



WORKSHOP

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Future Automotive Aftertreatment Solutions: The 150°C Challenge Workshop Report

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With

Greatly Appreciated and Significant Contributions and Efforts
of
The Workshop Session Participants

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TABLE OF CONTENTS

1) Introduction (Challenge and Mission)	3
2) Executive Review	3
3) Macro View – The 150°C Challenge (Background and Importance)	6
4) Micro View - The 150°C Challenge (Needs)	14
Overview Session 1) Modeling	14
Overview Session 2) Materials	17
Overview Session 3) Industry and Supplier Needs	18
Overview Session 4) System Integration and Architecture	19
5) Global View - The 150°C Challenge (The Benefit)	20
6) Workshop Structure	20
7) Technology Progression from Basic Science to Product Application	23
8) Session Reports (Recommended Pathways and Priorities)	26
9) Workshop Summary	27
10) Recommended Path Forward	27
11) Appendix	29

1. Introduction (Challenge and Mission)

With future fuel economy standards enacted, the U.S. automotive manufacturers (OEMs) are committed to pursuing a variety of high risk/highly efficient stoichiometric and lean combustion strategies to achieve superior performance. In recognition of this need, the U.S. Department of Energy (DOE) has partnered with domestic automotive manufacturers through U.S. DRIVE to develop these advanced technologies. However, before these advancements can be introduced into the U.S. market, they must also be able to meet increasingly stringent emissions requirements. A significant roadblock to this implementation is the inability of current catalyst and aftertreatment technologies to provide the required activity at the much lower exhaust temperatures that will accompany highly efficient combustion processes and powertrain strategies. Therefore, the goal of this workshop and report is to create a U.S. DRIVE emission control roadmap that will identify new materials and aftertreatment approaches that offer the potential for 90% conversion of emissions at low temperature (150°C) and are consistent with highly efficient combustion technologies currently under investigation within U.S. DRIVE Advanced Combustion and Emission Control (ACEC) programs.

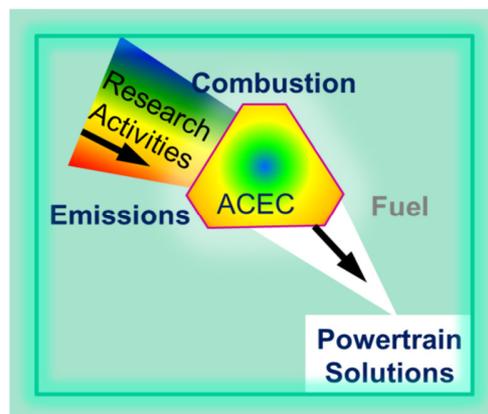


Figure 1. ACEC Vision

2. Executive Review

U.S. automotive manufacturers are continually faced with challenges related to simultaneously achieving higher engine efficiencies, lower exhaust emissions, greater fuel flexibility, and an array of powertrain strategies at economical costs. The U.S. DRIVE Partnership goal is to “significantly improve the efficiency of vehicles powered by advanced internal combustion powertrains (including hybrids) and vehicle fuel systems while protecting the environment.” Consistent with this mission, the ACEC 2020 U.S. DRIVE research target is as follows: “A 20% improvement in engine efficiency, compared to a 2010 baseline. Engine concepts shall be commercially viable and meet 2020 emissions standards.” In an attempt to improve the efficiency of pre-competitive research and development (R&D) at the domestic OEMs and leverage national resources, the U.S. DRIVE consortia have shown that they can develop fundamental knowledge and promising technology solutions for future engine and aftertreatment needs. Through these partnerships, cooperative and pre-competitive research and development activities can be conducted at the institutions and facilities most capable or efficiently providing the required technologies in a parallel manner instead of each OEM serially addressing similar

challenges. Although major challenges still lie ahead in the areas of advanced engines and alternative fuels, this workshop report specifically addresses potential aftertreatment solutions required to overcome technical barriers presented by highly efficient future powertrain running on a variety of fuels.

On November 29-30, 2012 at the US Council for Automotive Research (USCAR) HQ in Southfield Michigan, a workshop was conducted to address “The 150°C Challenge” related to future automotive emission control or “aftertreatment”. New fuel economy and greenhouse gas emission standards are challenging automotive manufacturers to produce more fuel efficient engines, but in many cases, the fuel efficiency improvements result in lower exhaust temperatures where conventional aftertreatment systems are not suitable. Thus, catalysts that are active at lower exhaust temperatures are needed to enable future U.S. EPA emission compliant aftertreatment systems. Fifty-five scientists and emissions aftertreatment specialists from universities, national laboratories, and industry gathered for the two-day workshop to discuss low temperature aftertreatment challenges facing the automotive community and to develop “roadmap” guidance for approaches that offer potential solutions for low temperature aftertreatment. The Low Temperature Aftertreatment Group of the U.S. DRIVE ACEC Tech Team hosted the workshop; the objective of the workshop was to:

- Create a roadmap for the discovery and development of catalytic materials and systems capable of functioning at 150°C and consistent with ACEC goals.
 - Note: This document serves as an aftertreatment roadmap, therefore by design, it is consistent with the U.S. DRIVE Advanced Combustion and Emissions Control Technical Team Roadmap published in June 2013 (http://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/acec_roadmap_june_2013.pdf).
- Sub-objectives were:
 - Determine goals for catalysts that would support and harmonize with ACEC goals for the year 2020 related to engine efficiency.
 - Identify key barriers to emission control technology as related emissions compliance; specifically, address barriers related to key required performance metrics such as: activity, selectivity, cost-effectiveness, and durability.
 - Recommend technical approaches that can overcome limitations in current catalyst technologies to provide >90% emissions reduction efficiency at 150°C.
 - Define roles and collaborations that will enable fundamental science research in the field of catalysis to support innovative research and development of catalysts by applied research and engineering entities.
 - Ensure essential vehicle engineering requirements are considered during the development of new materials and systems.
 - Provide OEM guidelines in determining the feasibility of materials and systems in order to enhance the probability of industry adoption.

To achieve these objectives and provide future emission compliant solutions, the workshop breakout sessions were focused on four key areas that the ACEC Low Temperature Aftertreatment Group considered essential. These areas include:

- A) Modeling from Molecular to System Level
- B) New Materials and Research Directions
- C) Industry and Supplier Needs (From Discovery to Market)
- D) System Engineering and Architecture (Controls, Sensors, and OBD)

Low Temperature Workshop Focus Areas

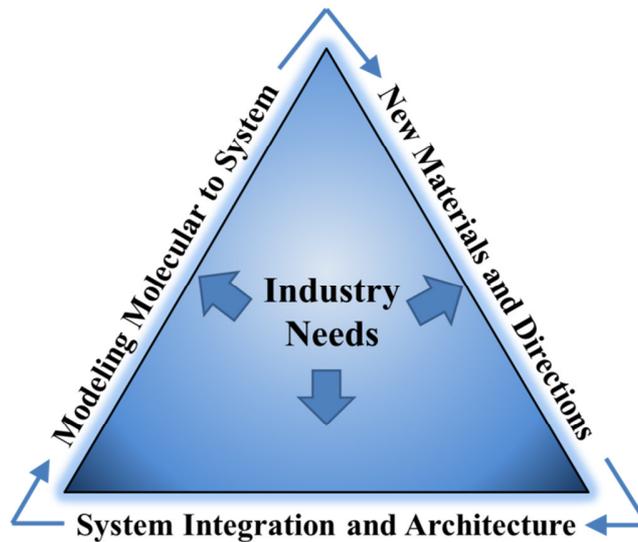


Figure 2. Interaction of Workshop Focus Areas

The main objectives or functions of each of these sessions were:

- Modeling from Molecular to System Level
 - Lessons learned from previous/current approaches
 - Accelerate the discovery of materials
 - Accelerate the predictive capability of system performance
 - Create a method to apply to other search and discovery applications
 - Identify search parameters
- New Materials and Research Directions
 - Assess current material technologies
 - Determine feasibility of 150C activity
 - Define areas of research requiring innovation (traps, NO_x, etc.)
 - Determine anticipated properties of new material solutions
 - Provide potential pathways of discovery
 - Define scope of effort
 - Identify resources and natural partnerships for effective discovery
- Supplier and Industry Needs (From Discovery to Market)
 - Material Requirements
 - Sustainability/Durability

- Component Availability
 - Cost
 - Manufacturability/Scalability
- Product Development Requirements
 - Research areas of interest
 - OEM and supplier roles during R&D process
 - Commonization of testing procedures
 - Commonize test conditions (temp, SV, exhaust composition, etc.)
- System Engineering and Architecture (Controls, Sensors, and OBD)
 - Define OBD requirements
 - Determine ability to diagnose new materials and systems
 - Determine methods of diagnosing materials and systems
 - Identify new technology to enable OBD of catalytic solutions (sensors/controls)
 - Packaging requirements for successful integration

3. Macro View - The 150°C Challenge (Background and Importance)

In the United States, several factors are driving increases in the fuel economy of transportation vehicles. Lower imports of petroleum are desired for national energy security. Reductions in greenhouse gases are being pursued to minimize manmade contributions to climate change. Increasing fuel prices due to increased global fuel demand are affecting consumers. These factors have led to new fuel economy and greenhouse gas emission standards for light-duty vehicles set by the U.S. Environmental Protection Agency (EPA) and the Department of Transportation's National Highway Traffic Safety Administration (NHTSA). The rules affect model year 2017-2025 passenger cars, light-duty trucks, and medium-duty passenger vehicles; fuel economy requirements over this period increase with model year. In addition to these light-duty rules, the EPA passed rules in 2011 related to heavy-duty vehicles for fuel economy. Although the focus of the efforts presented here is specific to light-duty vehicles, many technology advancements in the light-duty size classes will be transferable to the heavy-duty size classes. Together, light-duty, medium-duty, and heavy-duty vehicles represent over 60% of total petroleum consumption and 82% of total transportation petroleum consumption in the U.S. [Transportation Energy Data Book, Edition 31, July 31, 2012].

While electric vehicles (EVs) have been commercialized and are expected to gain market acceptance, vehicles based on internal combustion engines are expected to continue to dominate the market.[*DOE Quadrennial Review 2011; Energy Information Agency, Annual Energy Outlook, 2011; Review of the Research Program of the U.S. DRIVE Partnership: 4th Report, NRC 2013*] The cost effectiveness, versatility (over broad vehicle applications), and fuel-based convenience of the internal combustion engine either alone or as part of a hybrid electric vehicle (HEV) results in an acceptable product for customers, and new evolutions of the internal combustion engine are enabling continued market success. However, in order to commercialize future fuel-efficient vehicles, emission regulations must be met. The combination of advanced engines with catalytic emission control systems are required to meet both the fuel economy and pollutant emission regulations. Of critical importance to advanced engines is the fact that as

internal combustion engines become more fuel efficient, less exhaust heat is produced, thereby creating challenging conditions for catalyst systems to achieve emissions reduction.

Vehicles meet both fuel economy standards and emission regulations via demonstration of performance on a vehicle chassis dynamometer drive cycle test that entails transient operation representative of real world driving conditions. Other requirements include demonstration of durability (at emission regulation level) to 150k mileage levels and on-board diagnostics to insure ongoing compliance in the field. During the FTP transient drive cycle, which is required for emissions certification, the most challenging portion is at the beginning where the vehicle is required to undergo a cold start. In this phase, catalyst temperatures begin at room temperature and rapidly rise to higher temperatures (known as “light-off” temperatures) where catalytic activity increase to the 50% conversion level for HCs, CO, and NO_x. During this phase, significant emissions are emitted from the vehicle and are a major contributor to the total emissions over the entire drive cycle. Thus, maximizing catalyst efficiency at this time to meet SULEV 30 emissions standards is critical and lowering the light-off temperature for catalyst components greatly benefits this critical process. Nominally, most catalyst systems began becoming effective at ~200°C in today’s vehicles; however, more fuel efficient vehicles are resulting in lower exhaust temperatures. Based on exhaust temperature expectations for future engine technology, industry representatives predict light-off temperatures of ~150°C will be required to meet emission regulations for new engines used to meet vehicle fuel economy standards. This lowering of the temperature to ~150°C, at which catalysts become active, is extremely difficult and forms “The 150°C Challenge”. An ACEC Low Temperature Aftertreatment Group presentation by Mike Zammit of Chrysler to the ACEC Tech Team in November 2011 summarizes the challenge (appendix*).

Current emissions regulations in the U.S. for passenger vehicles are based on the Tier 2 Vehicle and Gasoline Sulfur Program (www.epa.gov/tier2) and associated rules and regulations passed in 2000. Under this program, the emissions limits for all passenger cars, light trucks, and medium-duty passenger vehicles are set; here medium-duty passenger vehicles include vehicles up to 10,000 pounds gross vehicle weight. Also, under this program, the sulfur level for gasoline sold in the U.S. capped at 80 ppm (by 2006). Pollutants specified in the regulation include the “criteria” pollutants non-methane organic gases (NMOG), oxides of nitrogen (NO_x), carbon monoxide (CO), formaldehyde (HCHO), and particulate matter (PM). The term “hydrocarbons” (HCs) is often used interchangeably with NMOG since hydrocarbon emissions other than methane generally make up the NMOG pollutants.

Tier 2 emissions standards are demonstrated on a FTP 75 (Federal Test Procedure) transient drive cycle with the full vehicle. Emissions measured on a g/mile basis must not exceed the regulation levels at both intermediate life (5 years/50,000 miles) or full useful life (120,000 miles) levels. Multiple bins of emissions levels are set and allow automotive manufacturers to meet overall emissions requirements through the sale of mixtures of vehicle models that certify to the various bins. Bins are numbered from 1 to 11 with the lowest bin (1) representing a zero-emissions vehicle. On average, vehicles sold by the manufacturers must meet Tier 2 Bin 5 level emissions targets; thus, sale of vehicles with emissions higher than Bin 5 levels must be offset by sale of vehicles with correspondingly lower emissions levels than Bin 5.

In addition to the requirement to demonstrate emissions below the regulatory levels, automotive manufacturers are also required to perform on-board diagnostics (OBD) over the vehicle life to insure that the vehicle maintains the expected performance. The OBD process helps prevent excessive emissions due to tampering, an accident, or part failure in the field once the vehicle is out of the control of the manufacturer. Although the details of OBD requirements will not be presented here, it is important to note that meeting OBD requirements entails a degree of understanding of the functionality of the catalysts and other components in the emission control system. Thus, automotive manufacturers require science-based understanding of exhaust chemistry processes to meet the OBD elements of regulations.

The state of California has established their own emissions regulations which in general force lower emissions than U.S. federal regulations in order to address air quality issues associated with dense population areas in California. California's current emissions regulations are called Low Emission Vehicle II (LEV II) Standards and establish four different emissions categories including: LEV (low emission vehicle), ULEV (ultra-low emission vehicle), SULEV (super ultra-low emission vehicle), and PZEV (partial zero emission vehicle). Furthermore, California requires gasoline sulfur levels to not exceed 20 ppm. Several other states have adopted California's emissions standards as well.

Compared with other countries, the U.S. and California emission standards demand lower vehicle emissions. However, both the U.S. and California are both seeking lower emissions regulations to address potential increases in emissions from greater vehicle miles travelled and, in general, assure that various regions of the country are in attainment of air quality standards. California finalized the new LEV III standards in 2012 which calls for reduced emissions beginning in MY2015 in California and ultimately requires a 30 mg/mile fleet average for NMOG and NO_x emissions by 2025. In addition, California will require PM emissions to be less than 1 mg/mile starting in 2025. The U.S. EPA has announced a Tier 3 proposed standard and has released the proposed rulemaking for public comment at this time. Based on the new California standards and potential new federal standards, current emission goals for the Advanced Engine and Emission Control Tech Team of US DRIVE are U.S. EPA Tier 2 Bin 2 emission levels. As such, the goals for the research and development activities outlined in this document will also be U.S. Tier 2 Bin 2 levels. Note that the Bin 2 levels represent a >70% reduction in NO_x emissions and >85% reduction in NMOG emissions compared to the Bin 5 level; these levels of emission reduction are extremely challenging.

Fuel Economy

Light-duty-vehicle fuel economy regulations are now in place to 2025. The current regulations require a US fleet average of 250-g CO₂ per mile in 2016 (equivalent to 35.5 miles per gallon) and 163-g CO₂ per mile in 2025 (equivalent to 54.5 miles per gallon). This is a 40% increase and more than a 100% increase in miles per gallon versus a 2008 baseline of 25 miles per gallon in 2016 and 2025, respectively. Each manufacturer has a different fuel economy target depending on the vehicle mix and volume sold. Each vehicle has a fuel economy target based on the vehicle footprint.¹

¹ Credits for other CO₂ reduction technologies and business decisions can reduce the CAFE target. Examples of these credit and incentive opportunities are: reduced refrigerant leakage from air conditioner; flex fuel (credit

Manufacturers do not assume that the engine alone will provide the necessary CAFE improvements. Instead, a combination of technologies at a vehicle level will be used to meet the regulation. Customer demand will play a role in technology selection. Technology areas that will improve CAFE include:

- Engine (dilute gasoline, clean diesel, LTC, boosting and downsizing, and other advanced fuel injection and combustion approaches)
- Transmission (automatic, manual, dual clutch, ...)
- Vehicle (mass, tires, aerodynamics, ...)
- Hybrid (strong, mild, ...)

Specific CAFE plans and technology selections for each manufacturer are confidential. However, achieving the goals of the ACEC Tech Team is critical for all OEMs to meet fuel economy mandates likely after 2016.

Emissions

Tier 2 emissions regulations apply to vehicles in the U.S. fleet today. Most light-duty vehicles today are certified to Bin 4 or Bin 5 levels to meet requirements. Emission control system warranty requirements are 120,000 miles and 10 years. California emissions regulations are more stringent than federal, with an emphasis on hydrocarbon (HC) emissions. Their standard requires a decreasing level of HC in the fleet. This is achieved by certifying a growing percentage of vehicles in bins lower than 5. Today, California vehicles certify at emission levels in the range from LEV to SULEV. PZEV vehicles have SULEV emissions, additional evaporative emission control, and a 150,000 mile warranty. In the future, the number of SULEV vehicles (roughly Bin 2 equivalent) required by the regulations is set to increase for states that have adopted California emission levels.²

Current particulate measurements are based on mass measurements (gram/mile) of particulate matter (PM) collected on a filter. The baseline stoichiometric SI engine technology meets current PM regulations. Advanced combustion strategies may result in higher engine particulates, which could require new emission control devices to comply with the existing regulations. The size, chemistry, and morphology of PM vary with combustion techniques and fuels requiring sophisticated analytical techniques to properly characterize the complex PM.

Fuels

Another aspect of technology relevant to emission control is fuel. Fuel chemistry has a direct impact on combustion properties but also affects downstream exhaust chemistry as well. In particular, different hydrocarbon species in the fuel lead to different “unburned” hydrocarbons in the exhaust as emissions, and the oxidation efficiency of catalysts varies for different hydrocarbon species. Thus, understanding exhaust chemical composition and the species-based

declines to zero in 2016); BEV, PHEV and fuel cell vehicles; natural gas vehicles; credit transfer between car/truck fleets or future/previous model years; credits purchased from other OEM's.

² California Low Emission Vehicle Regulation – LEV III (Proposed for model years 2017 -2025)

dependencies of catalysis processes is critical to insuring emission control over a range of fuel types.

The ACEC Tech Team Roadmap addresses fuels as an important element of powertrain technology and specifically focuses on the utilization of fuels for efficient combustion. Emphasis in the roadmap is placed on reducing petroleum-based fuel by using alternative fuels as well as determining fuel characteristics that enable more efficient combustion and emission control technologies.

In the U.S., the use of ethanol in gasoline has grown and is a critical aspect of meeting the Renewable Fuel Standard and other aspects of the Energy Independence and Security Act passed in 2007. Currently, ethanol content in gasoline up to 10% (E10) is found at most fuel stations, and the EPA has granted partial waivers to approve sale of gasoline with up to 15% ethanol content (E15) in 2010 (appendix*). Furthermore, automotive manufacturers sell flex fuel vehicles which are capable of operating with up to 85% ethanol content in gasoline (E85). While fuel used in real-world operation is growing in ethanol content, existing emission control standards are still met with 100% gasoline (or “certification gasoline”) fuels during the transient drive cycle test to demonstrate emissions. The ethanol content will affect both fuel economy and emissions during the drive cycle test; so, automotive manufacturers are challenged by the varying degree of ethanol in the fuels used in compliance testing and real-world operation. Recent studies have also shown that ethanol content in gasoline impacts the amount of PM emissions created with a reduction in PM associated with higher ethanol content in fuel.

Fuel chemistry can significantly affect catalyst activity and durability. Impurities in fuel can have a large impact on catalyst durability. Sulfur is a known catalyst poison and is present in both gasoline and diesel fuels at 80 ppm and 15 ppm maximum levels, respectively. Over the course of time, catalysts are exposed to integrated amounts of S resulting from fuel combustion even if the S content in fuels is low. The S impacts can range from increasing light-off temperatures for oxidation processes to completely blocking NO_x adsorption processes in lean NO_x trap catalysts. Although the industry has developed on-line protocols to remove sulfur in processed known as “desulfation”, the processes typically entail operation at higher catalyst temperatures which can damage the active precious metal components via sintering processes. Lubricants are also sources of S that lead to catalyst poisoning. Phosphorous and zinc are other lubricant-born poisons commonly found in oil additives that lead to catalyst degradation.

Engine Efficiency Strategy (Harmonization with Aftertreatment)

Research of advanced powertrain technologies will be ongoing at automotive manufacturers to meet the fuel economy and emission standards. The powertrain technologies of interest will vary depending on vehicle design and function. In order to meet the fuel economy standards over the wide range of vehicle products consumers have interest in, automotive manufacturers must investigate many powertrain options. The ACEC Tech Team has established a roadmap to achieve the goal of “20% improvement in engine efficiency, compared to a 2010 baseline”. The target date for achieving the goals is the year 2020 at which time the precompetitive research results can be funneled into product development programs as the automotive manufacturers. The roadmap addresses three main types of combustion anticipated for internal combustion

engines including: dilute gasoline combustion, clean diesel combustion, and low-temperature combustion. Each combustion technique will result in a unique combination of emissions and exhaust temperatures and thus require a unique emission control solution. While more detail about each combustion technique is provided in the ACEC Tech Team Roadmap, a synopsis of the combustion techniques and associated emission control needs are presented here.

a) Dilute Gasoline Combustion

In dilute gasoline combustion, fuel efficiency gains are attained by diluting the fuel-air mixture with greater amounts of either exhaust or air. The cases for dilution with exhaust or air greatly affect the emission challenges. For dilution with exhaust, the three-way catalyst (TWC) technology commonly found on the majority of passenger cars today can be effectively utilized to control the pollutants; however, lower exhaust temperatures from combustion may result requiring catalysts with lower light-off temperatures to control pollutants effectively during cold start. For dilution with air, the exhaust will contain high levels of oxygen that will prevent the TWC technology from performing. Thus, dilute gasoline combustion with air will require NO_x reducing catalysts for lean, oxygen-rich exhaust.

b) Clean Diesel Combustion

Diesel engine and emission control technology has made great progress over the last decade due to heavy-duty emissions regulation requirements and the lowering of sulfur in diesel fuel to <15 ppm (from a previous 500 ppm S cap). Fuel economy and emissions standards for light-duty passenger car vehicles will continue to push clean diesel combustion and emission control technologies. Diesel engines will operate net-lean and produce oxygen-rich exhaust for all operation modes thereby requiring lean NO_x emission control as well as effective CO and NMOG oxidation catalysts which operate at low light-off temperatures that are associated with the low exhaust temperatures of diesel engines. Furthermore, PM emissions will need to be addressed. Diesel particulate filters (DPFs) are proven technologies to meet heavy-duty PM control needs, but may need further development for light duty Tier II vehicles that will operate with cooler exhausts environments during while meeting 3mg/mi standards.

c) Low-Temperature Combustion

Low-temperature combustion represents a variety of combustion techniques that utilize a more homogeneous fuel-air mixture to achieve lower gas temperatures in the engine cylinder during combustion to reduce NO_x and PM formation during the combustion process. Such engines, which may operate on a variety of fuels, emit lower NO_x and PM emissions but may also emit higher levels of CO and NMOG emissions (and particularly in some cases formaldehyde). Thus, the challenges for net lean, oxygen-rich, emission control shift in comparison to lean combustion via dilute gasoline and clean diesel techniques. Furthermore, the exhaust temperatures for low-temperature combustion can be significantly lower requiring lower light-off temperatures for catalysts.

Powertrain Efficiency Strategies

Another complicating factor for effective aftertreatment is the variability of powertrain strategies to meet future fuel economy standards. OEMs are now introducing vehicles that include hybrid technology, engine start/stop schemes, cylinder deactivation capability, and more extensive use of turbo charging to provide even greater fuel economy and performance. These approaches, together with employing advanced combustion processes, have further complicated aftertreatment solutions by lower heat energy in the exhaust for emission control devices.

a) Hybrid

Hybrid vehicles are continuing to enter the marketplace in increasing numbers despite their inherent cost disadvantage relative to conventional gasoline powertrains. The main driver for these vehicles is the increased fuel economy associated with operating these vehicles. Typical hybrid SUVs and cars are capable of running solely on battery power for most daily driving needs, implying little fuel use. However, when the hybrid gasoline engine is engaged to charge the battery or provide additional power assist, exhaust emissions are created. Since the engine is run infrequently, the exhaust aftertreatment is exposed to many more cycles of low temperature conditions requiring increased performance at lower temperatures to meet emissions standards. This is particularly challenging from the cost perspective. Usually, heavily PGM loaded catalysts are required to successfully remediate cold start exhaust emissions. Aftertreatment solutions that incorporate less costly new materials that will operate at low temperature would improve the cost disadvantage of hybrid vehicles.

b) Start/Stop Technologies

Strategies now being employed by automotive manufacturers to improve fuel economy include engine start/stop technologies when the vehicle is not moving. In a typical application, as a vehicle comes to a stop at a traffic intersection, normally, the engine continues to expend fuel by idling, but producing no useful work. The fuel cost associated with engine idling is estimated to be between 1–3%. By employing engine start/stop technologies, this fuel use can be eliminated. However, as with hybrid technologies, this strategy repeatedly deprives exhaust aftertreatment systems during normal driving. This creates the situation where exhaust catalysts are not operating at temperatures high enough for maximum performance. Current solutions require additional PGM to help compensate for the loss of exhaust heat. Potential cost effective alternatives include non-PGM materials or systems that possess high activity for TWC under these conditions or materials that adsorb and release HCs or NO_x at desirable temperatures.

c) Cylinder Deactivation

Employing engine cylinder deactivation to conserve fuel under cruising conditions does not, by itself, create challenging conditions for the aftertreatment system. Normally, temperatures are high enough and the catalytic system is sufficiently warmed up to cause a performance issue for traditional catalysts. Even if this strategy is combined with the aforementioned powertrain

methods for enhancing fuel economy, potential aftertreatment solutions would not require technologies not already present in the industry.

d) Turbo Charging

In addition to developing efficient combustion technologies, both lean and stoichiometric, OEMs are expanding their use of turbo charging to boost engine horsepower. These combined strategies allow vehicle manufacturers to employ smaller, more efficient engines, without sacrificing performance. However, the use of turbo charging and more efficient smaller engines significantly lowers the heat energy available in exhaust systems for emissions control catalysis. Also, the added thermal mass of the turbocharger and extraction of energy to create the boosted intake pressures decreases exhaust temperatures for downstream catalysts. This loss of exhaust energy is especially critical during the cold start portion of the FTP cycle where the activity of the catalyst is already challenged by low temperatures. Therefore, having noticeably reduced exhaust energy available for emission control catalysis will further complicate potential aftertreatment solutions and, based on currently available technologies, add greatly to the cost to meet more stringent emission standards. As an example, typical turbo chargers can lower the temperature of exhaust gas by much greater than 100°C even if a turbo bypass strategy is employed, at an additional cost, to maintain heat to downstream aftertreatment.

Common Needs for Low Temperature Performance

The need for low temperature emission control performance is common to all of the powertrain strategies of interest for meeting the new fuel economy standards. In addition, by nature, more efficient combustion will decrease the amount of wasted energy that exits the combustion cylinder in the form of heat in the exhaust. Thus, more fuel efficient engines and powertrains will create lower temperature conditions in the exhaust.

Alternative approaches for supplying additional heat to existing catalyst technologies, such as various post or late fuel injection strategies, may help attain emission regulation. However, this option is not preferred as providing heat by this method erodes the fuel benefits associated with greater combustion efficiencies enabled by the engine. Thus, modifying catalyst technology to meet the lower temperature conditions of the engine is greatly preferred to modifying the exhaust temperature to meet the catalyst needs. Therefore, regardless of the powertrain approach chosen to meet fuel economy standards, lower temperature catalyst performance will be required.

Reduced Development Time and Cost

Domestic automotive OEMs are continually attempting to shorten product cycles to compete with an ever increasing number of global manufacturers. This requires advanced powertrain work to be performed more efficiently and at costs that will not burden the multitude of vehicle programs that always under development. Recent economic events in the domestic automotive market have also required U.S. car companies to scale down their engineering staffs to maintain their viability in future year. This has increased the stress level on internal resources to support current and future product development. One way by which US manufacturers can more

effectively manage critical and limited resources would be to participate in pre-competitive activities for future products, such as those in the fields of engine and aftertreatment.

Improved Understanding

As mentioned, unlike earlier generations, current automotive OEMs have more limited internal capability to pursue a wide range of inception stage research into innovative materials and new technologies in the field of catalysis. This lack of resources creates a “knowledge gap” in the discovery process of new materials and the fundamental understanding of how these materials and systems would function in future exhaust environments. With the participation of the OEMs, the National Labs, and universities, the likelihood of bridging this gap and providing better solutions in a timely manner can be significantly improved.

4. Micro View – The 150°C Challenge (The Need)

An overview of each of the four sessions, that was the main focus of this workshop, is presented in this section. An extended, more detailed report for each of the sessions is accessible through the links provided in section 8.

Session 1: Modeling

In general, industry efforts to uncover new materials and processes are inherently time consuming and resource intensive. This holds especially true for chemical engineering. Past strategies, that relied mostly on the intuition of the investigators and prior art, often required years of research and experimentation to derive potentially viable solutions for chemical processes. In today’s competitive automotive landscape, the luxury of time is no longer available for discovery and product advancement to market. Therefore, advanced research and engineering organizations must rely on more sophisticated methods to more quickly locate and mine regions of the “material universe” to provide catalytic solutions.

Modeling at all levels (from atomistic to vehicle scales) is necessary to systemize our knowledge of aftertreatment and fully exploit current and future engine technologies that maximize fuel efficiency while meeting environmental constraints. The modeling breakout group constructed Figure 3 to illustrate this point. The type of computational simulation required to overcome the barriers stemming from the expected low exhaust temperatures of the future will require a vertically integrated approach for linking these different scales.

Aftertreatment modeling has already been employed in many ways. Examples of strengths in the current state of the art include:

- Widely published heterogeneous catalysis reaction mechanisms;
- Extensive pre-competitive collaborations and reference lab and dynamometer data and catalyst sharing among labs, universities, and industry (e.g., CLEERS);
- Advanced experimental capabilities to measure local and global reaction rates and intermediate species;
- Powerful software and algorithms for computational simulations of dynamic device and

- vehicle systems performance;
- DOE & NSF support of both fundamental catalysis science and applied aftertreatment;
- Government-sponsored high performance computers capable of highly detailed atomistic-scale simulations.

However, there are important limitations in the current state of aftertreatment modeling and simulation which need to be recognized and addressed, including:

- Incomplete leveraging among fundamental and applied catalyst R&D programs in DOE and between DOE and NSF.
- Limited application of molecular simulation and microkinetic modeling as tools for mechanistic analysis and for new catalyst discovery
- Incomplete access and utilization of the advanced computing capabilities at national labs and universities for simulating catalyst chemistry and physics; and
- Incomplete utilization of the full range of advanced synthetic and experimental measurement techniques currently available at national labs and universities for catalyst model development and validation;
- The lack of explicit shared values for key kinetic rate parameters for reference catalysts;
- The unavailability of detailed transient laboratory and dynamometer measurements of catalyst performance under well-defined conditions that are directly relevant to the full range of exhaust conditions generated by advanced light and heavy duty engines in both conventional and hybrid vehicles;

In the modeling breakout session, the following specific recommendations for addressing the above limitations were identified:

- Low-T limits of current aftertreatment technology need to be accurately established including, for example, fundamental studies aimed at determination of reaction mechanisms and catalyst structure/function;
- R&D to link atomistic and system scale models needs to be accelerated;
- Closer integration between modeling and experiments is needed and should include:
 - Standard conditions/parameters across the research community
 - Integration of models with advanced *operando* catalyst characterization
 - Cross validation of modeling discovery and approaches
 - More effective sharing of pre-competitive data and models
- Experiments and models should be hypothesis/question driven (e.g., Does CO inhibition limit low-T TWC, does NH_4NO_3 decomposition set low-T SCR limit, is NO oxidation limiting SCR performance?);
- Government support of both vertically structured proprietary and pre-competitive aftertreatment R&D is needed to maximize chances of meeting the needs of the next generation of commercial vehicles.

Specific performance targets for future low-temperature aftertreatment modeling R&D should include:

- Catalyzed NO_x reduction;
- Catalytic HC, NO and CO oxidation;
- Passive storage of NO_x, HC, and CO;
- Soot filter regeneration;

- Fuel effects on the above (e.g., alternative and renewable fuels); and
- Integrated catalyst architectures (e.g., layered or segmented catalysts).

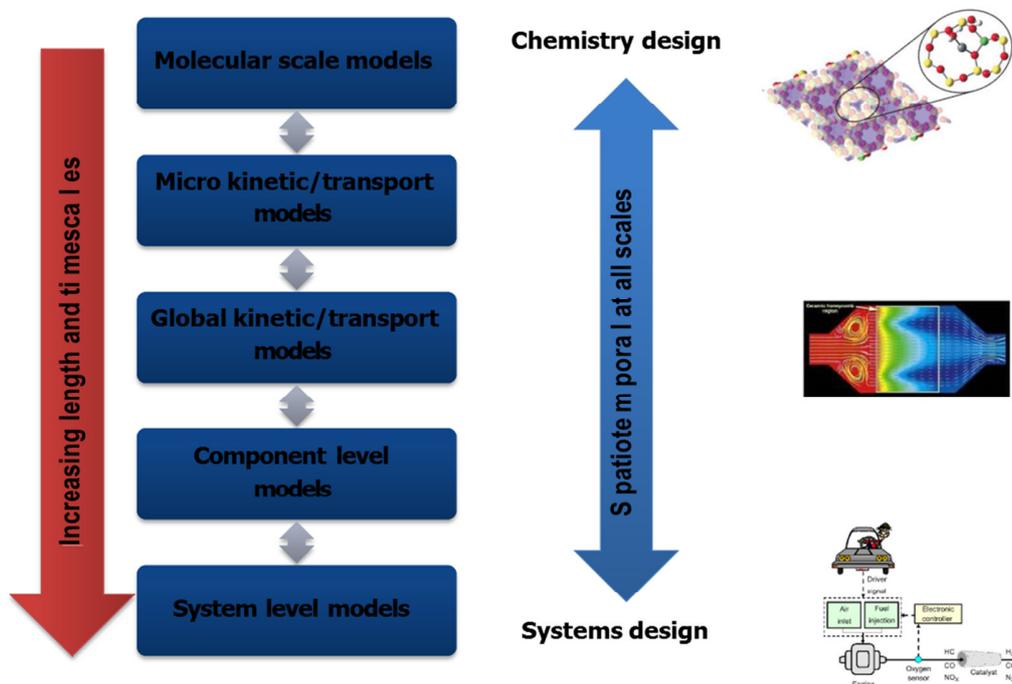


Figure 3. Modeling Program Links - Aftertreatment modeling must account for the effects of multiple scales, because there are multiple physical processes which can limit low temperature performance. At the atomistic level, the energetics and kinetics of the surface chemistry constrain what reaction products are possible and how fast the pollutant species are converted. At the vehicle scale, the dynamic interactions between the aftertreatment devices and engine determine the actual exhaust temperatures and species inputs experienced by the catalysts under driving conditions. Multiple heat and mass transport steps occur in between.

Session 2: Materials

The primary aftertreatment emission control technique is catalysis which relies heavily on a wide range of materials. The core chemical reactions to convert pollutant emissions to inert species occur on the surface of active metal nanoparticles and metal oxides. Proper selection, manufacture, and design of these materials is critical to achieving high catalyst performance; furthermore, keeping the catalyst surface stable and free from poison agents is also critical to maintaining low emission performance over the life of the catalyst.

Two main drivers are challenging existing catalyst material performance. As engines become more efficient through the implementation of advanced combustion techniques, the engine exhaust is, on a load-specific basis, cooler in comparison to more conventional engine technology. Another main challenge related to achieving emissions standards for SULEV vehicles is controlling the exhaust emissions occurring during vehicle startup and the subsequent

“warm up” period. Current estimates show that >99% conversion efficiency must be obtained over the entire FTP drive cycle in order for the most stringent emissions targets to be met. This cannot occur without 90% conversion efficiency achieved during the lightoff and warm up portions of the drive cycle. The combination of lower engine exhaust temperatures (from more efficient engines) and higher importance of controlling cold start emissions (to meet strict emission regulations) prevents current aftertreatment from meeting required emission levels. Current catalysts exhibit significantly lower catalytic activity below 200°C, which would occur during significant portions of the startup and subsequent portions of the drive cycle (figure 4).

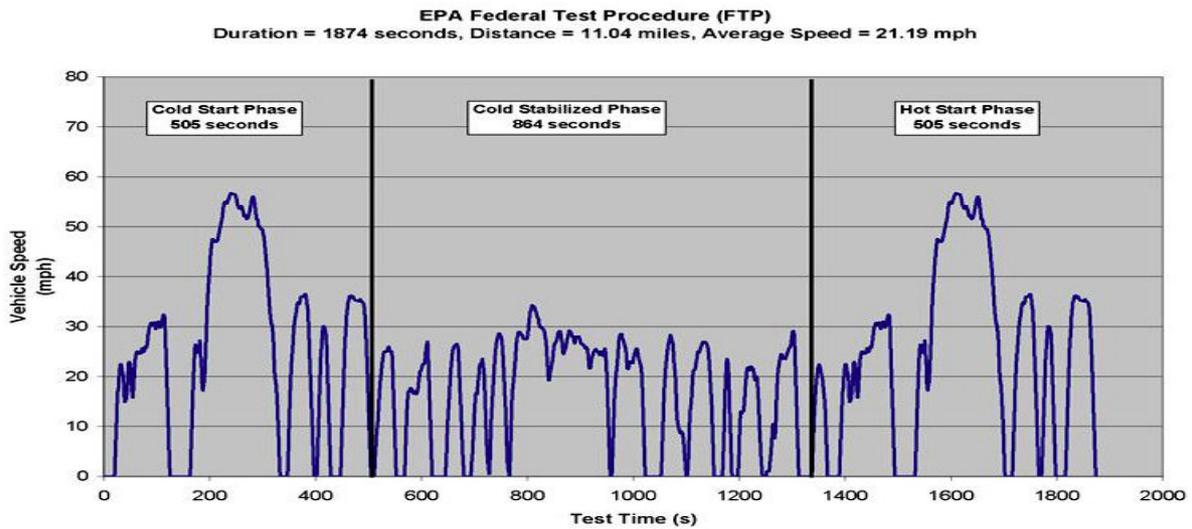


Figure 4. FTP Emissions Drive Cycle (www.epa.gov)

This is evident for both PGM and base metal formulations. Also, thermodynamic limitations or energy barriers may preclude materials from having catalytic capability at 150°C. This aspect has not been addressed satisfactorily yet, but would be an integral component of this roadmap of uncovering and characterizing materials that exhibit potential for low temperature activity.

In addition to low temperature performance, the same catalyst solutions must maintain high conversion efficiencies over as wide a temperature range as possible to capture emissions occurring under various engine operating conditions during required drive cycle performance. The process of uncovering and developing new catalytic materials that are chemically active at 150°C with an appropriate temperature window of operation is not an evolutionary development in catalyst technology. Rather, this characteristic of catalyst behavior would be a revolutionary development in catalyst technology.

Catalyst product selectivity is equally important from a performance viewpoint. It is not sufficient for a catalyst or catalyst system to merely remove NO_x, HC, and CO from the exhaust stream. These species must be converted into species that meet EPA standards for emissions, GHG, and CO₂ gases. SULEV emissions standards targeted by this program for catalyst system technologies require meeting government mandated 0.030 g/mi of NMOG + NO_x.

Further increasing the challenge of aftertreatment development are engineering specifications within OEM organizations that require a safety margin of 10 to 30% of the emission standards effectively mandating 0.018g/mi to 0.027g/mi NO_x + NMOG over the FTP driving cycle. This

margin is required for commercialization by OEMs to ensure in-field performance of aftertreatment systems. LEV III program requirements stipulate 150K mile durability of the aftertreatment systems for vehicles entering the market in 2018. Additionally, these mandates apply to a variety of Phase II and III fuels that will be in the domestic marketplace. Ethanol blends in particular can create further hurdles to overcome especially during required 50°F testing. The lower energy content of these fuels provide less heat to the exhaust, delaying the onset of catalyst lightoff and contributing to vehicle emissions.

Addressing the collection of emission performance and durability challenges will require innovative advancements in catalyst material technology. This materials-focused section provides roadmap guidance for the material research and development activities of merit. In addition to catalytic materials, materials for adsorption or “trapping” of pollutants and/or pollutant reducing agents are included as adsorption-based approaches are also of significant interest.

Session 3: Industry and Supplier Needs

The overriding consensus of this session agreement was that the process of material discovery and development must be a closely coordinated effort among OEMs, suppliers, and research organizations. Traditionally, this has not occurred in non-OEM research facilities where research was typically geared toward a solution for a particular problem. However, this methodology, although effective at providing a potential solution, did not always take into consideration the needs of the industry. For a solution to be viable, it must meet the requirements of the end users in two areas:

- Material or component properties
- Product development process

In the automotive industry, where part volumes are normally in the tens of millions, any potential material or component technology must broadly possess the properties:

- Sustainability/Durability
- Availability
- Cost
- Manufacturability/Scalability

In addition, to material and component properties required by OEMs and suppliers, the product development process must also take into consideration OEM and supplier needs. This too requires more interaction between the industrial partners and the research and development organizations participating in projects related to low temperature aftertreatment. Highly efficient combustion strategies currently under investigation as part of ACEC activities will be generating different exhaust compositions and conditions as well as working under different cylinder environments than many previous stoichiometric combustion engines. As a result, every effort should be made to assure that potential solutions are consistent with the need of the industry. Therefore, the following areas must be thoroughly addressed in the product development process:

- Research areas of interest

- Supplier/OEM roles
- Commonized testing procedures
- Commonized testing conditions (T, SV, exhaust composition)

Session 4: System Integration

The representatives to the System Integration team concluded that the future powertrain architectures to address high fuel efficiency standards are by no means universally agreed upon. Numerous technologies are available (or are in development) that may ultimately be utilized. How the overall system is finally optimized will have a strong impact on the specific requirements from the aftertreatment system and, therefore, the unique catalytic challenges. For example, the ACEC technical team roadmap suggests three possible combustion approaches: dilute gasoline combustion, clean diesel combustion and low temperature combustion. Likewise, specific technologies/approaches may be brought to the market such as;

- down-sizing and down-speeding
- multi-mode combustion
- lean stratification
- increased use of turbocharging
- variable CR
- VVTs

To anticipate every possible solution and its impact on aftertreatment system requirements was beyond the scope of this workshop. The group felt that the ultimate approach will require an iterative process between the combustion, drivetrain and aftertreatment research organizations. In order to provide guidance to the initial definition of this process the group felt it was important to identify the likeliest candidates as seen from this moment in time. The consensus was that most of the automotive fleet would fall into one of the following two categories:

- Stoichiometric with EGR, DI, turbo, VVT
- Lean stratified DI with lean NO_x aftertreatment (LNT and/or SCR)

To varying degrees, any of the anticipated future system architectures will have to deal with the two critical aspects of exhaust temperature management:

- Getting the catalyst to operating temperature quickly after cold start with minimal fuel penalty
- Maintaining catalyst temperature in acceptable range
 - Avoid light out in light load conditions
 - Manage peak temperature to avoid thermal aging degradation.

In the case of stoichiometric operations, a general statement of criteria can be described as follows:

- temperature range needed from catalyst
 - TWC: 150C light off, tolerate 1000C (900C with full load cooled EGR or VCR)
 - trap materials: trap near ambient, release above TWC light off

While in the case of lean operations (case #2), a general statement of criteria can be described as follows:

- temperature range needed from catalyst

- LNT and/or NH₃ SCR and/or HC SCR and/or TWC: 150C light off, tolerate 1050C (900C with full load EGR or VCR)
- HC/passive NO_x trap: Trap from room temperature to hot enough for the rest of the system to remove as it desorbs.

5. Global View – The 150°C Challenge (The Benefit)

Lowering emissions from on-road vehicles touches many aspects of our domestic and global societies. These benefits are both broad in scope and far reaching. Chief among them, with respect to this workshop, is the enabling of highly efficient powertrains to enter the local and international markets. By US auto manufacturers successfully meeting the twin challenges of increasingly stringent fuel economy and emissions standards, a more competitive and healthy domestic auto industry will result providing greater opportunity for additional employment in the future. The downstream net effect of this can then be felt in a number of areas. With regard to the consumer, increasing fuel economy and the ability to operate a vehicle with a number of fuel sources, positively impacts the cost of ownership. For instance, a 10% increase in fuel economy from the base case of 23.0/17.1 mpg will result in saving 12.8 billion gallons gasoline annually, which is equivalent to \$47 billion/year (at \$3.68/gallon 2012 US price). This discretionary savings could then flow into the U.S. economy supporting domestic industries. In addition, by lowering the demand of traditionally imported energy sources, US energy independence and national security can be greatly improved. [Transportation Energy Data Book, Ed. 31, 2010].

Significant environmental benefits will also result from emissions enabled high efficiency engine and powertrain technologies. Tier II Bin 2 and SULEV emissions standards, which are goals of this work, will be the cleanest in the world. This will greatly lower the rate harmful emissions enter the atmosphere from automotive sources. Human health studies indicate that the resulting incidence of cancer and lung ailments will also decrease by instituting these standards. Additionally, as a result of 20% improvement in engine efficiency, also a goal of the ACEC roadmap, a corresponding decrease in CO₂ emissions will be realized. This slowing in the accumulation of the primary greenhouse gas in the atmosphere is expected to positively impact the rate of global warming and lessen adverse associated climatic effects.

The United States has always led global aftertreatment development to achieve very stringent emissions standards. However, the US image as a leading green country has diminished somewhat in recent years in the eyes of the world community due to the country's contribution to fossil fuel derived atmospheric CO₂. By increasing engine efficiency and reducing exhaust emissions targeted by ACEC-like activities, the US will improve its stance as a recognized leader in support of sustainable energy, transportation, and environmental policies.

6. Workshop Structure

Attendees (fields of expertise)

The 55 scientists and specialists from universities, government, and industry that participated in this workshop represented a number of areas in catalysis and aftertreatment research and development. Each attendee was chosen by the workshop organizers based on their recognized contributions to the focus areas of this workshop and/or their stature and responsibilities within

their respective communities. In addition, the composition of attendees was such that each session could be equally staffed to increase the likelihood that in-depth and high level discussions would take place within each session to yield a sound technical roadmap.

Represented Fields:

Four main areas of the catalysis community were represented at this event. The industry group included the automotive OEMs, GM, Ford, and Chrysler. This segment included both powertrain program directors and aftertreatment specialists. Also in attendance were members of the OEM aftertreatment supply chain. All three major suppliers of catalysts, Umicore, BASF, and Johnson Matthey, were well represented along with technical leaders from of Bosch, FEV, Cummins and many others that support aftertreatment activities with the domestic automakers.

Members of various U.S. government agencies were also able to attend. Chief among them were officials from the DOE, NSF, and BES which provided key insight into ongoing programs at the agencies in support of domestic automakers. In addition, well respected research scientists from PNNL and ORNL contributed heavily to the workshop discussions and provided their perspective on the problems and challenges.

Also contributing significantly to the workshop sessions were recognized leaders in the fields of catalysis and modeling from a dozen universities and private institutions. These individuals were critical to the success of this workshop because of their wide range of knowledge related to approaches and methods of new material discovery. A full list of attendees is provided in the **appendix***.

Session Focus Areas

Four topic areas were identified as critical to developing a low temperature aftertreatment technology roadmap for ACEC projects and programs. Although all four areas are required elements of a viable roadmap, the Industry and Supplier Needs component must drive the other three areas of research and development. The four areas referenced are:

- Modeling from Molecular to System Level
- New Materials and Research Directions
- Industry and Supplier Needs (From Discovery to Market)
- System Engineering and Architecture (Controls, Sensors, and OBD)

Workshop Program

Thursday – November 29, 2012

Meeting Welcome

08:00 - 08:10 Craig DiMaggio – Chrysler - Welcome, Workshop Purpose/Objectives, Agenda

Department of Energy (DOE) and Industry Overview

- 08:10 - 08:30 Ken Howden – DOE OVT – Perspective and Role of Office of Vehicle Technologies
- 08:30 - 08:50 Mike Harpster – GM R&D Propulsion Systems Research Lab, (Director, APTLC) – Industry view of the direction of powertrain development

Nature of the Problem from Industry Perspective

- 08:50 - 09:10 Christine Lambert – Ford - History of automotive emission control
- 09:10 - 09:30 Joe Kubsh – MECA – LEV_{III} and global emission requirements
- 09:30 - 09:50 Mike Zammit – Chrysler – The need for low temperature aftertreatment
- 09:50 - 10:10 Break

Specific Scientific and Technical Challenges

- 10:10 - 10:30 Chuck Peden – PNNL – The scientific challenge of low temperature aftertreatment
- 10:30 - 10:40 Dick Blint – N₂Kinetics – Combinatorial studies for high frequency testing - Lessons learned from successful CRADAS
- 10:40 - 11:00 Bill Schneider – University of Notre Dame - Catalytic reaction mechanisms
- 11:00 - 11:20 Dean Tomazic – FEV - System challenges for emission control

Potential Pathways

- 11:20 - 11:40 Abhaya Datye – University of New Mexico – Evidence of highly active catalytic materials
- 11:40 - 12:00 BASF Tian Luo – Low Temperature Light-off Challenge for Three-Way Conversion Catalysts

Workshop Plan

- 12:00 - 12:20 Session Chairs objectives/instruction (5 min/session)
- 12:20 – 01:30 Lunch (room setup)

Day 1 Breakout sessions

- 01:30 - 04:00 Day 1 breakout session (may include break)
- 04:00 - 05:00 Interim report drafting, plan for Friday

Friday – November 30, 2012

- 08:00 - 11:30 **Day 2 Breakout sessions**
- 08:00 - 08:40 Interim reports (4) and day 2 objectives
- 08:40 - 10:40 Day 2 breakout sessions
- 10:40 - 11:00 Break
- 11:00 - 12:00 Report drafting

12:00 - 01:00	Lunch
01:00 - 02:00	Reports and Technology Roadmap
02:00 – 02:15	Departing Comments and Adjournment

a) Session Chairs

- Session 1: **Dick Blint / Stuart Daw / Bill Schneider**
Modeling from Molecular to System Level
- Session 2: **Galen Fisher / Mark Crocker / Steve Overbury**
New Materials and Research Directions
- Session 3: **Tim Johnson / Joe Kubsh**
Industry and Supplier Needs (From Discovery to Market)
- Session 4: **Dean Tomazic / John Hoard / Magdi Khair**
System Engineering and Architecture
(Controls, Sensors, and OBD considerations)

b) Session Goals

Breakout Session #1 (Day 1):

Overall objective: Brainstorm to define the key scientific and technical needs and challenges to address, and what approaches are best suited for the program.

Breakout Session #2 (Day 2):

Overall objective: Draft a program scope related to the session topic based on Day 1 discussion including specific activities and goals with timelines.

- Commence assembling main elements of each session into a preliminary technology roadmap outline for low temperature aftertreatment
- Propose natural working groups or partnerships and their roles in providing effective research and development solutions

7. Technology Progression from Basic Science to Product Application

The general consensus, based on discussions and information presented at this workshop, is that catalytic materials and components capable of reducing NO_x and oxidizing HCs and CO with >90% efficiency at 150°C in an automotive exhaust environment is not an evolutionary development of current technologies. Rather, this effort would be a revolutionary departure to new approaches requiring inception stage research and development efforts. If this R & D endeavor is to be adopted, it must first begin with identifying the research institutions and partnerships that will search for these new materials. The proposed process of intelligently searching the “material universe” for possible solutions, should begin with a well-organized modeling/search algorithm to expedite discovery and laboratory activities that are used to filter high throughput testing of potential candidates. However, as can be seen in the figure 5 below, the entire project timeline is compressed relative to past efforts. The inception stage work, which normally requires 5-10 years, would be limited to a 3 year timeframe where multiple

parallel pathways would be investigated. This is equivalent to passing research from TRL 1 to TRL 3 levels within the national laboratories research ladder. Promising technologies passing this phase would enter the 2016/2017 window where the effort level would begin to transition to industry led groups to scale-up and test under exhaust-like conditions. This activity would be the equivalent of a TRL 4 to TRL 8 program within the national laboratories. Finally, in 2020, an industry and supplier led effort at the vehicle level or simulated vehicle level demonstration would act as a proof of concept for technologies surviving to this stage. The contributions from the different project participants are shown in figure 6.

Timeline of ACEC Aftertreatment Development

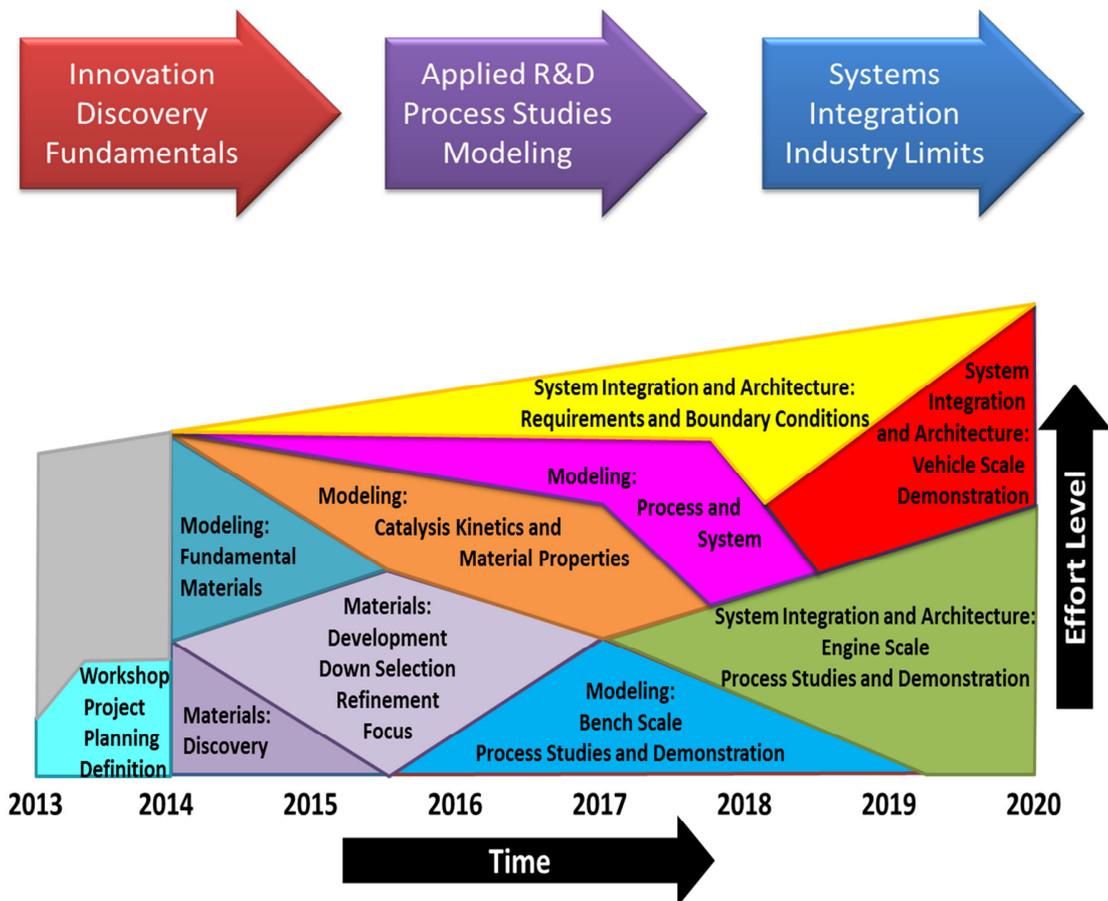


Figure 5. Resource Allocation Timeline

Materials: Discovery	NSF, BES; National Labs, Universities, Material Suppliers; Innovative Approaches
Materials: Development, Down Selection, Refinement, Focus	EERE; NLS, Universities, Tier 1, Industry; Selection and Development
Modeling: Fundamental Materials	NSF, BES; National Labs, Universities; Atomic Level Modeling
Modeling: Catalyst Kinetics and Material Properties	BES, EERE; National Labs, Universities; Modeling Core Functionality
Modeling: Process and System	EERE; National Labs, Universities; Modeling Catalyst as Component in system
Modeling: Bench Scale Process Studies and Demonstration	EERE; National Labs, Tier 1, Industry; Understanding Process, Function
Sys. Int. & Arch.: Engine Scale Process Studies and Demonstration	EERE; National Labs, Tier 1, Industry; Devices in Real Exhaust, Fuel Penalty
Sys. Int. & Arch.: Vehicle Scale System Integration and Demonstration	EERE, Industry: Tier 1; Prototype Vehicle Systems under Transient Cycles
Sys Int. & Arch.: Requirements and Boundary Conditions	Industry, Tier 1 and 2 Suppliers; Reality Checks, Feedback, Guidance

Figure 6. Resource Activities

Coordinated or complementary development efforts, within the DOE laboratory structure, would begin with inception stage research in the Office of Science (Basic Energy Sciences) where fundamental technology and techniques are first generated (figure 7). Partnerships should be proposed between this DOE office and those entities previously mentioned so that a combined effort can leverage the research strengths of the participating organizations to expedite the process of discovery. As the newly developed technologies transition from basic laboratory investigations to scaled or proof of concept level, more of the development will be performed with participation of the Office of Vehicle Technology (OVT) within the DOE as shown below. Final stage development, with a vehicle or total system simulation, would then be undertaken with the automotive OEMs leading this effort. Internal resources at the automakers along with their suppliers would provide the necessary technology and specifications required to demonstrate a functional system.

Research & Development Technology Movement from BES to OVT

Relationships Between the Science and the Technology Offices in DOE

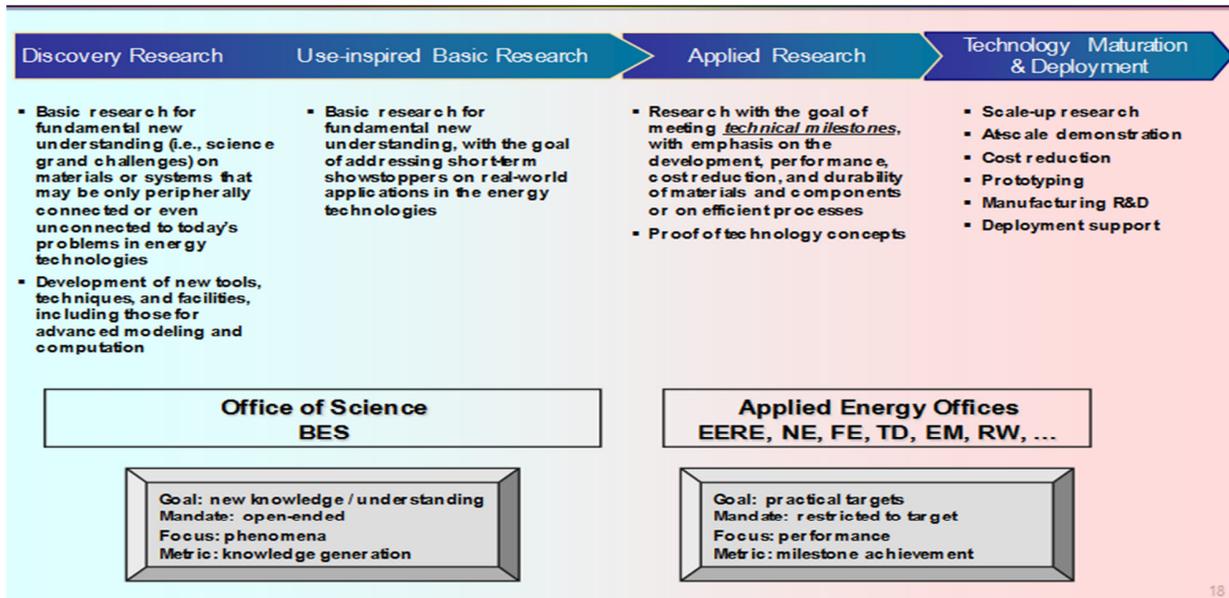


Figure 7. Technology Development Progression (BES – OVT)

8. Session Reports (Recommended Pathways and Priorities)

- **Session 1: Modeling from Molecular to System Level**

Dick Blint / Stuart Daw / Bill Schneider



(Modeling_Appendix_for_workshop_report_May6.pdf)

- **Session 2: New Materials and Research Directions**

Galen Fisher / Mark Crocker / Steve Overbury



(Materials_Approach_Section_20130318.pdf)

- **Session 3: Industry and Supplier Needs (Discovery to Market)**

Tim Johnson / Joe Kubsh



(Session_3_Industry_and_Supplier_Needs_Report_033113.pdf)

- **Session 4: System Engineering and Architecture**

Dean Tomazic / John Hoard / Magdi Khair



(Workshop_report_systems_breakout_March_15th.pdf)

9. Workshop Summary (Roadmap)

Traditionally, the United States has always led the world in the implementation of emissions control technologies due to highly restrictive vehicle exhaust emissions that have been mandated by congress. To maintain that leadership role and to meet the timeline of increasing stringent emissions standards, advanced catalytic materials and approaches must be pursued and developed within a shorter period of time. This challenge is further heightened by the emergence of highly efficient combustion processes, powertrain strategies, and a more complex mix of fuels to achieve mandated fuel economy targets. All these developments have stressed currently available aftertreatment solutions by robbing significant heat energy from the exhaust system. Therefore, to effectively meet the mandated twin hurdles of powertrain efficiency and emissions reduction, catalytic materials and systems must be uncovered that will function at greater than 90% efficiency at much lower temperatures. The stretch goal set by this workshop consortium was to obtain this efficiency at 150°C, which would represent a grand challenge in catalyst technology and push the thermodynamic limits of any catalytic material.

To achieve the goal of 90% efficiency at 150°C will require close cooperation between the national laboratories, universities, and the OEM community on projects. In general, the main highlights of this workshop include:

- Enhance computation modeling tools to significantly reduce the time for discovery and development of new materials that possess the appropriate characteristics for low temperature functionality.
- Create system modeling tools to determine the performance of the aftertreatment system in addition to component activity is critical.
- Research new methods of enhancing precious metal activity and stability at low temperatures while improving poison resistance.
- Develop alternative PGM materials capable of supporting HC, CO, and NO_x conversion reactions under exhaust conditions that will be present in future powertrains.
- Uncover materials that can adsorb and release HC, CO, and NO_x species at challenging points in emission test cycles for greater aftertreatment efficiency.
- Provide standardized testing and screening methods and guidelines for uncovering potential catalytic solutions to ensure OEM needs are captured in research activities.
- Develop system controls and sensors using materials that have the ability to function at the temperatures, conditions, and are compatible with aftertreatment components.
- Understand and account for fuel effects on the efficiency and selectivity of catalyst based technologies.

10. Recommended Path Forward

Based on the discussions held at the workshop, the following recommendations for technical and organizational paths forward are presented:

Technical Path Forward:

Achieving the “90% Conversion at 150°C Goal” requires:

- Promoting innovative catalytic solutions via partnership with DOE BES activities
 - Special emphasis on chemical and thermal catalyst stability in these studies to insure potential solutions are practical ones
- Effective simulation and modeling for design and understanding of processes from nanoscale to full scale
- Performing research on new “trap” technologies as an alternate approach (to lower temp conversion)
- Performing system level research and integration to determine practical solutions that perform under realistic exhaust conditions

Organizational Path Forward:

- Increase total program level of effort to accelerate progress for better alignment with OEM timelines
- USDRIVE ACEC Tech Team to promote and coordinate national labs, universities, and industry activities
- Periodically assemble broader R&D technical teams to review progress and discuss challenges
- Co-funded government/industry teams to provide consistent system requirements and guide down-selection of technology R&D
- Ensure access to DOE User Facilities



ACEC “150°C Challenge” Workshop Participants

11. Appendices:

See VROOM Folder