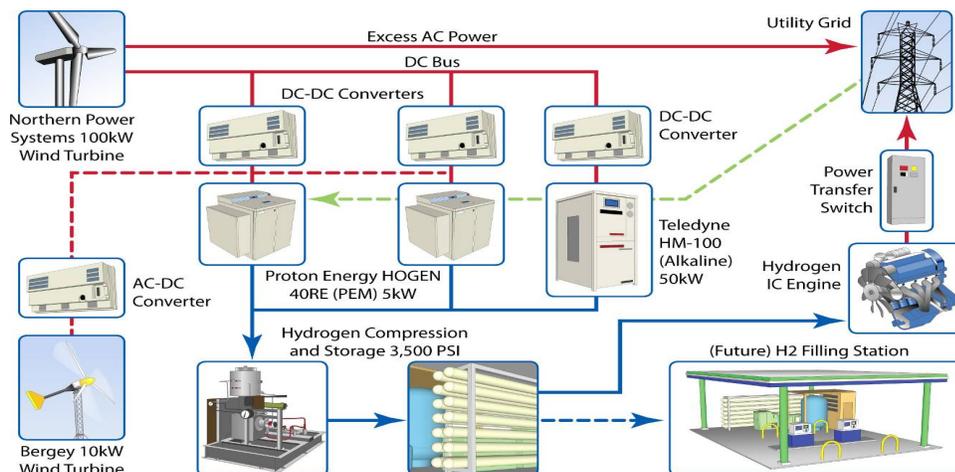
## Wind Powered Electrolysis

National Renewable Energy Lab and Xcel Energy

Installation and dedication of the Wind2H2 Demonstration Center was completed at NREL with ongoing operational testing. Funded by the DOE Hydrogen Program and Xcel Energy, this multi-year collaborative project is designed to gain knowledge and insight about producing hydrogen by electrolysis for use as a fuel and as “stored wind” energy. It will fill important knowledge gaps that the electric utility industry has concerning its potential role in supplying and delivering hydrogen. These gaps include the ability of wind generated hydrogen to address the intermittent nature of wind power and the extent hydrogen can support the electric grid through off-peak production and storage of hydrogen.

Hydrogen will be produced directly from wind turbines as well as from the electric grid via electrolysis. In addition, the project will examine compressing and storing the hydrogen during off-peak demand and then using it to put electricity back onto the grid during periods of higher electricity demand. Several unique features of the planned wind-electrolysis system will be analyzed including:

- Direct feed of direct current (DC) from the wind turbine to the electrolyzer to enable system efficiency gains and capital cost reductions;
- Concurrent feed of alternating current (AC) to the electrolyzer to provide clear comparison to direct DC feed performance;
- Comparison of alkaline and PEM electrolyzer technologies, commercial grade higher pressure electrolyzer and low/medium pressure range compression & storage for reduced operability risk;
- Use of a hydrogen engine/generator for peak power demand reduction; and
- System transportability for redeployment for Xcel Energy use after research & development.



# *2006 FreedomCAR and Fuel Partnership Highlight*

## *Hydrogen Behavior and Interface Information*

Codes and Standards Tech Team

### **Hydrogen Behavior: Sandia Hydrogen Compatibility Work**

A reference internet accessible database for hydrogen compatible materials is now included on Sandia's web site and includes existing knowledge of hydrogen compatibility needs and published data on hydrogen-assisted fracture of engineering alloys. Additional materials' testing is ongoing and the technical reference website will be updated as new data is generated. This data can be accessed at the following website: <http://www.ca.sandia.gov/matlsTechRef>.



### **Fuel-Vehicle Interface**

- H2 Quality: There has been significant progress in fuel cell testing of contaminants (hydrogen sulfide) by LANL (funded by the DOE Fuel Cell activity) and baseline testing of some of the SAE J2719 constituents by the University of Hawaii and the University of South Carolina. In addition, progress has been made by ASTM in the development of standard test procedures for hydrogen quality. A draft hydrogen quality standardization timeline has been developed with target timing for a common SAE/ISO standard by mid-2009.
- 70 MPa Hydrogen Fueling Testing: SAE coordinated initial hydrogen tank testing for the purpose of evaluating fueling targets proposed in SAE J2601. The study utilized supplier tanks to determine the limits of "fast" hydrogen fueling at 70 MPa. This testing showed that precooling and/or communications would be needed at certain ambient conditions to allow for a complete fill in a relatively short amount of time (at least equal to the time to fill a gasoline vehicle). This study was directional as these supplier tanks were not the 'production intent' designs that are planned for deployment on the next generation of OEM vehicles. The results from this study are guiding future work.



# 2006 FreedomCAR and Fuel Partnership Highlight

## National Codes and Standards Template and National Hydrogen-Fuel Cell Codes and Standards Coordinating Committee

National Renewable Energy Laboratory

A key success of national hydrogen and fuel cell codes and standards developments efforts is the creation and implementation of a national template for Vehicle Systems and Refueling Facilities (Figure 1). Through the template, all key stakeholders coordinate the preparation of critical standards and codes for hydrogen and fuel cell technologies and applications, and maintain a coordinated national agenda for hydrogen and fuel cell codes and standards.

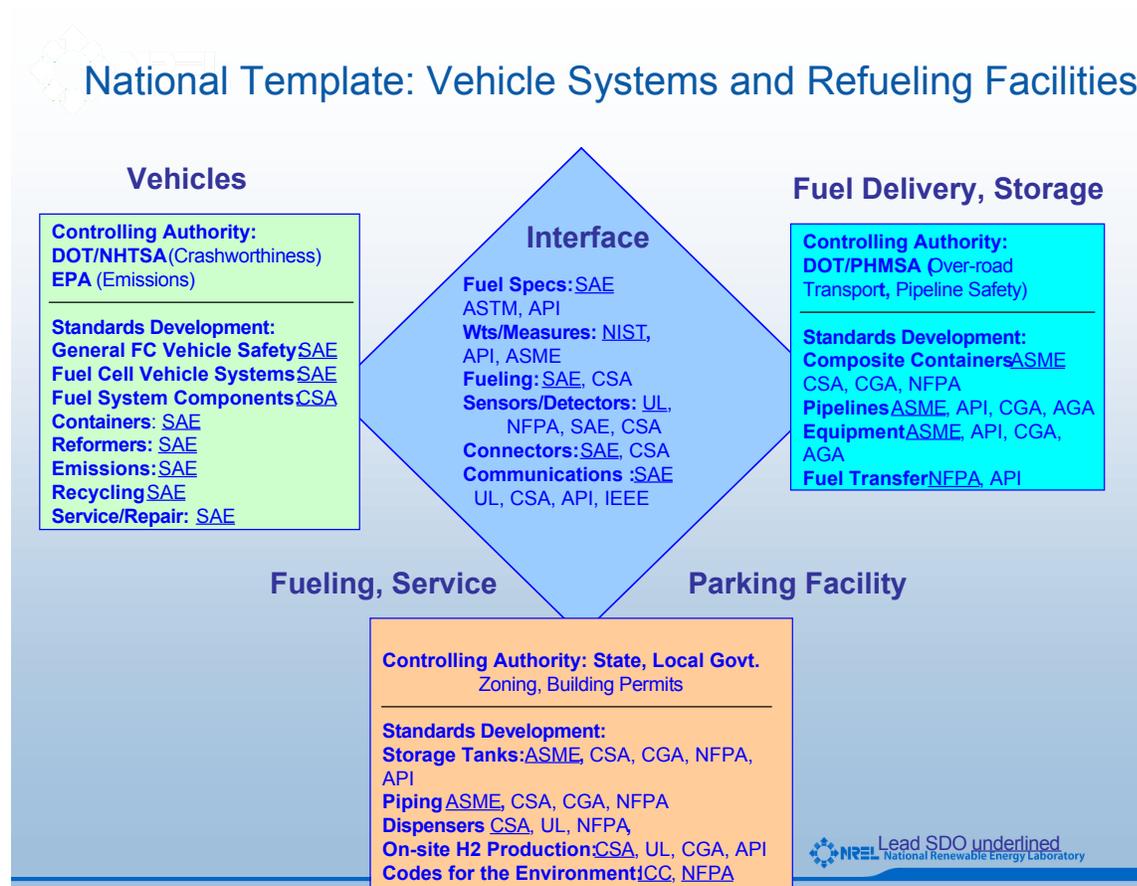


Figure 1: The template and the National Hydrogen and Fuel Cells Codes and Standards Coordinating Committee, managed by DOE, NHA, and the USFCC to implement the template, have enabled a “virtual national forum” for standards and model code development organizations, industry, government, and interested parties to address critical codes and standards issues, both immediate and long-term.

# 2006 FreedomCAR and Fuel Partnership Highlight

## DOE Hydrogen Safety Databases

National Renewable Energy Laboratory &  
Pacific Northwest National Laboratory

Hydrogen has an extensive safety record as a chemical feedstock, yet experience with its safe use as an energy carrier remains to be thoroughly established. To help establish a safety record, the Department of Energy's (DOE) Hydrogen Safety, Codes and Standards program has published information resources compiling hydrogen incidents and hydrogen safety literature to share and promote lessons learned (Figures 1- 2).

In May 2006, the Pacific Northwest National Laboratory launched the Hydrogen Incidents Database. This database catalogs hydrogen safety incidents and near-misses in projects funded by the DOE Hydrogen Program and other organizations. All the reports include details of the incidents but are non-attributed to ensure anonymity. By sharing safety information, DOE aims to prevent the occurrence of similar incidents at other facilities and organizations involved in the advancement of hydrogen technologies. The database can be found online at: <http://www.h2incidents.org>.

In response to a recommendation by the National Research Council — DOE published the Hydrogen Safety Bibliographic Database in May 2006. Maintained by the National Renewable Energy Laboratory, the database currently contains over 400 hydrogen safety articles and presentations published by industry, academia, and governments from around the world. This collection allows researchers, code officials and stakeholders to learn from a wide variety of experiences. The database can be found online at: [http://www.hydrogen.energy.gov/biblio\\_database.html](http://www.hydrogen.energy.gov/biblio_database.html).

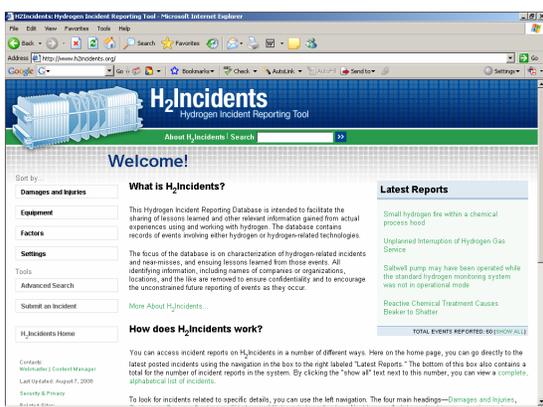


Figure 1: Hydrogen Incidents Database. [www.h2incidents.org](http://www.h2incidents.org)

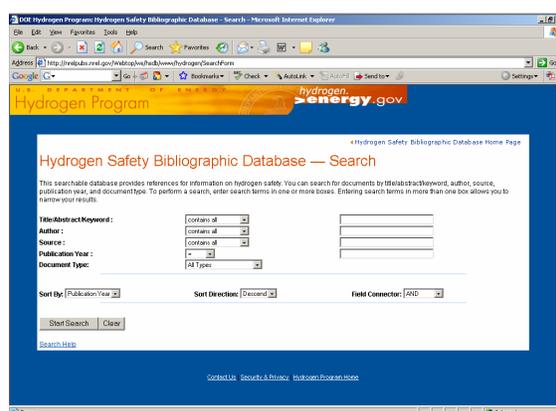


Figure 2: Hydrogen Safety Bibliographic Database. [www.hydrogen.energy.gov/](http://www.hydrogen.energy.gov/)

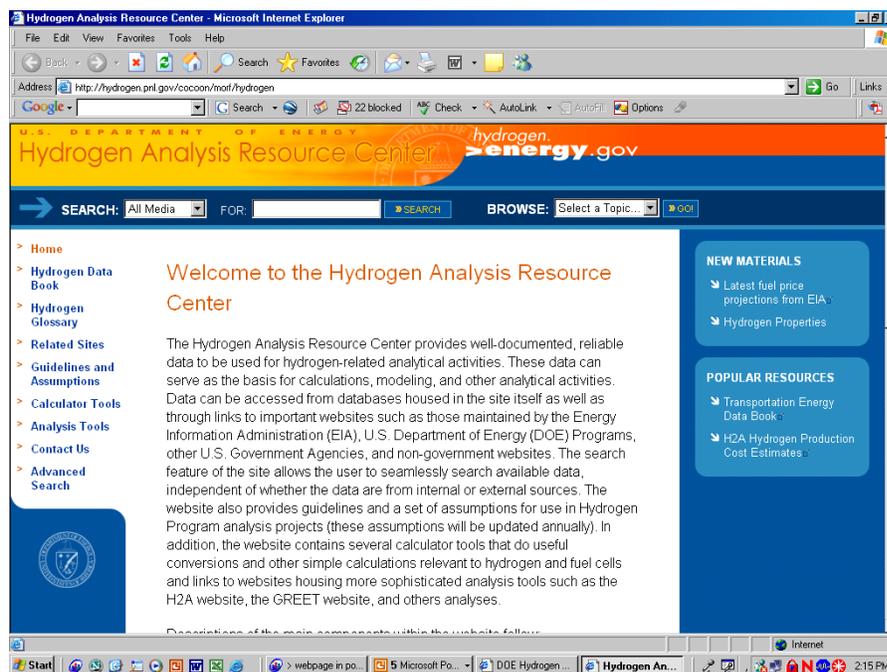
# 2006 FreedomCAR and Fuel Partnership Highlight

## Hydrogen Analysis Resource Database

In 2006, the US Department of Energy (DOE) completed and issued the Hydrogen Analysis Resource Center (HyARC) of hydrogen-related data to a public website. HyARC contains well-documented, reliable data to be used for associated hydrogen analytical activities and serve as the basis for calculations, modeling, and other analyses. The effort to develop this hydrogen resource center brought DOE, national laboratories, and industry together to provide transparent and consistent data for hydrogen related analysis and information dissemination.

HyARC provides data that can be accessed from data files housed in the website, as well as through links to important websites such as those maintained by the Energy Information Administration, DOE Programs, other U.S. Government Agencies and non-government sources. A “search” feature is provided to enable the user to seamlessly search available data from internal and external sources. Guidelines and the set of assumptions used in the Hydrogen Program analysis projects, which are updated annually, are available. In addition, the website contains several “calculator” tools that perform useful conversions and other calculations relevant to hydrogen and fuel cells, and links to websites housing more sophisticated analysis tools.

The Hydrogen Analysis Resource Center resulted from the database design by the Pacific Northwest National Laboratory, and the collaboration between the Department of Energy, NIST, DOT, national laboratories (National Renewable Energy Laboratory, Argonne National Laboratory, and Pacific Northwest National Laboratory), and industry. Expert feedback on the HyARC data and calculation methodology was provided to DOE by member of the energy companies in the FreedomCAR and Fuel Partnership. HyARC website address is [www.hydrogen.energy.gov/resource\\_center.html](http://www.hydrogen.energy.gov/resource_center.html).



<http://hydrogen.pnl.gov/cocoon/morf/hydrogen>