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VEHICLE TECHNOLOGIES PROGRAM

ADVANCED COMBUSTION ENGINE TECHNOLOGIES

U.S. Department of Energy
Energy Efficiency and Renewable Energy
Bringing you a prosperous future where energy is clean, abundant, reliable, and affordable

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FY 2008 PROGRESS REPORT FOR ADVANCED COMBUSTION ENGINE TECHNOLOGIES

Energy Efficiency and Renewable Energy
Office of Vehicle Technologies

Approved by Gurpreet Singh
Team Leader, Advanced Combustion Engine R&D
Office of Vehicle Technologies

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I. INTRODUCTION

I. Introduction

DEVELOPING ADVANCED COMBUSTION ENGINE TECHNOLOGIES

On behalf of the Department of Energy's Office of Vehicle Technologies (VT), we are pleased to introduce the Fiscal Year 2008 Annual Progress Report for the Advanced Combustion Engine Research and Development (R&D) Sub-Program. The mission of the VT Program is to develop more energy-efficient and environmentally friendly highway transportation technologies that enable the United States to use less petroleum. The Advanced Combustion Engine R&D Sub-Program supports this mission by removing the critical technical barriers to commercialization of advanced internal combustion engines for passenger (cars and light trucks) and commercial (medium and heavy trucks) vehicles that meet future Federal emissions regulations. Improving the efficiency of internal combustion engines is the most promising and cost-effective approach to increasing vehicle fuel economy (miles traveled per gallon of fuel) in the next 10 to 20 years or until such time that plug-in hybrid electric or fuel cell hybrid vehicles dominate the market. Improved fuel economy with advanced combustion engines will reduce our transportation fuel consumption, thereby improving our energy security, environment, and economy.

Advanced internal combustion engines are a key element in the pathway to achieving the goals of the FreedomCAR and Fuel Partnership for transportation. Advanced engine technologies being researched will allow the use of hydrogen as a fuel in highly efficient and low-emission internal combustion engines, providing an energy-efficient interim hydrogen-based powertrain technology during the transition to hydrogen/fuel cell-powered transportation vehicles. Hydrogen engine technologies being developed have the potential to provide diesel-like engine efficiencies with near-zero air pollution and greenhouse gas emissions.

This introduction serves to outline the nature, recent progress, and future directions of the Advanced Combustion Engine R&D Sub-Program. The research activities of this Sub-Program are planned in conjunction with the FreedomCAR and Fuel Partnership and the 21st Century Truck Partnership (21CTP) and are carried out in collaboration with industry, national laboratories, and universities. Because of the importance of clean fuels in achieving high efficiency and low emissions, R&D activities are closely coordinated with the relevant activities of the Fuel Technologies Sub-Program, also within VT.

BACKGROUND

Advanced combustion engines have great potential for achieving dramatic energy efficiency improvements in light-duty vehicle applications, where they are suited to both conventional and hybrid-electric powertrain configurations, and can accept non-petroleum fuels like ethanol, biodiesel, and hydrogen. Light-duty vehicles with advanced combustion engines are projected to have energy efficiencies that are competitive with hydrogen fuel cell vehicles when used in hybrid applications. The primary hurdles that must be overcome to realize increased use of advanced combustion engines in light-duty vehicles are the higher cost of these engines compared to conventional engines and compliance with the U.S. Environmental Protection Agency's (EPA's) Tier 2 regulations which are phasing in from 2004-2009. The Tier 2 regulations require all light-duty vehicles to meet the same emissions standards, regardless of the powertrain. Compliance can be achieved with advanced combustion engines through the addition of catalytic emission control technologies, though these technologies are much less mature than gasoline engine catalysts and are severely affected by sulfur from the fuel and lubricant. Even the recent reduction of diesel fuel sulfur content to below 15 ppm does not assure that catalytic emission control devices will be durable and cost-effective. The Advanced Combustion Engine R&D Sub-Program focuses on developing technologies for light-, medium-, and heavy-duty internal combustion engines (ICEs) operating in advanced combustion regimes, including homogeneous charge compression ignition (HCCI) and other modes of low-temperature combustion (LTC), which will increase efficiency beyond current advanced diesel engines and reduce engine-out emissions of nitrogen oxides (NOx) and particulate matter (PM) to near-zero levels.

The heavy-duty diesel engine is the primary engine for commercial vehicles because of its high efficiency and outstanding durability. However, the implementation of more stringent heavy-duty engine emission standards, which were phased in starting in 2007 (100% implementation in 2010), is anticipated to cause a reduction in fuel efficiency due to the exhaust emission control devices needed to meet emissions regulations for both NOx and PM. Heavy-duty vehicles using diesel engines also have significant potential to employ advanced combustion regimes and a wide range of waste heat recovery technologies that will both improve engine efficiency and reduce fuel consumption.

Advanced engine technologies being researched and developed by the Advanced Combustion Engine R&D Sub-Program will also allow the use of hydrogen as a fuel in ICEs and will provide an energy-efficient interim hydrogen-based powertrain technology during the transition to hydrogen/fuel cell-powered transportation vehicles.

Given these challenges, the Advanced Combustion Engine Technologies Sub-Program is working toward achieving the following objectives:

- Advance fundamental combustion understanding to enable design of engines with inherently lower emissions, and eventually advanced engines operating predominantly in low-temperature or HCCI combustion regimes. The resulting technological advances will reduce the size and complexity of emission control devices and minimize any impact these devices have on vehicle fuel efficiency. A fuel-neutral approach is being taken, with research addressing gasoline-based LTC engines as well as diesel-based advanced engines.
- Increase overall engine efficiency through fundamental improvements such as advanced combustion processes, reduction of parasitic losses, and recovery of rejected heat.
- Improve the effectiveness, efficiency, and durability of engine emission control devices to enable these engines to achieve significant penetration in the light-duty market and maintain their application in heavy-duty vehicles.
- Develop highly efficient hydrogen engine technologies with near-zero NOx, PM and greenhouse gas emissions.
- Identify that any potential health hazards associated with the use of new vehicle technologies being developed by VT will not have adverse impacts on human health through exposure to toxic particles, gases, and other compounds generated by these new technologies.
- Develop advanced thermoelectric technologies for recovering engine waste heat and converting it directly to useful energy that will significantly increase vehicle fuel economy.

Technology Status

Continuing advances in fuel injection and combustion systems have made the diesel engine very attractive for light-duty vehicle use by reducing the combustion noise associated with diesel engines, and consumers are discovering that modern turbocharged diesel engines offer outstanding driveability and fuel economy. The change-over to ultra-low-sulfur diesel fuel enabled catalytic exhaust treatment devices that virtually eliminate the offensive odors associated with diesel engines and further improve their prospects for wider use in light-duty vehicles.

Current heavy-duty diesel engines have efficiencies in the range of 42-43%. Moderate progress in efficiency has continued in the last decade while achieving NOx and PM emission reductions on the order of 90%, which is overall a great success. Improvements in a wide variety of engine components such as for boosting, thermal management, and recovery of rejected thermal energy are expected to enable efficiencies to reach 50% if aggressive R&D is able to proceed. The fuel efficiency of heavy-duty diesel engines is highly valued and emission controls reduce efficiency, increase fuel consumption (e.g., fuel used for regeneration of NOx catalysts, or both).

In early 2007, the U.S. EPA finalized its guidance document for using selective catalytic reduction (SCR) employing urea for regeneration (urea-SCR) technology for NOx control in light- and heavy-duty diesel vehicles and engines. This opens the door for the introduction of SCR technology in Tier 2 light-duty vehicles, heavy-duty engines, and in other future diesel engine applications in the United States. The U.S. EPA has put regulations in place to assure that users of urea-SCR vehicles don't operate them without replenishing the urea, which makes the catalysts ineffective. Using urea-SCR, light-duty manufacturers will be able to meet Tier 2, Bin 5 which is the "gold standard" at which diesel vehicle sales do not have to be offset by sales of lower emission vehicles. Heavy-duty diesel vehicle manufacturers are attracted to urea-SCR since it has a broader temperature range of effectiveness than competing means of NOx reduction and allows the engine/emission control system to achieve higher fuel efficiency.

Both light-duty vehicle and heavy-duty engine manufacturers have responded positively to these regulations. On the light-duty vehicle side, Mercedes-Benz is offering 2008 diesel passenger cars using urea-SCR that meet the Tier 2, Bin 8 standard. For 2009, Mercedes-Benz has already certified these vehicles and diesel sport utility vehicles (SUVs) to Tier 2, Bin 5 and California LEV-II making them available in all 50 states. Volkswagen and Audi plan to offer diesel SUVs using urea-SCR, a diesel oxidation catalyst (DOC), a diesel particulate filter (DPF), and a NOx sensor which will allow them to be certified to the Tier 2, Bin 5 standard. On the heavy-duty engine side, all the engine manufacturers except for Navistar have indicated that they plan to employ urea-SCR to certify their engines to 2010 regulations. For PM control, both light-duty vehicles and heavy-duty engines are relying on DPFs, often paired with DOCs to facilitate passive or active regeneration. DPFs are typically capable of reducing PM emissions by 95% or more.

The other technology being considered for NOx control from diesel engines is lean-NOx traps (LNTs), also known as NOx adsorbers. LNTs appear to be favored by light-duty manufacturers given that Volkswagen has certified its 2009 diesel Jetta to Tier 2, Bin 5 and California LEV-II using one in conjunction with exhaust gas recirculation (EGR), an oxidation catalyst and DPF. Honda plans to introduce a diesel passenger car to the U.S. in 2009 that meets the Tier 2, Bin 5 standard using NOx adsorber technology and a particulate filter. These products are the direct result of regulation to reduce fuel sulfur content and R&D to develop advanced emission control technologies. LNTs have a larger impact on fuel consumption than urea-SCR but light-duty vehicle manufacturers prefer LNTs since overall fuel efficiency is less of a concern than for heavy-duty engine manufacturers, and because urea replenishment represents a larger concern for light-duty customers than for heavy-duty vehicle users. Other drawbacks to LNT use on heavy-duty vehicles are that they are larger in relation to engine displacement (being over twice as large as those required for light-duty vehicles), the "not-to-exceed" operating conditions generate higher exhaust temperatures which degrade durability, and the fuel used for regeneration adds to operating costs. Research on LNTs has decreased this fuel "penalty," but it is still in the range of five percent of total fuel flow. This problem is exacerbated by the need to periodically drive off accumulated sulfur (even using ultra-low-sulfur fuel) by heating the adsorber to high temperatures, again by using fuel (desulfation). In addition, the high temperature of regeneration and desulfation has been shown to cause deterioration in catalyst effectiveness. LNTs additionally require substantial quantities of platinum group metals, and the cost of these materials has been rising at a concerning rate.

An optimum solution to diesel engine emissions would be to alter the combustion process in ways that produce emissions at levels that don't need ancillary devices for emissions control, or greatly reduce the requirements of these systems, yet maintain or increase engine efficiency. This is the concept behind advanced combustion regimes such as HCCI, pre-mixed charge compression ignition (PCCI) and other modes of LTC, which result in greatly reduced levels of NOx and PM emissions (emissions of hydrocarbons and carbon monoxide still exist and must also be controlled – the lower exhaust temperatures associated with these combustion modes can make hydrocarbon and carbon monoxide control difficult). Significant progress is being made in these types of combustion systems, and performance has been demonstrated over increasingly larger portions of the engine speed/load map. In recent years, DOE has adopted the term "high-efficiency clean combustion" (HECC) to include these various combustion modes since the boundaries among them are difficult to define. The major issues of this R&D include fuel mixing, control of air intake flow and its temperature, control of combustion initiation, and application over a wider portion of the engine operating range. Control of valve opening independent of piston movement appears to be highly desirable for such engines. Most heavy-duty engine manufacturers are employing some sort of HECC in engines designed to meet the 2010 emission standards. Ford has announced that it intends to release a light-duty diesel engine employing HCCI before 2012 which may not include any NOx aftertreatment devices.[1] Ford is also demonstrating that HCCI can accommodate methanol and ethanol as fuels while others have demonstrated hydrogen and dimethyl ether are possible HCCI fuels.[2] General Motors has demonstrated two driveable concept vehicles, a 2007 Saturn Aura and Opel Vectra, with light-duty HCCI engines using gasoline.[3]

Complex and precise engine and emission controls require sophisticated feedback systems employing new types of sensors. A major advancement in this area for light-duty engines has been the introduction of in-cylinder pressure sensors integrated into the glow plug. NOx and PM sensors are under development and require additional advances to be cost-effective, accurate, and reliable. Start-of-combustion sensors (other than the aforementioned pressure sensor) have been identified as a need, and several development projects are underway.

Advanced fuel formulations and fuel quality are also crucial to achieving higher energy efficiencies and meeting emissions targets. The EPA rule mandating that the sulfur content of highway diesel fuel be reduced to less than 15 ppm is a great benefit to the effectiveness, efficiency, and durability of emission control devices. Since October 15, 2006, diesel fuel being sold for highway use in most of the country has less than 15 ppm sulfur (complete phase-in is anticipated by 2010 as small refiner exemptions are phased out). The addition of non-petroleum components such as biodiesel can have beneficial effects on emissions while providing lubricity enhancement to ultra-low-sulfur diesel fuel. Recent tests have shown that biodiesel lowers the regeneration temperature of particulate traps and increases the rate of regeneration with the potential for avoiding or reducing the need for active regeneration and its associated fuel economy penalty. On the other hand, biodiesel use has resulted in some operational problems as well. Fuel filter plugging has been reported under cold conditions for fuels with as little as 2% biodiesel because the biodiesel was not made to specification for blending with diesel fuel. Biodiesel is certain to become more prevalent in diesel fuel due in part to the Renewable Fuel Standard, which calls for 0.5 billion gallons in 2009 increasing to 1.0 billion gallons by 2012.

Waste heat recovery is being implemented in heavy-duty diesel vehicles. New engines being introduced by Daimler Trucks include turbo-compounding technology that uses a turbine to extract waste energy and add to engine power output. The addition of turbo-compounding and other engine changes result in a claimed 5% improvement in vehicle fuel economy. Testing has shown that waste heat recovery has the potential to improve vehicle fuel economy by 10% and heavy-duty engine efficiency also by 10%.

Vehicular thermoelectric generators directly converting engine waste heat to electricity are on a path to commercialization. BMW intends to introduce thermoelectric generators in their 5 and 7 Series cars in the 2010-2014 timeframe in both Europe and North America. The system currently tested by BMW generates 750 W during highway driving, equivalent to a 5% improvement in fuel economy, and about half of that amount in city driving.

DOE/NETL contracts with Ford and General Motors will pursue the concept of a zonal, dispersed thermoelectric cooling system which will cool an occupant with 630 W compared with the 3,500 to 4,000 W used by conventional mobile air conditioning systems.

Future Directions

Internal combustion engines have a maximum theoretical fuel conversion efficiency that is similar to that of fuel cells and considerably higher than the mid-40% peak values seen today. The primary limiting factors to approaching these theoretical limits of conversion efficiency start with the high irreversibility in traditional premixed or diffusion flames, but include heat losses during combustion/expansion, untapped exhaust energy, and mechanical friction. Multiple studies agree that combustion irreversibility losses consume more than 20% of the available fuel energy and are a direct result of flame front combustion. Analyses of how “advanced combustion regimes” might impact the irreversibility

[1] “Ford, PSA Developing HCCI Diesel” by William Diem, WardsAuto.com, October 11, 2006.
[2] “Ford, Brunel Studying CAI Combustion with Methanol and Ethanol in Direct Injection Engine,” Green Car Congress, June 23, 2008.
[3] “GM Takes New Combustion Technology Out of the Lab and Onto the Road” GM Press Release, August 24, 2007.

losses have indicated a few directions of moderate reduction of this loss mechanism, but converting the preserved availability to work will require compound cycles or similar measures of exhaust energy utilization. The engine hardware changes needed to execute these advanced combustion regimes include variable fuel injection geometries, turbo- and super-charging to produce very high manifold pressures, compound compression and expansion cycles, variable compression ratio, and improved sensors and control methods. Larger reductions in combustion irreversibility will require a substantial departure from today's processes but are being examined as a long-range strategy.

The other areas where there is large potential for improvements in ICE efficiency are losses from the exhaust gases and heat transfer losses. Exhaust losses are being addressed by analysis and development of compound compression and expansion cycles achieved by valve timing, use of turbine expanders, regenerative heat recovery, and application of thermoelectric generators. Employing such cycles and devices has been shown to have the potential to increase heavy-duty engine efficiency by 10% to as high as 55%, and light-duty vehicle fuel economy by 10%. Heat transfer losses may be reduced by HECC, and interest in finding effective thermal barriers remains valid.

Most of the basic barriers to high engine efficiency hold true for both gasoline- and diesel-based engines. Recognizing the dominance of gasoline-type spark ignition engines in the U.S., VT intends to increase emphasis on their improvement. Gasoline-based engines, including E85 flex-fuel, can be made at least 20-25% more efficient through direct injection, boosting/downsizing, and lean-burn. Real-world fuel savings might be even higher by focusing attention on the road-load operating points.

Hydrogen engine efficiencies of roughly 45% have been projected based on single-cylinder engine data. The underlying reasons for these impressive levels suggest a case study for applicability to other fuels.

Emission control devices for diesel engines to reduce PM and NOx will become commercially widespread over the next few years. Much work still needs to be done to make these devices less costsly and to lessen their impact on fuel consumption. Information about how best to employ these emission control devices also continues to evolve with new developments leading to more efficient operation. As engine combustion becomes cleaner, the requirements of the emission control devices will change as well.

Thermoelectric generators that directly convert engine waste heat to electricity have great potential to improve engine efficiency and vehicle fuel economy, and reduce criteria and greenhouse gas emissions. The electricity generated can be used to drive engine accessories, operate emission control equipment, or used directly to propel the vehicle. The challenges facing implementation of thermoelectric devices include scale-up, manufacturing techniques, and durability to withstand extremes of heat and vibration typical of vehicle environments. The fact that in spacecraft, thermoelectric generators endure the launch stress and then operate continuously for over 30 years bodes well for long life and low maintenance in vehicle applications.

Technical Targets

The Advanced Combustion Engine R&D Sub-Program has two activities:

- Combustion and Emission Control R&D
- Solid State Energy Conversion

Combustion and Emission Control R&D

The Combustion and Emission Control R&D activity focuses on enabling technologies for energy efficient, clean advanced combustion engines for passenger and commercial vehicles using clean hydrocarbon-based and non-petroleum-based fuels and hydrogen. R&D has been focused on developing technologies that will enable advanced combustion engines to operate at efficiencies that are better than those of diesel engines but with very low or near-zero emissions. These operating conditions are possible with homogeneous charge compression ignition (HCCI) and other modes of low-temperature combustion (LTC).

Fuel efficiency improvement is the overarching focus of this activity, but resolving the interdependent emissions challenges is a critical integrated requirement. (Penetration of even current-technology diesel engines into the light-duty truck market would reduce fuel use by 30-40% per gasoline vehicle replaced.) The major challenges facing diesel emission control systems across all three platforms are similar: durability, cost, and fuel penalty (or in the case of urea-SCR, urea infrastructure development). Full-life durability in full-scale systems suitable for 2010 regulations has yet to be demonstrated for either light- or heavy-duty systems, with the exception of very recent announcements by Cummins of a 2007 chassis certified heavy-duty diesel engine certified to the 2010 emission regulations.

The VT technical targets for advanced combustion engines suitable for passenger vehicles (cars and light trucks), as well as to address technology barriers and R&D needs that are common between passenger and commercial (heavy-duty) vehicle applications of advanced combustion engines include:

- By 2010, for passenger vehicles, develop the understanding of novel low-temperature engine combustion regimes needed to simultaneously enable engine efficiency of 45 percent with a fuel efficiency penalty of less than 1 percent while meeting prevailing EPA emissions standards.
- By 2017, increase the thermal efficiency of heavy truck engines to 55 percent while meeting prevailing EPA emissions standards.

Presented in the following tables are the technical targets (consistent with the goals) for the Combustion and Emission Control R&D activity as of FY 2008. The FreedomCAR and Fuel Partnership goals for both hydrocarbon- and hydrogen-fueled ICEs are shown in Table 1. These apply to passenger vehicles (cars and light trucks). The technical targets for heavy truck engines for commercial vehicles are shown in Table 2.

TABLE 1. Technical Targets for Passenger Vehicle Engines

Characteristics	Fiscal Year		
	2007	2009	2010
Reference peak brake thermal efficiency[a], %	32	34	35
Powertrain cost[b,c], $/kW	35	30	30
FREEDOMCAR AND FUEL PARTNERSHIP GOALS			
ICE Powertrain			
Peak brake thermal efficiency, % (Diesel/H_2–ICE) (H_2–ICE)			 45/45 45 (2015)
Cost, $/kW - (Diesel/$H_2$–ICE) ($H_2$–ICE)			30/45 30 (2015)
Target peak brake thermal efficiency/part-load brake thermal efficiency (2 bar BMEP[d] @1,500 rpm), %	42/29	44/30	45/31
Emissions[e], g/mi	Tier 2, Bin 5	Tier 2, Bin 5	Tier 2, Bin 5
Durability[e], hrs	5,000	5,000	5,000
Thermal efficiency penalty due to emission control devices[f], %	<3	<1	<1

[a] Current production, EPA-compliant engine.
[b] High-volume production: 500,000 units per year.
[c] Constant out-year cost targets reflect the objective of maintaining powertrain (engine, transmission, and emission control system) system cost while increasing complexity.
[d] Brake mean effective pressure.
[e] Projected full-useful-life emissions for a passenger car/light truck using advanced petroleum-based fuels as measured over the Federal Test Procedure as used for certification in those years.
[f] Energy used in the form of reductants derived from the fuel, electricity for heating and operation of the devices, and other factors such as increased exhaust back-pressure, reduce engine efficiency. A cycle average thermal efficiency loss of 1 to 2% is equivalent to a 3 to 5% fuel economy loss over the combined Federal Test Procedure drive cycle.

TABLE 2. Technical Targets for Heavy Truck Diesel Engines

Characteristics	Year			
	2002 baseline	2006	2009	2013
Engine thermal efficiency, %	>40	50	51	55
NOx emissions,[a] g/bhp-hr	<2.0	<0.20	<0.20	<0.20
PM emissions,[a] g/bhp-hr	<0.1	<0.01	<0.01	<0.01
Stage of development	Commercial	Prototype	Prototype	Prototype

[a] Using 15-ppm sulfur diesel fuel

Recovery of waste energy from the engine exhaust represents a potential for 10% or more improvement in overall engine thermal efficiency. Turbochargers strongly influence engine efficiency in several ways, including recovery of part of the exhaust energy. Turbochargers currently have efficiencies of around 50 to 58%, which could be increased to 72 to 76% with enhancements such as variable geometry. Turbo-compounding can be configured to produce mechanical shaft power or electric power for additional waste heat recovery. Direct thermal-to-electric conversion could also improve the overall thermal efficiency. Bulk semiconductor thermoelectric devices are currently 6 to 12% efficient. Recent developments in quantum well thermoelectrics suggest a potential improvement to over 20% is possible. A Rankine bottoming cycle for heat recovery is being evaluated in one of the heavy-duty truck engine efficiency projects.

Enabling technologies being developed by the Combustion and Emission Control R&D activity focus on fuel systems, engine control systems, and engine technologies. Fuel systems R&D focuses on injector controls and fuel spray development. The fuel injection system pressure and fuel spray development influence the spray penetration and fuel-air mixing processes and thus combustion and emissions formation within the combustion chamber. Engine control systems R&D focuses on developing engine controls that are precise and flexible for enabling improved efficiency and emission reduction in advanced combustion engines. These control system technologies will facilitate adjustments to parameters such as intake air temperature, fuel injection timing, injection rate, variable valve timing, and exhaust gas recirculation to allow advanced combustion engines to operate over a wider range of engine speed/load conditions. Engine technologies development will be undertaken to achieve the best combination that enables advanced combustion engines to meet maximum fuel economy and performance requirements. These include variable compression ratio, variable valve timing, variable boost, advanced sensors, and exhaust emission control devices (to control hydrocarbon emissions at idle-type conditions) in an integrated system.

The Combustion and Emission Control R&D activity performs the critical role of elevating potential health issues related to advanced combustion engine technologies to the attention of industry partners and DOE/VT management. This portion of the activity ensures that the development of new vehicle technologies, rather than just enabling compliance with existing standards, also considers the possibility of causing negative health impacts:

- To provide a sound scientific basis underlying any unanticipated potential health hazards associated with the use of new powertrain technologies, fuels and lubricants in transportation vehicles.
- To ensure that vehicle technologies being developed by VT for commercialization by industry will not have adverse impacts on human health through exposure to toxic particles, gases, and other compounds generated by these new technologies.

Solid State Energy Conversion

The Solid State Energy Conversion activity focuses on developing advanced thermoelectrics for converting waste heat from engines directly into useful electrical energy to improve overall vehicle energy efficiency and reduce emissions. Effective use of waste heat from combustion engines would significantly increase vehicle fuel economy. In current production passenger vehicles, roughly over 70% of the fuel energy is lost as waste heat from an engine operating at full power. About 35 to 40 percent is lost in the exhaust gases and another 30 to 35 percent is lost to the engine coolant. There is an opportunity to recover some of the engine's waste heat using thermoelectric materials that will convert it directly to electricity for operating vehicle auxiliaries and accessories.

The goal of this activity is to develop advanced thermoelectric technologies for recovering engine waste heat and converting it to useful energy that will improve overall engine thermal efficiency to 55% for Class 7 and 8 trucks, and 45% for passenger vehicles while reducing emissions to near-zero levels. More specifically,

- By 2014, achieve at least 25 percent efficiency in advanced thermoelectric devices for waste heat recovery to potentially increase passenger and commercial vehicle fuel economy by a nominal 10%.

This activity also supports the overall engine efficiency goals of the FreedomCAR and Fuel Partnership, and 21st CTP. The technical targets for Solid State Energy Conversion are shown in Table 3.

TABLE 3. Solid State Energy Conversion Technical Targets

Characteristics	Year		
	2003 Status	2008	2010
Thermoelectric Devices			
Efficiency, % • bulk semiconductor • quantum well	5–7	– >15	– >20
Projected cost/output, $/kW (250,000 production volume)	--	500	180
Passenger Vehicle Application			
Fuel economy improvement, %	<4	>7	>12
Power, kW	<0.8	>1.0	>2.0
Projected component life, hours	<10	>5,000	>10,000
Commercial Vehicle Application			
Fuel economy improvement, %	<3	>8	>10
Power, kW	<10	>18	>20
Projected component life, hours	<10	>5,000	>20,000

Achieving these targets requires reduction in the cost of thermoelectrics, scaling them up into practical devices, and making them durable enough for vehicle applications.

PROJECT HIGHLIGHTS

The following projects highlight progress made in the Advanced Combustion Engine R&D Sub-Program during FY 2008.

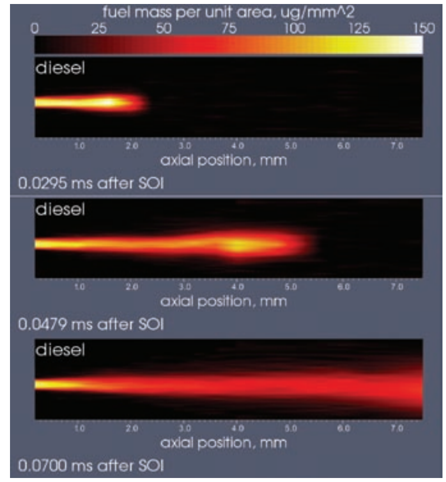
Advanced Combustion and Emission Control Research for High-Efficiency Engines

A. Combustion and Related In-Cylinder Processes

The objective of these projects is to identify how to achieve more efficient combustion with reduced emissions from advanced technology engines.

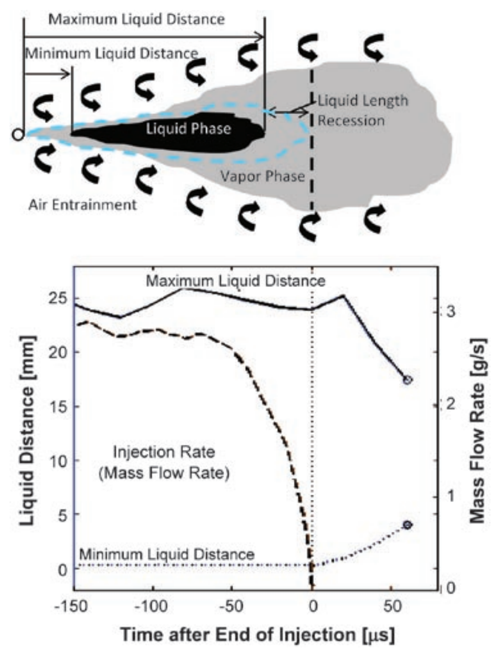
- Argonne National Laboratory (ANL) made a significant discovery that uses a quantitative measurement of the fuel distribution to show how diesel fuel injection spray width changes as ambient pressure is increased. This discovery clears up a discrepancy in the spray literature, and extends knowledge about spray behavior to the near-nozzle region. This discovery will allow spray models to more accurately predict fuel distribution. Due to advances in X-ray optics, ANL was able to measure the fuel distribution from a diesel injector under high density conditions without a fuel additive. This is a significant step, since several industrial partners have requested tests of pure diesel fuel. (Powell, ANL)

- Sandia National Laboratories (SNL) used homogeneous reactor simulations employing detailed chemical kinetic mechanisms to clarify the impact of mixture equivalence ratio and temperature on carbon monoxide (CO) and unburned hydrocarbon (UHC) yield with LTC. The results show that CO emissions will be more difficult to eliminate than UHC emissions in both mixing- and kinetically-controlled combustion regimes. They also used planar laser-induced fluorescence to observe the spatial distributions of CO and UHC within the cylinder. The results have been compared with the predictions of multi-dimensional simulations. The comparison has identified specific aspects of the models that should be examined and possibly modified to improve the simulation accuracy. (Miles, SNL)



These ANL measurements are the first that have been made without the use of a fuel additive to improve the image contrast. (Powell, ANL)

- SNL is improving understanding of rapid leaning near the injector after the end of injection that causes UHC emissions for LTC. They found that (1) jet-jet interactions create fuel-rich regions, which lead to soot formation, and (2) fuel-lean regions near the injector do not burn to completion, leading to UHC emissions. Jet-jet interaction increases with a smaller bowl, pushing hot combustion farther into the center of the combustion chamber, thus displacing the fuel-lean regions of UHC into the hot combustion zones, which may help to consume unburned fuel. (Musculus, SNL)
- SNL demonstrated that shortening the fuel injection duration to one-half of the quasi-steady liquid length time reduces the liquid-phase penetration of the spray, providing an understanding needed to prevent liquid wall impingement and its negative impacts on emissions and combustion efficiency. They discovered that the maximum liquid penetration recedes towards the injector after the end of injection. The cause of the liquid length recession is an entrainment wave of enhanced fuel-ambient mixing that occurs during the injection-rate ramp down. They also provided new insight into diesel lift-off stabilization by using laser-ignition upstream of the natural lift-off length. Ignition stabilizes lift-off upstream for a substantial period of time, effectively controlling lift-off length for LTC. (Pickett, SNL)

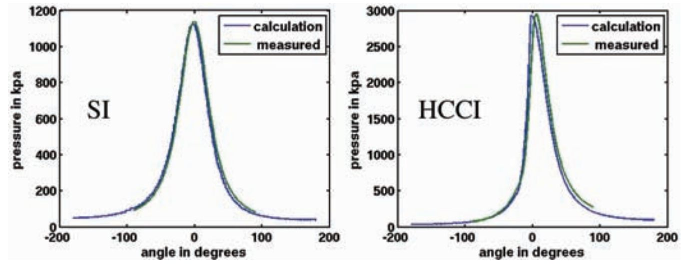


Maximum and minimum liquid penetra-tion distances along with a fuel mass flow rate before and after end of injection. (Pickett, SNL)

- Oak Ridge National Laboratory (ORNL) was successful at providing new insight into the implementation of HECC operation with multi-cylinder engines that is an important component to demonstrating 2010 FreedomCAR efficiency and emissions milestones using light-duty diesel engines. Specific accomplishments are as follows: (1) completed mixed-source EGR experiments and the effect of intake charge temperature on emissions and efficiency, (2) evaluated three LTC strategies on multi-cylinder engine for emissions, brake thermal efficiency (BTE), and stability and (3) characterized thermodynamic availability of conventional diesel combustion and LTC operation. (Wagner, ORNL)
- SNL developed a new tabulation approach for treatment of complex hydrocarbon fuels based on the Linear Eddy Model and developed a high-fidelity model for high-pressure direct injection

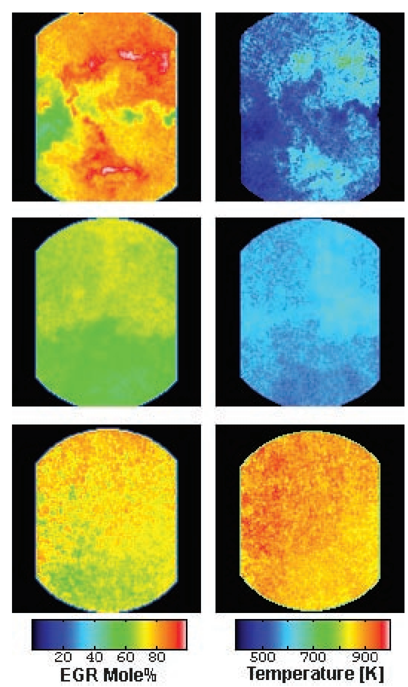
processes and completed validation studies in collaboration with Ghandhi et al., University of Wisconsin. Comparisons between large eddy simulation (LES) and particle image velocimetry data for a hydrogen engine were made. (Oefelein, SNL)

- Lawrence Livermore National Laboratory (LLNL) developed and tested detailed 3-dimensional meshes for analysis of partially stratified combustion in experimental engines at Sandia Livermore and conducted detailed analysis of HCCI combustion in the Sandia engine. The LLNL multi-zone model was migrated to KIVA4 enabling parallelization and unstructured meshes enabling faster execution. They also developed a new analysis tool for modeling of spark ignition to HCCI transition experiments being conducted at ORNL. (Aceves, LLNL)



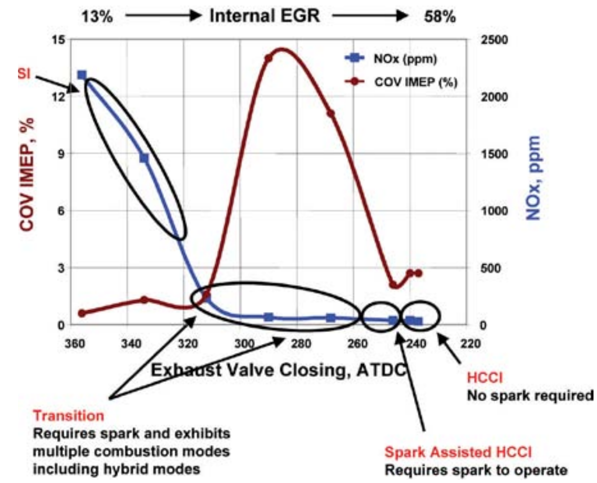
Comparison between ORNL experimental results and LLNL numerical results for SI combustion at low residual gas fraction (20%, left) and HCCI combustion at high residual gas fraction (60%, right). (Aceves, LLNL)

- SNL determined the effect of EGR/residuals on HCCI heat-release rates and NOx formation for well-mixed HCCI by isolating these effects from the other effects of EGR. This showed that EGR offers little direct benefit for extending the high-load limit. The high-load limits for single- and two-stage ignition fuels were determined, and three different mechanisms for these limits, depending on fuel type were identified. In addition, detailed exhaust-speciation analysis for well-mixed operation at a variety of loads and for stratified operation at low loads with iso-octane fueling was completed (with LLNL). A detailed exhaust-speciation analysis was completed for both well-mixed and mixture-stratified operation, and an electro-hydraulic variable valve actuation system was completed and tested on the engine. These efforts are related to technical barriers of poor combustion efficiency (and HC and CO emissions) at low loads and combustion-phasing control, respectively. (Dec, SNL)
- SNL expanded operation of their automotive HCCI optical engine to include the negative valve overlap (NVO)-HCCI strategy for low loads, and a useful range of operating conditions was been mapped. An operating procedure was developed to quickly attain steady operating conditions and enable optical measurements. Development and application of Stanford's two-wavelength planar laser-induced fluorescence diagnostic was continued and has produced viable in-cylinder measurements of temperature and composition during fired operation. In addition to air-seeded EGR measurements, the fuel-seeded laser-induced fluorescence technique was used to obtain measurements during the difficult NVO period. Spatially averaged temperatures obtained with the diagnostic will be useful for validating models of their HCCI engine. (Steeper, SNL)
- ORNL determined that the combustion variability observed during spark ignition (SI)-HCCI operation is driven by competition between SI and HCCI combustion modes. Stabilizing SI-HCCI operation relies on the ability to maintain a balance between these two modes. A low-order model was been developed which is capable of simulating the complex dynamics observed experimentally on a single-cylinder engine. The next phase of this activity involves adapting these concepts to a multi-cylinder engine (a Delphi Automotive System four-cylinder gasoline engine with advanced powertrain components and



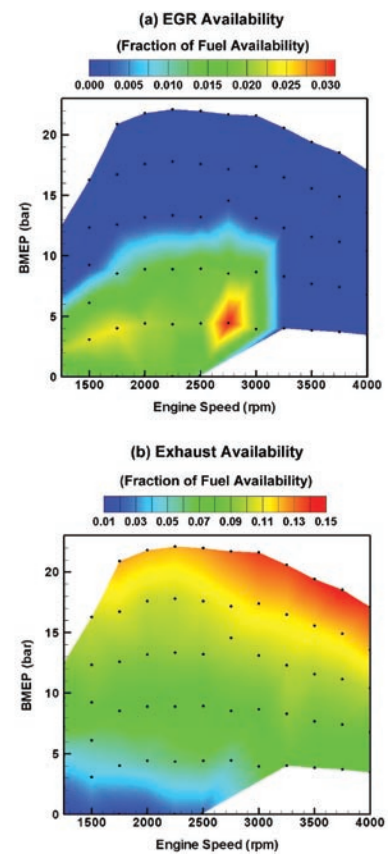
Simultaneous single-shot EGR and temperature images recorded during NVO operation. (Steeper, SNL) controls) for the development and implementation of adaptive control strategies. (Wagner, ORNL)

- Los Alamos National Laboratory (LANL) completed a parallel LES implementation of KIVA-4. Calculations were performed which compared the LES model against the k-epsilon model in a vertical valve engine. A parallel multi-zone model in KIVA-4 was implemented. Calculations were performed and results compared very well with the LLNL multi-zone KIVA-3 model in a 3-dimensional (3-D) sector mesh. The University of Wisconsin's (UW's) chemistry and spray submodels were tested in a constant volume 3-D geometry. Results compared very well with UW's code. Pressure histories of KIVA-4, KIVA-3V and experimental data were compared in a Caterpillar 3401 engine running at different loads and injection timings. Soot calculations were performed with KIVA-4 in a constant volume chamber and compared against Pickett and Siebers' experimental data. Partitioning strategies were implemented and tested in four different engine geometries. A paper was submitted to Computers and Fluids. (Torres, LANL)



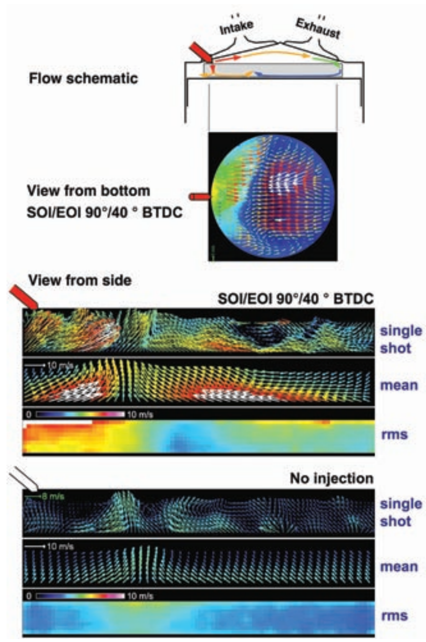
General combustion trends observed in the SI-HCCI transition experiments for 1,600 rpm, 3.4 bar BMEP. Internal EGR referenced in the figure was estimated using a full engine simulation code. (Wagner, ORNL)

- LLNL validated a low- and high-temperature mechanism for normal alkanes from C8 to C16, including n-hexadecane, a primary reference fuel for diesel engines. A detailed chemical kinetic mechanism for a large biodiesel surrogate was further validated. A reduced mechanism for a large biodiesel surrogate for use in computational fluid dynamics (CFD) codes was developed. (Pitz, LLNL)
- ORNL achieved and demonstrated the 2008 FreedomCAR milestones of 43% peak BTE and 27% part-load BTE using a light-duty diesel engine. The thermodynamic availability of engine systems (e.g., exhaust system, EGR, etc.) was characterized across the speed-load operational range of a light-duty diesel engine and potential fuel economy improvements over the Federal Test Procedure (FTP) drive cycle were estimated. A thermal energy recovery model of an organic Rankine cycle was developed and a bench-scale system was constructed which will be transitioned to an engine in early FY 2009. A well-defined path to meeting FY 2010 efficiency and emissions milestones was developed. (Wagner, ORNL)
- SNL continued development of a free-piston generator with a projected fuel-to-electricity conversion efficiency of 50% at 30 kW output using hydrogen as the fuel. The project has progressed by conducting idealized combustion experiments, designing and procuring the linear alternators required for control and power conversion, and conducting computational fluid dynamics design of the inlet/exhaust processes. The design has evolved into a dynamically balanced configuration suitable for seamless incorporation into an automotive application. (Van Blarigan, SNL)



Thermodynamic availability of the (a) EGR and (b) exhaust systems on a GM 1.9-L engine shows a significant amount of fuel energy is discarded to the environment and potentially available for recovery. (Wagner, ORNL)

- ANL determined that the injector location has significant influence on the efficiency and emissions behavior of a hydrogen engine. It was also discovered that the injection strategy and nozzle design are closely related and highly dependent on injector location. The potential of water injection for NOx emissions reduction was evaluated and found that an emissions reduction of up to 50% with no significant loss in engine efficiency is feasible. (Wallner, ANL)
- SNL aims to provide the science base for the development of high-efficiency hydrogen-fueled vehicle engines. The technical focus is on direct-injection strategies, using laser-based in-cylinder measurements closely tied to advanced numerical simulations. A 2-dimensional measurement technique to quantify in-cylinder fuel distribution was improved substantially to be able to make measurements under more realistic operating conditions and evaluation of injection strategies, coordinated with metal-engine experiments at Argonne, is in progress. Detailed velocity measurements in two orthogonal planes were made to help understand interaction of intake-induced and injection-induced flow. (Kaiser, SNL)



The injection event has a strong influence on the in-cylinder flow, increasing charge velocities of hydrogen engines by more than a factor of two. (Kaiser, SNL)

- Cummins achieved a 13% to 15% improvement in efficiency compared to the project target of 10% using HECC-developed technology with SCR NOx aftertreatment while meeting U.S. EPA 2010 emissions for Class 6, 7, and 8 commercial vehicles. Without NOx aftertreatment the efficiency improvement is reduced to 8%. Additional fuel consumption improvements of 3%-4% can be achieved through better integration of the engine with the transmission and vehicle systems. (Stanton, Cummins)
- Caterpillar continued their efforts to apply HECC. They identified the relationship between liquid fuel impingement, efficiency and emissions, and completed single-cylinder engine testing of gasoline/diesel fuel blends. Emissions and fuel consumption benefits under laboratory conditions of PCCI combustion with a Caterpillar C15 engine were demonstrated. A jacket water boiling model was developed and validated to allow accurate prediction of heat transfer to engine coolant. The cause of variable compression ratio (VCR) engine bearing failure was identified and design changes were proposed to eliminate failure. (Gehrke, Caterpillar)
- Navistar applied LTC to their 6.4L V8 engine and achieved 5 to 15% better efficiency than the conventional engine. The load target of 12 bar bmep was surpassed to 16.5 bar bmep by managing charge temperatures, dilution ratios, and fuel injection strategies. Testing was closely coordinated with CFD-KIVA studies which correlated well with experiments, and provided a fundamental understanding of the combustion process. NOx levels were limited to below 0.2 g/bhp-hr with soot levels adequate for a DPF. (de Ojeda, Navistar)
- ORNL continued their efforts to analyze and define specific pathways to improve the energy conversion efficiency of internal combustion engines from nominally 40% to as high as 60%. They developed a conceptual design for a bench-top cyclic constant volume combustor for demonstrating low-irreversibility combustion based on regenerative preheating with thermochemical recuperation, and characterized performance of a reforming catalyst provided by an industrial partner in a flow reactor. (Daw, ORNL)
- Detroit Diesel Corporation (DDC) demonstrated 5% thermal efficiency improvement on a multi-cylinder engine using advanced PCCI combustion concept at one engine operating point while maintaining the same emissions level. DDC also demonstrated over 4% fuel economy benefit on a multi-cylinder engine over the transient FTP cycle while simultaneously reducing PM by 25% and NOx by 15%, using validated next generation model-based control. (Zhang, DDC)

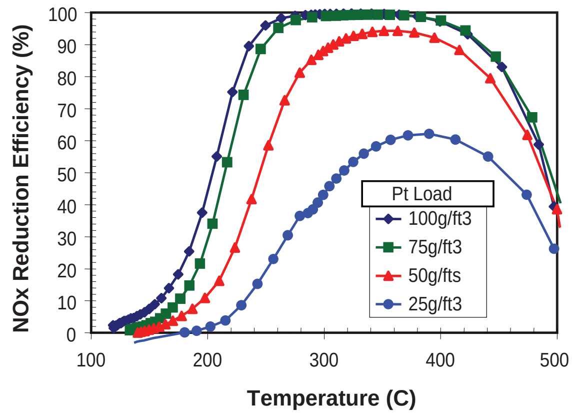
- GM developed and demonstrated prototype gasoline and diesel engine hardware which enables operation of HCCI combustion for improved fuel efficiency and emissions performance. In the zone of operation for gasoline engine in HCCI mode, fuel efficiency improvements in the range of 8% to 20% were demonstrated, depending on the specific engine operating condition. Fuel efficiency of the diesel engine was improved by about 1% over the Federal Test Procedure (FTP) cycle and 0.5% over the US06 cycle. Smoke emissions were reduced by approximately 40% over the US06 cycle and ~50% over the FTP cycle. (Patton, GM)
- Cummins developed and calibrated an engine cycle simulation model for their light-duty diesel engine. The model was expanded beyond the base engine to simulate variable valve actuation (VVA) functions on both the intake and exhaust. The model has been used primarily to evaluate the relative emissions and efficiency trade-offs of VVA functions to specify and procure a multi-cylinder VVA prototype. Advanced air handling and EGR components are also being evaluated and will be used to specify and procure hardware for engine tests beginning in 2009. (Frazier, Cummins)
- Ford is developing optimal system solutions to address boost system challenges, such as efficiency degradation and compressor surge, etc., in diesel combustion/emission control system development to enable commercialization of advanced diesel combustion technologies. The first round of design, analysis and flow bench test made limited achievements. Even though the flow bench test was interrupted due to turbocharger failure, the test data from one speed line still provided valuable correction/validation for the compressor and turbine design and analysis which will guide the future design optimization for better efficiency and wider flow range. The first round exercise focused on compressor blade, diffuser vane and mixed flow turbine design optimization. The next step will focus on using fewer moving parts in the compressor to achieve the widest operation range with minimal efficiency penalty. (Sun, Ford)

B. Energy-Efficient Emission Controls

The following project highlights summarize the advancements made in emission control technologies to both reduce emissions and reduce the energy needed for emission control system operation.

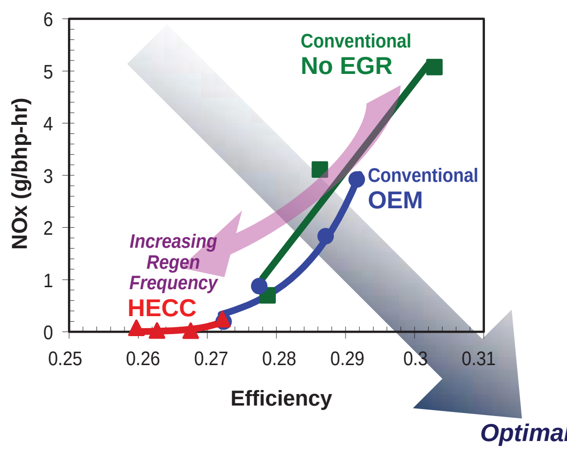
- PNNL studied the specific structures associated with the monolayer of $Ba(NO_3)_2$ that forms on the alumina surface of LNTs using both experiments and computational modeling. Ultra-high resolution transmission electron microscopy (TEM) at the High Temperature Materials Laboratory at ORNL confirmed that initially BaO monomers dispersed on the γ-alumina support surface by anchoring to penta-coordinated Al sites. The results from this combined experimental and computational study has allowed PNNL to unambiguously determine the nature of “surface” and “bulk” nitrates that were identified in prior studies and that have shown to be important in determining the optimum practical behavior of Ba-based LNT catalysts. Using a one-of-a-kind very high field nuclear magnetic resonance instrument at PNNL, the role of specific surface sites on the γ-alumina catalyst support surface in its high temperature stability to phase transformation has been determined. (Peden, PNNL)
- PNNL continued their efforts to identify mechanisms of sulfur poisoning of NOx adsorber materials. It was observed that a simple liquid water treatment applied to fresh and thermally aged Pt(2 wt%)-BaO(20 wt%)/Al_2O_3 LNT catalysts at room temperature induces morphological and structural changes in the barium species, resulting in the increase in the NOx uptake. It was found that the sulfur species at low sulfur loading are less likely to be removed as H_2S and have more tendency to be transformed to sulfide species (as BaS) on the material, thus demonstrating the significant effect of sulfation levels on the desulfation behavior of LNT materials. It was also found that ceria-based catalysts have a) much higher sulfur tolerance and b) excellent resistance against Pt sintering when they are compared to the widely used alumina based catalysts. (Peden, PNNL)
- ORNL developed a LNT regeneration strategy based on PCCI combustion mode for use at low loads. Low temperature desulfation (onset at ~300°C) of a Ce-based LNT formulation on a bench flow reactor was demonstrated, and the NOx reduction performance characterized. The impact of precious metal loading on LNT performance as a function of temperature on a bench flow reactor was also characterized. (Parks, ORNL)

- ORNL with CRADA partner Navistar developed a protocol that provides the critical transient and steady-state model parameters for SCR catalysts, implemented a subset of the protocol on commercial-intent SCR catalyst, and coordinated modeling efforts with Michigan Technical University. (Toops, ORNL)
- ORNL continued their NOx abatement research and development CRADA with International Truck and Engine Co./Navistar Inc. They developed a protocol that provides the critical transient and steady-state model parameters for SCR catalysts, implemented a subset of the protocol on a commercial-intent SCR catalyst, and coordinated modeling efforts with Michigan Technical University. (Toops, ORNL)



NOx Reduction Efficiency as a Function of Temperature for Four Different Pt Loadings (Parks, ORNL)

- ORNL is developing a diagnostic for rapid, on-engine measurements of oil dilution by fuel and applying it to a CRADA-partner's engine development facility. Ammonia formation and utilization within LNT catalysts during regeneration was studied and clarified: (1) first direct experimental evidence of fast NH_3 generation and intermediate-NH_3 regeneration pathway, (2) provided detailed data necessary to better understand and model NH_3 chemistry, and (3) provided detailed data necessary to develop improved NH_3-management protocols; e.g., via formulation tuning, active control, design and modeling. (Partridge, ORNL)
- ORNL demonstrated the benefits of HECC in conjunction with an LNT to achieve EPA Tier 2, Bin 5 NOx emissions with only a slight drop in fuel efficiency as compared with conventional combustion modes. Two technical challenges were identified to be addressed with HECC-related systems: low temperature CO and hydrocarbon emission control and EGR system fouling. (Parks, ORNL)



NOx Tailpipe Emissions vs. Thermal Efficiency for all Combustion Modes at 2,000 rpm and 2.0 bar BMEP (Parks, ORNL)

- ORNL continued co-leading the Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Planning Committee and facilitation of the SCR, LNT, and DPF Focus Group telecoms with strong domestic and international participation. Key R&D priorities from the CLEERS community were identified, including coordination of a second R&D priorities survey with response from 16 DOE Diesel Cross-cut Team companies and their supplier and energy company partners in 2008. Web site functionalities, security, and data were maintained to facilitate Web meetings and serve Focus Group interactions. (Daw, ORNL)
- ORNL made detailed spatially resolved capillary inlet mass spectrometer (SpaciMS), microscopy, and temperature programmed reaction measurements of model and Umicore reference LNT catalysts to resolve critical details about the impact of sulfation and desulfation. This information was used to develop a low-order LNT model capable of systems simulation studies. Diffuse reflectance infrared Fourier-transform spectroscopy (DRIFTS) measurements were continued of the fundamental mechanisms involved in sulfur poisoning and desulfation of LNTs – a detailed kinetics model of combined LNT NOx capture and stored-NOx regeneration is being developed in collaboration with SNL. (Daw, ORNL)

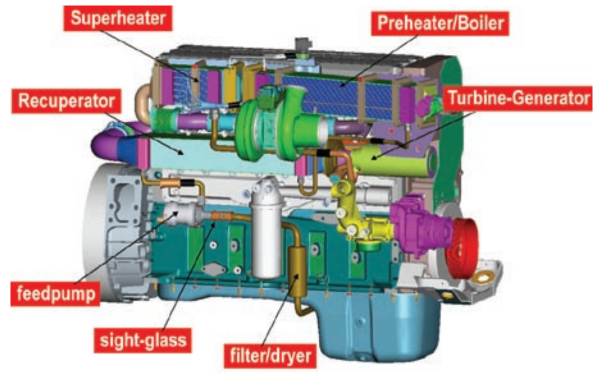
- PNNL developed techniques for loading individual filter walls and single channel samples of DPFs with aerosolized salt particles or lab-generated soot particles for fundamental filtration studies. Energy dispersive X-ray spectroscopy scans of fractured filter walls loaded with aerosolized salt particles were performed to characterize particle penetration into the filter microstructure. The particle capture model of the micro-scale filtration simulation tools was enhanced and studies with varying capture probability were performed. (Stewart, PNNL)

C. Critical Enabling Technologies

VVA, variable compression ratio (VCR), and combustion sensors are enabling technologies for achieving more efficient engines with very low emissions. The following highlights show the progress made during FY 2008.

- An optimal, cost-effective, VVA system for advanced low-temperature diesel combustion processes was designed and tested. A dual cam design was selected from concept designs and all dynamic analyses were completed. An original equipment manufacturer (OEM) confirmed that the proposed dual cam design is a cost-effective and production feasible design. The package size was reduced to require minimal change to the OEM engine envelope. A single-cylinder device was built and installed on a free-running lab engine. The mechanism was tested and demonstrated the capability of meeting all design requirements. (Gutterman, Delphi)
- Envera LLC reduced the hydraulic pressures in the actuator system of its VCR system by 86% through system optimization. The reduction in pressure significantly relaxes the demands that will be placed on the hydraulic system and enables cost to be reduced. Test results indicated that compression ratio can be reduced from 18:1 to 8.5:1 in ~0.35 seconds, and increased from 8.5:1 to 18:1 in ~0.70 seconds. On average 0.074 seconds is projected to elapse for each point increase in compression ratio. Finite element analysis of the production-intent 4-cylinder VCR engine predicts that the crankcase meets all stiffness, robustness and durability requirements for mass production. (Mendler, Envera LLC)
- Streamline Automation, LLC focused on designing and developing fabrication methods for an all-new planar type voltammetric NOx gas sensor. A miniature real-time support instrument (electronics) to couple with the new sensing element is being developed. An on-engine installation and characterization plan is under development. (Vogt, Streamline Automation, LLC)
- TIAX LLC is developing an accelerometer-based start of combustion (SOC) sensor which provides adequate SOC event capture to control an HCCI engine in a feedback loop. Three engines of the same model line/different serial number were installed to verify engine-to-engine repeatability of the SOC sensor system (a potential drawback of accelerometer-based systems), including two dynamometer setups and one vehicle setup. An initial real-time version of the SOC algorithm has been developed to optimize the algorithm for accuracy and processing speed. Data over the operating range of interest (the expected HCCI operating envelope of low to medium speed, low to medium load) has been recorded. (Smutzer, TIAX LLC)
- Westport Power, Inc. is developing an accelerometer-based SOC sensing system including a method to minimize sensor-to-sensor variation. The average sensor-to-sensor variation over all modes was reduced to 0.36 crank angle degree (CA°) at the 98.9% confidence level which exceeds the initial target of sensor-to-sensor variation of 0.5 CA°. The mode-averaged total error (based on one standard deviation) was reduced to 0.41 CA° which exceeded the initial target to achieve total error of measured SOC timing of 0.5 CA°. The capability of the accelerometer-based combustion sensing system was extended to capture not only the SOC timing but also the complete in-cylinder pressure trace. (Mumford, Westport Power, Inc.)
- Cummins Inc. completed assembly of the first-generation R245fa-based Organic Rankine Cycle energy recovery system on a model year 2007 Cummins ISX engine. Using EGR-only energy recovery a 6% fuel economy benefit was successfully demonstrated. An effective integrated control system to operate the energy recovery system through practically all engine operating conditions was developed. Stable and repeatable steady-state and transient control of the system was demonstrated. A number of critical system features and control techniques were identified to insure that system operation was stable and robust against system disturbance. (Nelson, Cummins)

- Caterpillar Inc. is developing technologies that will reduce all forms of exhaust energy loss, including: blowdown losses, aero machinery losses, fluid frictional losses, losses due to pulsating exhaust flow, heat transfer losses, and losses of energy out the exhaust stack to achieve a 10% improvement in engine thermal efficiency. The Caterpillar approach for achieving a 10% improvement in engine thermal efficiency breaks down as follows: +4% from implementation of turbocompound to recover stack waste heat, +3.7% from improving turbocharger efficiencies, +1.3% from intercooling the series turbocharging system, +0.5% from insulating the engine exhaust ports, and +0.5% from reducing exhaust piping flow losses. (Kruiswyk, Caterpillar)



Cummins ISX Engine Shown with EGR-Only WHR System Hardware (Nelson, Cummins)

D. Health Impacts

The Health Impacts activity studies potential health issues related to new powertrain technologies, fuels, and lubricants to ensure that they will not have adverse impacts on human health. The following are highlights of the work conducted in FY 2008.

- ORNL measured mobile source air toxics (MSATs) from several light-duty vehicles operating on intermediate blends of ethanol (E10, E15 and E20). It was found that higher ethanol blends increase ethanol emissions over a driving cycle but the overall non-methane hydrocarbons and non-methane organic gases emissions are largely unchanged. Higher ethanol blends increase acetaldehyde emissions but formaldehyde emissions were only slightly increased over the driving cycle. Additionally, ORNL characterized MSATs from two HECC diesel engines equipped with catalytic aftertreatment. The goal was to determine if higher engine-out levels of CO and HCs affected the destruction of MSATs by the catalyst. Both PCCI and HCCI engines were investigated. Despite high levels of CO and HCs, MSATs were efficiently removed except when catalyst temperatures fell below 225°C. MSATs and particulate emissions from small non-road engines operating were characterized on intermediate blends of ethanol and gasoline. E20 dramatically reduced particle emissions for in-use utility engine while increasing acetaldehyde emissions. (Parks, ORNL)
- The National Renewable Energy Laboratory (NREL) is quantifying the role of engine lubricating oil on PM and semi-volatile organic compound emissions from in-use motor vehicles fueled with gasoline, 10% ethanol in gasoline (E10), diesel, biodiesel, and compressed natural gas while operating on fresh and used crankcase lubricants. Both "normal" and "high-emitting" vehicles are being tested. To date, vehicle testing has been completed on the light-duty "normal" and "high-emitters." (Lawson, NREL)
- The Health Effects Institute (HEI) made progress in their management of the Advanced Collaborative Emissions Study. Detailed characterization of four engines that are employing new technologies to substantially reduce PM and NOx was completed. A representative engine was identified to generate the test atmosphere for the animal exposures during the chronic inhalation bioassay. In parallel, the back-up engine has been tested, thereby completing the experimental work of Phase 1, and developed the protocol for testing the selected engine and characterizing the exposure atmosphere in the inhalation chambers. (Greenbaum, HEI)

Solid State Energy Conversion

Several projects are being pursued to capture waste heat from advanced combustion engines in both light- and heavy-duty vehicles using thermoelectrics. Following are highlights of the development of these technologies during FY 2008.

- General Motors Research & Development Center (GM) in the past year has focused on several areas: design of the thermoelectric (TE) waste heat recovery generator; design of electrical power management system for the TE generator; development of vehicle-level algorithms to optimize potential fuel economy gains; and the search for high-performance, mechanically-robust, and cost-effective TE materials and modules. The geometry and position of various components including heat exchangers have been defined for the generator design, in addition, the generator position and exhaust bypass geometry have been defined and integrated with the selected GM vehicle. A trade-off study was completed to determine the electrical topology of the generator and the direct current (DC)-to-DC converter architecture. The selected design maximizes reliability and efficiency over the driving cycles and minimizes system cost. Vehicle level control algorithms have been developed for electrical power management and thermal management to achieve optimized fuel economy gains. (Yang, GM)
- BSST continued their efforts to develop a thermoelectric generator (TEG) for use on light-duty vehicles. Several activities were completed during the year including: (1) thermal cycling of TE subassemblies was completed that supported the high-temperature TEG build, (2) the power control system designed and built in 2007 was successfully tested, (3) a high-temperature TEG was built and tested that provided 125 watts of power using 600°C gas, (4) characterization techniques for TE subassembly electrical interfaces were developed and applied by Ford that provided an important tool and basis for further improving the technology, (5) initial assessment of the application of TEG technology in a hybrid vehicle platform was completed and fuel economy improvement predictions made by Ford, and (6) the system performance model was updated to incorporate a transient TEG model and more efficient BMW engine. (LaGrandeur, BSST)
- Michigan State University (MSU) is conducting an in-depth effort aimed at determining the viability of using advanced TE materials implemented in an electric generator to recover waste heat from an over-the-road (Class 8) truck. Bulk mechanical properties and micro-structural analysis of hot pressed lead, antimony, silver, lead, antimony, silver, and tellurium (LAST)/LAST+tin (LASTT) and skutterudites have been evaluated. The TE system for a number of lead and tellurium (PbTe)-based systems has been evaluated with typical performance characterized. Performance improvements for an over-the-road truck have been accessed based upon the performance of TE material which has been synthesized and tested. (Schock, MSU)

University Research

- The University of Michigan (UM) is using experiments and modeling to acquire the knowledge and technology to extend the load range of LTC engines. Progress during the year include (1) extension of the high-load limit from 1 bar net mean effective pressure to near 6 bar in both single- and multi-cylinder tests, (2) it was found that ignition at the low-load limit on the next cycle can be advanced or retarded depending on the overall oxygen concentration and the negative valve overlap temperature, (3) A GT-Power® model was developed and predicts that the high-load limit can be extended without knock provided the mixture is leaned-out or diluted as pressure is increased, (4) for direct injection and partially premixed compression ignition engine applications an improved flamelet combustion model has been developed to describe the interaction between spray and combustion, (5) a thermodynamic analysis has been carried out to delineate the combustion regimes for spark-assisted (SA)-HCCI, (6) a first generation model of a urea-SCR catalyst has been assembled using AVL Boost with appropriate chemical equations drawn in part from previous work at UM and from the literature, and (7) rapid compression ignition delay measurements have been made for a number of isomers of simple five and six carbon esters representative of future bio-derived fuels. (Assanis, UM)
- The University of Wisconsin-Madison is developing methods to optimize and control LTC that offers the potential of nearly eliminating engine NOx and PM at reduced cost over traditional methods by controlling pollutant emissions in-cylinder. To this end, they have developed reduced mechanisms and efficient chemistry solvers have been developed for use in advanced CFD and engine system combustion models. New high resolution optical diagnostics have been developed for in-cylinder chemical species measurement and for combustion model validation. Advanced fuel injection concepts, such as variable pressure injection have been proposed and explored, and

injector models have been formulated. Ultra-low emissions and improved fuel efficiency have been demonstrated when operating a LTC diesel engine on gasoline fuel. (Reitz, University of Wisconsin-Madison)

- The University of Houston is utilizing a combination of experimental and theoretical tools to advance LNT technology. Systematic temporal analysis of products (TAP) studies were conducted and a mathematic model framework for elucidating reaction pathways and estimating kinetic parameters is being developed. Comprehensive steady-state and cyclic studies using hydrogen as a reductant on model NOx trap monolithic catalysts comprising Pt, Pt/Ba, and Ba are being conducted. A steady-state LNT model that incorporates the results on the complex regeneration kinetics from the TAP and bench-scale reactor studies has been developed, and this model has been applied to simulate steady-state bench-scale data. (Harold, University of Houston)
- The University of Kentucky is improving understanding of the mechanisms of LNT aging to understand the effect of washcoat composition on catalyst aging characteristics. The effect of ceria addition on the sulfation and desulfation characteristics of a model Ba-based LNT catalyst was studied. According to DRIFTS and NOx storage capacity measurements, ceria is able to store sulfur during catalyst exposure to SO_2, thereby helping to limit sulfation of the main (Ba) NOx storage phase and maintain NOx storage capacity. Model monolithic catalysts were aged on a bench reactor according to a protocol designed to simulate ca. 75,000 miles of road aging. The aged catalysts were then evaluated on a bench reactor in order to characterize their NOx storage-reduction characteristics and enable a comparison with the fresh (de-greened) catalysts. Spectacular improvement in LNT durability was observed for catalysts incorporating CeO_2 and $CeZrO_2$ (particularly the latter). (Crocker, University of Kentucky)
- Texas A&M University is using the second law of thermodynamics (in conjunction with the first law) to better understand the thermodynamics of internal combustion engines. The examination of hypothetical “reversible” combustion at high temperatures and pressures was completed, documented and presented. The results indicate possible scenarios where the availability destruction can be zero by preselecting the reactant composition such that at the end of compression the species are in equilibrium. Although availability is preserved, most of the availability remains in the exhaust gases and the engine efficiency is typically low. Turbocharging capabilities were added to the cycle simulation, and included the use of the first and second laws of thermodynamics. The new components included a compressor, turbine, and intercooler. In addition to adding the new components, an appropriate engine and operating conditions were selected. The enhanced simulation was used in a series of parametric studies. (Caton, Texas A&M University)
- MSU is studying a high-compression-ratio Atkinson-cycle engine using low-pressure direct injection and pneumatic-electronic valve actuation to demonstrate the technology needed to produce a highly efficient engine. A forward-backward mass air flow sensor has been developed and a patent application for the device has been submitted. This technology will have particular application in variable valve timing direct injection systems for internal combustion engines. LES and KIVA-based simulations were used in conjunction with flow visualizations in an optical engine to study fuel air mixing. During this effort a metric for quantifying fuel distribution has been devised. A low-pressure direct injection system was developed and successfully tested. (Schock, MSU)
- The University of Texas (UT) Engine Combustion Laboratory is refining and completing development of an on-board PM sensor, bringing it to a point where it can be commercialized and marketed. New sensor designs were developed that make use of new manufacturing technologies that bond electrodes directly to ceramic support posts which are electrically isolated in metal bases. By eliminating small diameter metal wire electrodes, vibration noise was significantly reduced. The new foil-type electrodes were found to enhance electric field strength, as well, resulting in higher sensitivity for the same size sensor. Measurements of sensor sensitivity found resolutions as low as approximately 3 mg/m^3 of dry PM, and improvements beyond this level are expected. The durability of the sensors has been greatly improved though the application of active heating of the electrode supports. The response of the sensor to PM emissions created during engine transients has been assessed and found to be less than 20 ms. A licensing agreement to commercialize the PM sensor technology was signed in February 2008 with Emisense, Inc. a division of Ceramatec, Inc., which is a division of Coorstek, Inc. UT is currently pursuing joint development of the

technology and is in the process of finding a large sensor original equipment manufacturer to partner with. (Hall, UT at Austin)

PROJECT FUTURE DIRECTIONS

Advanced Combustion and Emission Control Research for High-Efficiency Engines

A. Combustion and Related In-Cylinder Processes

The focus in FY 2009 for combustion and related in-cylinder processes will continue to be on advancing the fundamental understanding of combustion processes in support of achieving efficiency and emissions goals. This will be accomplished through modeling of combustion, in-cylinder observation using optical and other imaging techniques, and parametric studies of engine operating conditions.

- ANL will increase the impact of their fuel injection spray visualization work by fostering collaboration with outside groups. Collaborations with modeling groups will increase the fundamental understanding of the mechanics of the spray event, while collaborations with industry will enable development of a technique that is useful as a diagnostic for injection system manufacturers. Both of these will expand the impact of their research, and help to meet the program objectives of decreased emissions and increased efficiency. Improvements to the measurement technique will increase its applicability and accessibility in the future. Such improvements include faster data acquisition, processing, and analysis, improved X-ray detector systems, increased X-ray intensity, and greater automation. An experimental station dedicated to spray radiography will be commissioned at Argonne's Advanced Photon Source. This will greatly expand the scope of the work, allowing development of new X-ray diagnostics and to expand partnerships with industry. (Powell, ANL)
- SNL will develop and apply additional diagnostic techniques that yield information characterizing the stoichiometry and temperature of regions where UHC is observed in low-temperature combustion. Diagnostics to identify the presence of liquid fuel in the cylinder, stemming from both the main injection event as well as inadvertent secondary injections and injector sac dribble will be developed and applied. Correction techniques to compensate for out-of-plane velocity biasing effects on velocity data obtained within the piston bowl will be further quantified and developed. Planar fluorescence imaging and particle image velocimetry techniques will be applied to measure UHC, CO, and velocity fields in late-injection low-temperature combustion systems. The impact of squish height and spray targeting on CO and UHC emissions from low-temperature combustion systems will be investigated. The impact of strain and rotation dependent model coefficients on the modeling of the turbulent kinetic energy dissipation in flows with bulk compression will be assessed. (Miles, SNL)
- SNL will apply optical diagnostics for other LTC conditions including (1) compare single and split/pilot injection schemes for conventional and LTC combustion using multiple imaging diagnostics and (2) acquire and process in-cylinder soot data to understand the influence of end-of-injection mixing on soot formation and oxidation. The modeling collaboration with University of Wisconsin to improve computer model performance for LTC conditions will be maintained using experimental data to validate and improve computer models. Efforts will continue to extend the conceptual model of diesel combustion to LTC conditions. (Musculus, SNL)
- SNL will continue their investigation of fundamental causes of UHC and CO formation in LTC. They will determine how multiple injections can be used to affect ignition timing and minimize UHC at LTC conditions. Direct measurements of mixing (equivalence ratio) at the time of the premixed burn in constant-injection-duration diesel fuel jets for various EGR levels and multiple injection strategies will be performed. This investigation will show how mixing between injections affects the equivalence ratio and location of the premixed burn. In addition, how jet-jet interaction affects flame lift-off will be investigated. (Pickett, SNL)

- ORNL will further explore HECC strategies on their GM engine for comparison of technologies and compression ratio effects to the Mercedes-Benz engine extensively tested previously. Cylinder/cyclic dispersion sensitivity to HECC method and EGR/air maldistribution will be characterized and development of acoustic/vibration phenomenological model for combustion characterization and insight into the potential of noise damping will be continued. Support of efficiency and emission controls activities to ensure a collaborative path toward achievement of FY 2010 DOE FreedomCAR milestones will be continued. (Wagner, ORNL)
- SNL will continue development of high-fidelity simulations of their optical H2-ICE and systematically extend them to HCCI engine experiments. They will also continue high-fidelity simulations of the optical H2-ICE by (1) installing a new Ford direct-injection head and matching experimental activities, (2) validation of measured, modeled results using chemiluminescence imaging, particle image velocimetry, and planar laser induced fluorescence, and (3) joint analysis of data extracted from validated simulations to enhance basic understanding, improve engineering models, and hydrogen-injector pattern optimization. (Oefelein, SNL)
- LLNL will continue their combustion modeling development in the coming year. They will validate the KIVA multi-zone code at partially stratified conditions and demonstrate fast modeling of partially stratified combustion with an artificial neural network-based chemical kinetics model. An analysis tool will be demonstrated for modeling unstable SI-HCCI transition experiments: transitioning between SI and HCCI by advancing exhaust valve closing produces oscillatory behavior for intermediate residual gas fraction (30-50%). Work will continue with ORNL in developing chemical kinetics-based models that help in understanding this complex phenomenon. They plan to release and license LLNL analysis tools to collaborators: there is continuous interest from industry and academia in these tools. (Aceves, LLNL)
- SNL will continue HCCI combustion development by determining how natural thermal stratification develops in an HCCI engine, including its magnitude and distribution, which is critical for high-load HCCI operation. They will complete development of an appropriate planar temperature-imaging diagnostic and determine the potential of pressure-boost to extend the high-load range of HCCI by using EGR to control the pressure-induced combustion-phasing advance. The behavior of ethanol as an HCCI fuel over a range of loads, speeds, and intake-pressure boost conditions will be investigated. Detailed exhaust-speciation study over a range of loads for a representative two-stage ignition fuel will be continued and compared with previous data for single-stage fuels (with LLNL). The traces species that affect autoignition recovery from near misfire for single- and two-stage ignition fuels will be determined by using detailed exhaust-speciation analysis under these conditions. Cooperative work with LLNL on improving chemical-kinetic mechanisms for fuel constituents and surrogate fuels, and to support their CFD modeling work with data and analysis will be continued. (Dec, SNL)
- SNL will validate the University of Wisconsin CFD model of the SNL automotive HCCI engine using optical and conventional measurements over a range of NVO operating conditions. Optical diagnostics to characterize reforming reactions during the NVO period and correlate to main combustion will be applied and the tunable diode laser absorption diagnostic to permit in-cylinder measurement of water and carbon dioxide will be expanded. A new spray-guided direct injection head will be installed. (Steeper, SNL)
- ORNL will continue to map SI-HCCI regions of operation on a multi-cylinder engine located at Delphi Automotive Systems. The low-order combustion model will be refined with data from multi-cylinder engine experiments to facilitate the development of real-time predictive controls. Simulations of SI-to-HCCI transition to improve fundamental understanding of combustion modes and transitions will be continued. Simulations will be performed in-house as well as in collaboration with LLNL. (Wagner, ORNL)
- LANL will continue development of KIVA-4 by (1) enabling KIVA-4 to run with a cut-cell grid which will improve the numerical accuracy in the interior of the mesh and resolve rezoning issues, (2) developing a software package to produce a cut-cell grid from a stereolithographic surface, (3) performing parallel 3-D calculations with the KIVA-4 multi-zone method , and (4) performing calculations with the grid overset method in complex geometries. (Torres, LANL)

- LLNL will continue to develop detailed chemical kinetic models for fuel components used in surrogate fuels for diesel and HCCI engines. Surrogate fuel models are being developed to represent real fuels and model low-temperature combustion strategies in HCCI and diesel engines that lead to low emissions and high efficiency. The role of fuel composition on low-temperature combustion modes of advanced combustion engines will be characterized. A detailed chemical kinetic mechanism for heptamethylnonane, a primary reference fuel for diesel engines will be developed and validated. (Pitz, LLNL)
- ORNL will continue identifying pathways for improved engine efficiency to meet the 2010 FreedomCAR goals of 45% peak efficiency and Tier 2, Bin 5 emissions levels. In the coming year ORNL will continue component development of a thermal energy recovery (TER) system and evaluate it on the exhaust system of a light-duty diesel engine. A prototype turbo-compounding system being developed and supplied to ORNL by Woodward Governor will be evaluated. Approaches to LTC in combination with appropriate aftertreatment systems for improving overall system efficiency while meeting FY 2010 emissions targets will be explored. A vehicle systems model with integrated transient capable TER model using GT-Drive and/or PSAT to estimate the potential benefits of and manage implementation issues associated with TER on light-duty vehicle applications will be developed. (Wagner, ORNL)
- SNL will continue fabrication and assembly of a two-stroke, opposed-piston hydrogen engine research experiment utilizing optimized coupling of dual Magnequench linear alternators as a proof-of-concept tool. The research experiment will measure indicated efficiency in a continuous operation regime as well as the stability of the electrically-coupled opposed pistons. The flexibility and multi-fuel capability by operating on alternative fuels at various operating conditions (compressions ratios, equivalence ratios) will be demonstrated. The battery charging application will be optimized for higher power-to-weight ratios. (Van Blarigan, SNL)
- ANL plans to continue their optimization of direct injection hydrogen combustion engine performance using an endoscopic technique. The efficiency improvement of fast acting injectors (piezo-actuated) will be characterized. Improved injector nozzle designs for specific operation conditions (injector location, injection strategy) supported by optical engine results (SNL) and 3-D CFD simulation will be developed. The effects of external EGR on engine efficiency and emissions will be evaluated. A proposal has been submitted to evaluate hydrogen direct injection in a multi-cylinder engine. (Wallner, ANL)
- SNL will continue to provide the science base for the development of high-efficiency hydrogen-fueled vehicle engines. A new engine head, supplied by Ford R&D, will be installed featuring central or side injection and central ignition. Engine geometry will then be identical to that of collaborating labs at Ford and ANL. An extensive database of fuel distributions and velocity maps as a function of varying injector geometry and location, injection timing, speed, and load will be compiled. Data will be used to complement metal engine data and for simulation validation. Quantitative laser-based techniques will be supplemented with qualitative high-speed Schlieren "movies" to understand temporal development mixture formation. A hydroxyl ion planar laser-induced fluorescence will be used to investigate the influence of mixture formation on combustion, in particular with multiple injections per cycle. (Kaiser, SNL)
- Cummins will continue to design and develop advanced engine architectures capable of achieving U.S. EPA 2010 emission regulations while improving brake thermal efficiency by 10% compared to current production engines. Aftertreatment thermal management techniques and hardware to optimize the engine and aftertreatment system to minimize the impact on engine efficiency will be developed. A urea decomposition reactor to convert aqueous urea to gaseous ammonia to improve the SCR NOx catalyst conversion efficiency will be developed. On-board diagnostics associated with the implementation of the new HECC subsystem technology to achieve proper functioning during in-use operation will also be developed. (Stanton, Cummins)
- Caterpillar will continue their efforts to apply HECC. The activities to be conducted include: (1) single-cylinder engine testing of gasoline/diesel fuel blends with optimized engine hardware, (2) study evaporating and combusting sprays of gasoline/diesel fuel blends, (3) validate precision cooling design methodology and demonstrate reduced heat transfer to jacket water, (4) evaluate multi-hole spray impact on lifted flame diffusion combustion, (5) complete development and

validation of wall film model to improve simulation accuracy of combustion using early injection timing, such as PCCI, (6) optimization of PCCI combustion system hardware to extend operating range, and (7) complete bearing analysis of redesigned VCR and finalize design changes. (Gehrke, Caterpillar)

- Navistar will continue their efforts to apply LTC to their 6.4L V8 engine. An electro-hydraulic VVA system developed during the course of this project will be installed and used to explore the impact of valve timing on effective compression ratio and improved engine thermal efficiency. KIVA simulations will be used to further optimize combustion hardware and new boundary conditions to extend the operation of LTC. The engine will tested over the federal transient heavy-duty cycle. For this purpose, the project scope includes the development of a prototype electronic control unit to handle in-cylinder combustion diagnostics and feedback. (de Ojeda, Navistar)
- ORNL will continue their efforts to analyze and define specific pathways to improve the energy conversion efficiency of internal combustion engines. They will: (1) construct a regenerative air preheating with thermochemical recuperation (RAPTR) bench-top constant-volume combustor, (2) experimentally demonstrate low-irreversibility combustion in the RAPTR bench-top apparatus, (3) analyze data from RAPTR experiments to determine efficiency implications and appropriate ways to model exergy losses under different operating modes, (4) continue exploring better ways for recuperating exhaust heat and utilizing compound cycles for extracting work, and (5) continue exercising engine and combustion models to identify combustion modifications that would mitigate exergy losses. (Daw, ORNL)
- DDC will continue their efforts to explore advancements in engine combustion systems using HECC techniques to improve thermal efficiency while minimizing cylinder-out emissions. They plan to consolidate fuel injection strategy and multiple combustion modes to maximize thermal efficiency while maintaining the same or lower engine-out emissions as baseline, evaluate different advanced combustion concepts with advanced fuel injection system, continue steady-state advanced combustion development with implementation of genetic optimization recommendations for hardware procurement, continue transient combustion and control development using next-generation model-based control technology, and continue development and implementation of closed-loop real-time combustion control using novel in-cylinder sensors. (Zhang, DDC)
- GM will continue development and testing of their prototype gasoline and diesel engine hardware which enables operation of HCCI combustion for improved fuel efficiency and emissions performance. The enabling gasoline engine will continue to be used as the testbed for production-style cylinder pressure sensing subsystems and the fully-flexible engine will be built and demonstrated. The fully flexible valve actuation system using production-intent hardware will be updated and installed on the single-cylinder diesel engine. The emissions and fuel efficiency benefits found on the single-cylinder diesel engine will be validated using the multi-cylinder diesel engine. (Patton, GM)
- Cummins will develop an advanced combustion system that meets EPA Tier 2, Bin 5 emissions standards while demonstrating a 10.5% improvement in fuel economy over the FTP city drive cycle. Single-cylinder engine experiments will be conducted to optimize the combustion recipe and investigate NOx/brake specific fuel consumption trade-offs to determine what emissions compliance strategy enables the greatest improvement in fuel efficiency. A VVA system will be installed to validate and optimize its functionality for fuel economy improvement and emissions control. Multi-cylinder engine experiments to evaluate the potential benefits and develop algorithms for closed-loop combustion control and advanced model-based air handling controls will be conducted and suppliers of critical components for technology and commercial readiness will be assessed to ensure the technologies required for the planned architecture will be available for production. (Frazier, Cummins)
- Ford will continue their development of advanced engine boosting through evaluation of the low-speed flow bench data as well as the failure mode of the prototype turbocharger, revisiting the compressor and turbine design based on this preliminary flow bench test data and making improvements in simulation and further design iterations, if necessary, and conducting further flow bench testing on the C12 compressor wheel with three different casing treatments once the replacement turbine wheel is fabricated. (Sun, Ford)

B. Energy-Efficient Emission Controls

In FY 2009, work will continue on LNTs and urea-SCR to reduce NOx emissions. The focus of activities will be on making these devices more efficient, more durable, and less costly. For PM control, the focus will be on more efficient methods of filter regeneration to reduce impact on engine fuel consumption.

- PNNL will continue the studies of CO_2 and H_2O effects on BaO morphology changes and NOx storage properties of LNTs. Detailed characterization (e.g., Fourier transform infrared, transmission electron microscopy) of the roles (especially with respect to deactivation) and material properties of promoter species (such as ceria) will be made. Initial studies of interactions between multiple emission control devices (e.g., how to optimize LNT regeneration for ammonia production if a downstream urea-SCR catalyst system is present) will be conducted. (Peden, PNNL)
- PNNL will continue their efforts to identify mechanisms of sulfur poisoning of NOx adsorber materials by refining function-specific measures of 'aging', validating most-suitable function-specific measures on samples incrementally 'aged' under realistic conditions, applying the developed techniques to the commercial fresh and "aged" samples in the monolith form, and continuing to improve mechanistic understanding of sulfur removal processes. (Peden, PNNL)
- ORNL will continue their efforts to understand the complex chemistry that occurs during the regeneration processes for LNTs through experiments conducted on a full-size engine-LNT catalyst system. In the coming year, they will analyze the regeneration process in a hybrid LNT-SCR system and study LNT catalysis for lean gasoline applications. (Parks, ORNL)
- SNL will continue their efforts to develop chemical kinetics models for LNTs. They will complete parameter optimization for the sulfation/desulfation mechanism to allow a full quantitative description of catalyst poisoning and restoration. They will also account for the role of partial oxidation products as alternate reductant species during normal catalyst regeneration and use the validated reaction mechanisms to investigate coupling between an LNT and other devices in the aftertreatment train. (Larson, SNL)
- ORNL and their CRADA partner Navistar will (1) complete model development and protocol optimization, (2) evaluate model parameters with aged catalysts, and (3) investigate effects of hydrocarbons and SO_2 on model parameters. (Toops, ORNL)
- ORNL will continue their support of the NOx abatement research and development CRADA with International Truck and Engine Co./Navistar Inc. They will complete model development and protocol optimization, evaluate model parameters with aged catalysts, and investigate effects of hydrocarbons and SO_2 on model parameters. A decision to expand this CRADA to incorporate combustion efficiency will be made. (Toops, ORNL)
- ORNL will continue to develop a diagnostic for rapid, on-engine measurements of oil dilution by fuel. Activities to be completed include (1) quantify engine-system dispersion and mitigation strategies, (2) develop methods for in situ, on-engine-system assessment of catalyst state, and (3) investigate selected nitrogen-selectivity issues related to LNT regeneration and hybrid catalyst systems. (Partridge, ORNL)
- ORNL will continue their efforts to assess the relative merits of efficient emissions control for multi-mode lean direct injection engines. In the coming year they will investigate the potential to control the higher CO and hydrocarbon emissions associated with HECC by diesel oxidation catalysts and research the synergies between urea-SCR emission control and HECC combustion. (Parks, ORNL)
- ORNL will continue co-leading the CLEERS planning committee and co-leading the LNT Focus Group, and support the DPF and SCR Focus Groups as needed. ORNL will also continue providing standard reference LNT materials and data for Focus Group evaluation and continue assisting in refinement of CLEERS technical priorities, especially in regard to the balance between LNT and urea-SCR R&D and synergies between these two technology areas. ORNL will issue a final report on the 2008 R&D priorities survey and organize and conduct the 12th CLEERS workshop in the spring of 2009. Basic data and model exchange between CLEERS and other VT projects will be expanded and maintenance and expansion of the CLEERS Web site will be continued. (Daw, ORNL)

- ORNL will continue supporting the CLEERS joint development of benchmark kinetics by confirming primary chemical mechanisms and kinetics of sulfation and desulfation, implementing a combined LNT model that includes NOx capture and reduction and sulfation and desulfation in a form that can be used for systems drive cycle simulations and shared with the CLEERS community, and investigation of urea-SCR kinetics. Additional activities will include interface with CLEERS industry partners to determine if X-ray monitoring would be useful for DPF onboard diagnostics/model validation and continuing identification of synergies between LNT NH_3 generation kinetics and NH_3-SCR as a potential alternative to urea-SCR NOx control. (Daw, ORNL)
- PNNL will continue their CLEERS DPF modeling activities by (1) making improved measurements of particulate penetration into filter walls by immobilizing deposits with vaporized adhesive, potting with epoxy, and polishing wall cross-sections to a flat surface, (2) using computed tomography (CT) data to generate new DPF substrate reconstructions for pore-scale simulations, (3) comparing predictions made with CT geometries to those obtained with geometries generated by stochastic reconstruction, (4) exploring effects of pore structure variations (e.g. contributions of unusually large pores or cracks) in filter substrates, (5) examining effects of catalyst washcoat location and structure on flow, filtration, and regeneration, and (6) conducting filter regeneration experiments in a bench-scale reactor with catalyzed filter samples loaded with lab-generated soot and soot from diesel engines. (Stewart, PNNL)

C. Critical Enabling Technologies

The critical enabling technologies activities in FY 2008 include work on VVA, VCR systems, and combustion sensors.

- Delphi completed their project to design and build a cost-effective, VVA system for advanced low-temperature diesel combustion processes. (Gutterman, Delphi)
- Envera LLC will optimize their variable compression ratio hydro-mechanical system for improved performance and manufacturability. The existing/optimized variable compression ratio engine will be installed and tested in a vehicle. (Mendler, Envera LLC)
- Streamline Automation, LLC will continue their efforts to develop a workable NOx sensor for use in diesel engine exhaust systems. Verification and validation of the new instrument will be completed and a plan for installing it and testing it alongside commercial analyzers is planned. Modifications to the original calibration vs. a gas chromatograph will allow effort and time to install the new sensor on an experimental diesel engine to begin to gather real-time NOx emissions results. Specific activities include (1) complete verification and validation of latest sensor and instrument, (2) order and secure new diesel test engine, (3) instrument test engine with verified voltammetric gas microsensor(s), (4) compare and evaluate performance against existing NOx analyzers and measurement instruments, and (5) deliver example prototype sensors to Robert Bosch for commercial partner evaluation. (Vogt, Streamline Automation, LLC)
- TIAX LLC will implement LTC to evaluate their SOC sensor for HCCI engine operation (current data has been measured in diesel mode). The real-time SOC algorithm will be optimized for speed and accuracy. (Smutzer, TIAX LLC)
- Westport Power, Inc. will continue testing their SOC sensor by installing it on a light-duty Cummins ISB engine, a heavy-duty Cummins ISX HPDI engine, and onboard a Class 8 truck with a Cummins ISX engine. (Mumford, Westport Power, Inc.)
- Cummins has produced a first-generation waste heat recovery system which successfully demonstrated that the predicted fuel efficiency benefit of this concept could be achieved. Future work is focused on enhancing system performance and refining system architecture to be integrated into Cummins' future products. Activities in the coming year include (1) apply hardware test results to refine system performance models and continue with model-based system development and optimization, (2) create a refined second-generation hardware set which may be integrated into Cummins future engine products, (3) refine and develop system subcomponents including feed and boost pumps, integrated controls, and heat exchangers in order to demonstrate long-term durability, (4) proceed to in-vehicle system installation and operation, and (5) demonstrate the additional fuel economy benefit from additional exhaust energy recovery and also charge air energy recovery. (Nelson, Cummins)

- Caterpillar will continue their study of waste heat recovery systems to demonstrate significant progress toward the goal of a 10% improvement in thermal efficiency using prototype components. There will be two elements to this demonstration: first, an on-engine demonstration of a 5 to 7% improvement in thermal efficiency using advanced turbocharger technologies, intercooling, insulated exhaust ports, and mechanical turbocompound, and second, parallel developments of technologies for future integration into the system solution, including the mixed flow turbine and electric turbocompound. (Kruiswyk, Caterpillar)
- Volvo will conduct analysis of test results with simulation results and develop an advanced hybrid engine control strategy. (Kang, Volvo)

D. Health Impacts

The focus of the activities in Health Impacts is to identify and quantify the health hazards associated with exhaust from advanced combustion engines and put them in proper context with other air quality hazards, and to assess the relative hazards of emissions from different fuel, engine, and emission reduction technologies.

- ORNL will continue their study of health effects from advanced combustion and fuel technologies by characterizing particulate emissions from PCCI engines for evidence of soot precursors and changes in density and morphology, determining the efficiency of catalytic aftertreatment for reduction of MSATs from HECC diesel operation, and resolving differences in thermally-desorbed volatile fraction and solvent-desorbed volatile fraction of diesel PM. (Parks, ORNL)
- NREL will continue their collaborative lubricating oil study on emissions (CLOSE) project by testing a variety of light-, medium-, and heavy-duty vehicles over different driving test cycles at room (72°F) and cold (20°F) temperatures on chassis dynamometers. The complete vehicle and emissions testing project will be completed during FY 2009. (Lawson, NREL)
- HEI will continue management of the Advanced Collaborative Emissions Study. The Phase I final report will be prepared and the feasibility and timeline for beginning Phase 2 characterization of 2010-compliant engines will be assessed. Phase 3A emissions and exposure chamber characterization will be completed and a meeting of stakeholders will be held to discuss the results of Phase 3A chamber exposure characterization. Chronic bioassay in rats and associated biological screening studies in rats and mice will be initiated. (Greenbaum, HEI)

Solid State Energy Conversion

Research will continue in FY 2009 on thermoelectrics for converting waste heat from advanced combustion engines directly to electricity. Research will focus on development of practical systems that are suitable for future production.

- GM will continue to develop TE technology for automotive waste heat recovery by completing prototype TE module construction, starting performance tests of prototype TE modules, completing TE exhaust waste heat recovery subsystem prototype construction, and completing vehicle modification for TE generator performance testing. (Yang, GM)
- BSST will continue their efforts to develop a TEG for use on light-duty vehicles. They plan to: (1) test a 150 W high-temperature TEG on a single-cylinder engine dynamometer, (2) complete the build of a full-scale high-temperature TEG and perform testing on an engine dynamometer, and (3) finalize dynamometer performance results and evaluate the system on a vehicle. (LaGrandeur, BSST)
- MSU will continue their study of TE conversion of waste heat to electricity in an internal combustion engine powered vehicle. The design of a 500 Watt generator will be completed and demonstrated. Fixtures required to construct modules which will make up the 500 Watt generator will be designed and fabricated. Design and fabrication of power electronic systems that will be used in the demonstration of the 500 Watt generator will be completed. Evaluation of advanced systems will be continued and the 500 Watt system will be demonstrated. (Schock, MSU)
- Ford will test a 100 W thermoelectric panels on a single-cylinder test engine, then test an 800 W thermoelectric generator on 6-cylinder gasoline engine exhaust. (Maranville, Ford)

- GM and Ford will begin developing vehicular thermoelectric heating, ventilation, and air conditioning which will be particularly beneficial for hybrids, plug-in hybrids, and full electric vehicles as well as the conventional ICE-powered vehicles. (Yang, GM; Maranville, Ford)

University Research

In FY 2009, our university partners will continue their fundamental research into combustion and the chemistry of emission control devices.

- UM will perform the following activities during 2009: (1) carry out experimental work with single- and multi-cylinder engines to further extend upper and lower load limits, with consideration of constraints on knock, NOx and stability, (2) complete the validation of the GT-Power®-based LTC engine simulation tool with data from single-cylinder experiments on burn rate, combustion efficiency and stability limits, (3) complete modified KIVA/flamelet model of spark-assisted HCCI and explore potential benefits of the technology from the point of view of control and range extension, (4) refine SCR and DOC after-treatment models in conjunction with new bench test experiments carried out under simulated LTC conditions, and (5) extend ignition delay experiments on alternative fuels to include blends. (Assanis, UM)
- The University of Wisconsin-Madison will continue developing methods to optimize and control LTC diesel technologies that offer the potential of nearly eliminating engine NOx and particulate emissions at reduced cost over traditional methods by controlling pollutant emissions in-cylinder. (Reitz, University of Wisconsin-Madison)
- The University of Houston will continue their efforts to study regeneration kinetics of LNT catalysts. Activities in the coming years will include conducting bench-scale and TAP experiments on additional catalyst types, carrying out isotopic TAP studies of storage and reduction using ^{15}NO and $^{18}O_2$, carrying out evaluation of stratified monolith configurations, and carrying out testing of selected LNTs with engine exhaust in their dynamometer facility. (Harold, University of Houston)
- The University of Kentucky will continue their investigation of aging mechanisms in LNTs. They will do this by: (1) completing studies pertaining to the dynamics of LNT desulfation, (2) characterizing aged catalysts using standard physico-chemical techniques, in tandem with bench reactor tests, in order to correlate catalyst aging characteristics with washcoat composition, (3) applying SpaciMS to probe the transient behavior of aged catalysts (for comparison with results previously obtained on fresh catalysts), and (4) deriving a quantitative model that describes catalyst performance as a function of aging time. (Crocker, University of Kentucky)
- Texas A&M University will continue to use their engine cycle simulation to study diesel engines and to better understand the thermodynamics of internal combustion engines. The parametric examination of turbocharging from a first law and second law perspective will be completed. The cycle simulation with turbocharging will be used to examine other exhaust gas exergy recovery methods. In addition, the simulation will be used to explore other operating conditions such as low-heat-rejection which would result in higher exhaust energy and exergy which would then need to be recovered. (Caton, Texas A&M University)
- MSU has completed their project to develop and demonstrate a high-compression-ratio, Atkinson-cycle engine using low-pressure direct injection and pneumatic-electronic valve actuation enabled by ionization current and forward-backward mass air flow sensor feedback. (Schock, MSU)
- UT at Austin will continue efforts to design, develop, and commercialize an on-board engine exhaust PM sensor for HCCI and conventional diesel engines. Activities during the coming year will include: (1) evaluating new sensor designs to further evaluate and, if necessary, improve sensor durability and sensitivity, (2) completing our analysis of the effects of exhaust gas velocity on sensor output, (3) begin testing the sensor in a model-year 2007 6.7-liter Cummins diesel engine, (4) evaluating suitability for HCCI applications, (5) begin evaluations of the PM sensor applied to local Austin area school busses, and (6) continue commercialization efforts. (Hall, UT at Austin)

HONORS AND SPECIAL RECOGNITIONS

1. Paul Miles, Invited Lecture: 3rd Int. Symposium on Clean High-Efficiency Combustion in Engines, June 19–22, Tianjin, China.

2. Robert Wagner, activity contributed to 2008 Advanced Combustion & Emissions Control Technical Accomplishment in report to USCAR Board of Directors; "Demonstrated 2008 FreedomCAR engine efficiency milestones of 43% peak BTE and 27% road-load BTE on a light-duty engine" and "2nd Law thermodynamics perspective helps to define path to 45% peak BTE in light-duty internal combustion engines".

3. J.C. Oefelein invited presentation, "Toward high-fidelity simulations for clean and efficient combustion of alternative fuels," LES for Internal Combustion Engine Flows, December 1-2, 2008, Ruell-Malmalson, France.

4. J.H. Chen, J.C. Oefelein and R. Sankaran, invited presentation, "High-fidelity simulations for clean and efficient combustion of alternative fuels," Journal of Physics, SciDAC 2008, July 13-17, 2008, Seattle, WA.

5. Salvador M. Aceves invited to deliver a seminar at the SAE 2007 symposium on HCCI, September 2007, Lund, Sweden.

6. Daniel Flowers invited to deliver a seminar at the SAE 2007 symposium on HCCI, September 2007, Lund, Sweden.

7. Salvador Aceves invited to serve as an opponent in Ph.D. exam, Chalmers University, Gothenburg, Sweden, September 2008.

8. Nick Killingsworth invited to deliver a seminar at the "Advanced Engine Control Symposium," Tianjin, China, November 2008.

9. John Dec, invited topical review paper and lecture at the 32nd International Combustion Symposium, Montreal, Canada, August 2008.

10. John Dec, invited presentation at the 3rd International Symposium on Clean and High-Efficiency Combustion in Engines, Tianjin, China, June 2008.

11. John Dec, invited presentation for the Coordinating Research Council, Advanced Vehicle/Fuels/Lubricants Meeting, September 2008.

12. Robert Wagner, activity was recognized as 2008 DOE FreedomCAR and Fuel Partnership technical highlight "A Predictive Model has been Developed for the Practical Implementation of HCCI Combustion".

13. Charles K. Westbrook: 2008 Bernard Lewis Gold Medal award by the Combustion Institute.

14. Charles K. Westbrook: 2008 - 2012 President of the Combustion Institute.

15. William J. Pitz: Invited Plenary Lecture at the 2008 International Conference on Modeling and Diagnostics for Advance Engine Systems (2008 COMODIA), Sapporo, Japan.

16. Peden, C.H.F. "Fundamental Studies of Catalytic NOx Vehicle Emission Control." Invited Presentations made by Chuck Peden at the following locations:

1. Korea Institute of Energy Research, Daejon, South Korea, November 2007.
2. Argonne National Laboratory, Argonne, IL, December 2007.
3. Northwestern University, Evanston, IL, January 2008.
4. Annual DOE/EE/OVT Peer Review, February 2008.

17. Peden, C.H.F. "The Use of Ultrahigh Field NMR Spectroscopy to Study the Surface Structure and Catalytic Properties of Poorly Crystalline γ–Al_2O_3." Invited Presentations made by Chuck Peden at the following locations:

1. Annual Meeting of the Philadelphia Catalysis Club, Newark, DE, May 2008.
2. 14th International Congress on Catalysis, Seoul, South Korea, July 2008.
3. 236th American Chemical Society National Meeting, Philadelphia, PA, August 2008.

18. Peden CHF. "The Nanoscience of Next Generation Automobile Emission Control Catalysts." Invited Presentation made by Chuck Peden at the European Science Foundation Conference on "Nanotechnology for Sustainable Energy", Ötz Valley, near Innsbruck, Austria, June 2008.

19. J. Yang - National Academy of Engineering U.S. Frontiers of Engineering Symposium.

20. J. Yang – U.S. Department of Energy Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award.

21. J. Yang, March 2008, invited presentation, The Annual American Physical Society March Meeting, Opportunities in Energy Research Workshop, New Orleans, LA: "Thermoelectric Energy Conversion".

22. J. Yang, August 2008, invited presentation, The 27th International Conference on Thermoelectrics, Corvallis, OR: "Thermoelectric Materials for Automotive Applications".

23. J. Yang, September 2008, invited presentation, Department of Physics, Boston College, Chestnut Hill, MA: "Thermoelectric Materials by Design".

24. J. Yang, October 2008, invited presentation, 2008 MS&T conference, Pittsburg, PA, "Thermoelectric Materials for Automotive Applications".

25. J. Yang, December 2008, invited presentation, 2008 MRS Fall Meeting, Symposium W: Computational Materials Design via Multiscale Modeling, Boston, MA: "Thermoelectric Materials by Design".

26. J. Yang, December 2008, invited presentation, The 2008 IUMRS International Conference in Asia, Nagoya, Japan, "Thermoelectric Materials for Automotive Applications".

27. Q. Li, invited presentation, "Thermoelectric Materials with Potential High Power Factors" International Conference on Thermoelectrics, Corvallis, OR, USA, Aug. 3-7, 2008 (organized by International Thermoelectric Society).

28. L. Wu (invited talk), J. Zheng, J. Zhou, Q. Li, J. Yang and Y. Zhu, "Structural analysis of thermoelectric $AgPbmSbTe_2$+m using high resolution transmission electron microscopy" (MS&T08).

29. The SpaciMS received the 2008 R&D 100 Award, which recognizes the year's most significant technological innovations. The SpaciMS was developed in the Cummins-ORNL CRADA and sponsored by DOE\EERE\Vehicle Technologies and predecessor programs. The SpaciMS R&D100 team was ORNL, Cummins Inc., Queen's University Belfast, Hiden Analytical, and Y-12 National Security Complex. Hiden Analytical has commercialized the SpaciMS technology.

INVENTION AND PATENT DISCLOSURES

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2. Carl Hergart, et al., Caterpillar, "Extending Operating Range of a Homogeneous Charge Compression Ignition Engine via Cylinder Deactivation", US Patent No. 7,377,254, May 27, 2008.

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4. Kevin Duffy, et al., Caterpillar, "Dynamic Control of a Homogeneous Charge Compression Ignition Engine", US Patent No. 7,380,540, June 3, 2008.

5. Jia Ma, George Zhu, Harold Schock and Tom Stuecken, (MSU), "Method and Apparatus for Enhancing the Performance of a Camless Valve Actuator," Application made November 1, 2007. US Patent pending.

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7. The University of Texas at Austin, Patent Pending: 2443 - A Sensor to Measure Time-Resolved Particulate (soot) Exhaust Emissions from Internal Combustion Engines has been patented with coverage in the US in the form of a PCT that was nationalized in the US. Provisional: 7/19/2002, PCT conversion: 7/18/2003, Nationalization in the US: 1/19/2005.

8. Delphi Variable Valve Actuation Provisional Patents submitted:

1. System for Continuously Varying Engine Valve Duration.
2. Continuously Variable Valve Actuation System.
3. Electro-hydraulically actuated Variable Valve Duration System.

9. US Appl. No.: 12/137,964, "Laser-Induced fluorescence fiber optic probe measurement of oil dilution by fuel," ORNL Ref. No.: 1940.0, Filed 6/13/2008.

10. Xin He, Russell P. Durrett, “Reduce Diesel HC/CO Emissions at Low/Idle Loads by Using Internal EGR”. Provisional submitted, U.S. and international patent application in preparation.

The remainder of this report highlights progress achieved during FY 2008 under the Advanced Combustion Engine R&D Sub-Program. The following 54 abstracts of industry, university, and national laboratory projects provide an overview of the exciting work being conducted to tackle tough technical challenges associated with R&D of higher efficiency, advanced ICEs for light-duty, medium-duty, and heavy-duty vehicles. We are encouraged by the technical progress realized under this dynamic Sub-Program in FY 2008, but we also remain cognizant of the significant technical hurdles that lay ahead, especially those to further improve efficiency while meeting the EPA Tier 2 emission standards and heavy-duty engine standards for the full useful life of the vehicles.

Gurpreet Singh
Team Leader,
Advanced Combustion Engine R&D
Office of Vehicle Technologies

Roland M. Gravel
Office of Vehicle Technologies

Kenneth C. Howden
Office of Vehicle Technologies

John W. Fairbanks
Office of Vehicle Technologies

James Eberhardt
Chief Scientist,
Office of Vehicle Technologies

II. ADVANCED COMBUSTION AND EMISSION CONTROL RESEARCH FOR HIGH-EFFICIENCY ENGINES

II.A.1 Light-Duty Diesel Spray Research Using X-Ray Radiography

Christopher F. Powell (Primary Contact), Jin Wang
Argonne National Laboratory
9700 S. Cass Ave.
Argonne, IL 60439

DOE Technology Development Manager: Gurpreet Singh

Objectives

- Study the mechanisms of spray atomization by making detailed, quantitative measurements in the near-nozzle region of sprays from light-duty diesel injectors.
- Perform these measurements under conditions as close as possible to those of modern engines.
- Utilize the results of our unique measurements in order to advance the state-of-the-art in spray modeling.
- Provide access to a unique spray diagnostic to industrial partners in the spray and engine communities.

Accomplishments

- In Fiscal Year 2008 we made a significant discovery that uses a quantitative measurement of the fuel distribution to show how the spray width changes as ambient pressure is increased. This discovery clears up a discrepancy in the spray literature, and extends knowledge about spray behavior to the near-nozzle region. This discovery will allow spray models to more accurately predict the fuel distribution.
- Dr. Philippe Leick of Robert Bosch Corporate Research spent six weeks at Argonne working with our group. In June 2008, we performed X-ray measurements on sprays from several nozzle designs that are of interest to Bosch. Bosch is using these measurements to improve its computational spray modeling. The results of the measurements will be published and presented at the International Conference on Liquid Atomization and Spray Systems conference in July 2009.
- New techniques were developed that allow high speed X-ray imaging of the internal components of fuel injectors, and also of fuel droplet size and velocity. These measurements will prove invaluable to the computational modeling community for generation of accurate fuel nozzle geometries and validation of atomization models.
- In FY 2008 we arranged a new collaboration with the computational modeling group at the University of Wisconsin's Engine Research Center (ERC). In FY 2009, Prof. Christopher Rutland will send one of his Ph.D. students, Nidheesh Bharadwaj, to work at Argonne for two months. During this time, we will perform several measurements that are of interest to both Argonne and the ERC. After the completion of the measurements, Nidheesh will use the X-ray data to validate ERC's KIVA computational model, with the goal of improving the droplet drag modeling. This is a significant new development, as it has the potential to improve the industry's leading computational models.
- Due to advances in X-ray optics, we were able to measure the fuel distribution from a diesel injector under high density conditions without a fuel additive. This is a significant step, since several industrial partners have requested tests of pure diesel fuel. This is also an important step toward measuring evaporating sprays, since the effect of fuel additives might complicate measurements of sprays under high temperature conditions.

Future Directions

- Increase the relevance of our measurements by studying sprays under conditions even closer to those of modern diesel engines. We have made steady progress over the course of the project, continually increasing the ambient pressure and enabling the use of production nozzles. We plan to upgrade our fuel system to the latest generation of fuel injection equipment, and use full-production injectors that can also be run in the GM-Fiat 1.9 liter engine running in Argonne's Engine and Emissions group.
- Increase the impact of our work by fostering collaboration with outside groups. Our collaborations with modeling groups allow our work to increase the fundamental understanding of the mechanics of the spray event, while our collaborations with industry enable us to develop a technique that is useful as a diagnostic for injection system manufacturers. Both of these expand the impact of our research, and help to meet the program objectives of decreased emissions and increased efficiency.
- Improve the measurement technique. While we produce useful results today, improvements to the measurement technique will increase its applicability and accessibility in the future. Such improvements include faster data acquisition, processing, and

analysis, improved X-ray detector systems, increased X-ray intensity, and greater automation.

- In FY 2009, an experimental station dedicated to spray radiography will be commissioned at Argonne's Advanced Photon Source. This will greatly expand the scope of our work, allowing us to develop new X-ray diagnostics and to expand our partnerships with industry.

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Introduction

Fuel injection systems are one of the most important components in the design of combustion engines with high efficiency and low emissions. A detailed understanding of the fuel injection process and the mechanisms of spray atomization can lead to better engine design. This has spurred considerable activity in the development of optical techniques (primarily using lasers) for measurements of fuel sprays. Some of these optical techniques have become commercially available and can be readily applied to the testing and development of modern injection systems. Despite significant advances in spray diagnostics over the last 30 years, scattering of light from the large number of droplets surrounding the spray prevents penetration of visible light and limits such measurements to the periphery of the spray. This is especially true in the near-nozzle region of the spray, which is considered to be the most important region for developing a comprehensive understanding of spray behavior. Existing models of spray structure have only been compared with data acquired in the region relatively far from the nozzle. It is unknown how well these models apply in the crucial near-nozzle region. The limitations of visible light in the near-nozzle region of the spray have led us to develop X-ray diagnostics for the study of fuel sprays. X-rays are highly penetrative, and measurements are not complicated by the effects of scattering. The technique is non-intrusive, quantitative, highly time-resolved, and allows us to make detailed measurements of the spray, even in the dense droplet region very near the nozzle.

Approach

This project studies the sprays from commercially-available light-duty diesel fuel injectors. Our approach is to make detailed measurements of the sprays from these injectors using X-ray absorption. This will allow us to map the fuel distribution in these sprays, extending the existing knowledge into the near-nozzle region. The X-ray measurements are performed at the Advanced Photon Source at Argonne National Laboratory. A schematic of the experimental setup is shown in Figure 1; detailed descriptions of the experimental methods are given in [1] and [2]. The technique is straightforward; it is similar to absorption or extinction techniques commonly used in optical analysis. However, the X-ray technique has a significant advantage over optical techniques in the measurement of sprays: because the measurement is not complicated by the effects of scattering, there is a simple relation between the measured X-ray intensity and the mass of fuel in the path of the X-ray beam. For a monochromatic (narrow wavelength bandwidth) X-ray beam, this relation is given by

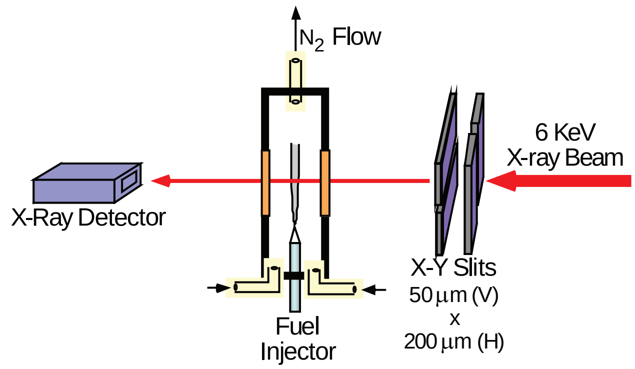

FIGURE 1. Schematic of the Experimental Setup

$$I/I_0 = \exp(-\mu_M M)$$

where I and I_0 are the transmitted and incident intensities, respectively; μ_M is the mass absorption constant; and M is the mass of fuel. The constant μ_M is measured in a standard cell, and the incident and transmitted intensities are measured as a function of time by the X-ray detector. This allows direct determination of the mass of fuel at any position in the spray as a function of time. It is the goal of our work to use the X-ray technique to measure sprays from our light-duty fuel injector at different injection pressures, different ambient pressures, and using different nozzle geometries. This will enable us to quantify how each of these variables affects the structure of the spray. We will also collaborate with spray modelers to incorporate this previously unknown information about the near-nozzle region of the spray into new models. This will lead to an increased understanding of the mechanisms of spray atomization and will facilitate the development of fuel injection systems designed to improve efficiency and reduce pollutants.

Results

In FY 2008 we made and published a significant discovery regarding the behavior of sprays under varying ambient pressure conditions. Several correlations exist in the literature for relating the width of the spray with the ambient density. However, these correlations vary considerably from one source to another, are only applicable far from the nozzle, and have only been validated with non-quantitative data. Quantitative, unambiguous X-ray measurements have demonstrated that the spray width varies as the square root of the density ratio (see Figure 2). This has been shown for several different nozzles, injector pressures, and densities. This important discovery quantifies the behavior of the spray as the in-cylinder pressure is changed, a correlation that will allow computational models of sprays to better predict the fuel distribution, ultimately leading to more accurate engine simulations.

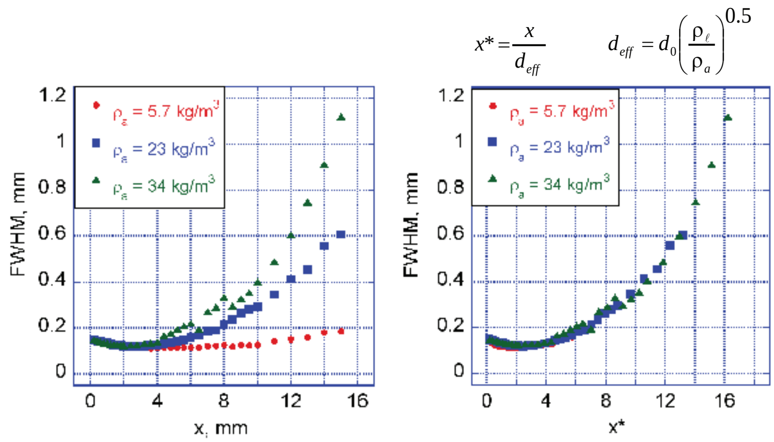

FIGURE 2. Spray width as a function of distance from the nozzle for the raw data (left) and normalized data (right). The normalization captures the dependence of width on ambient density.

In FY 2008 we made significant advances in effort to make measurements of sprays under conditions similar to those in a real engine. For the first time, X-ray measurements were performed using pure diesel fuel without additives. Past measurements have relied on a cerium or other additive to improve the X-ray contrast, but the additive causes slight changes to the fuel properties. In collaboration with a group from Monash University, Australia, we achieved high resolution data on diesel fuel sprays without a fuel additive (see Figure 3). While the effects of the additive are small for non-evaporating sprays, its different boiling point might cause difficulty in interpreting the results of spray measurements at elevated temperature. By demonstrating this capability, we clear an important technical hurdle and enable direct comparison of our data to real-world fuels.

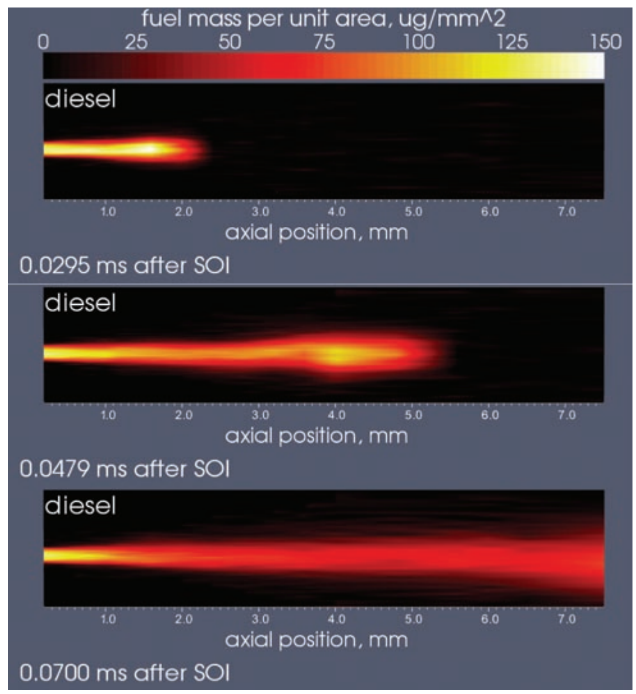

FIGURE 3. Fuel distributions of pure diesel fuel at three different times after start of injection measured under an ambient density of 25 kg/m^3. These measurements are the first that have been made without the use of a fuel additive to improve the image contrast.

Our group's collaboration with Robert Bosch GmbH had another milestone in FY 2008. Dr. Philippe Leick of Bosch Corporate Research spent five weeks at Argonne and participated in two weeks of X-ray experiments. Dr. Leick's expenses and salary were paid by Bosch, while Argonne provided his lodging. In addition, Bosch donated a large number of fuel system components to Argonne, including spray nozzles that were custom-built to Argonne's specifications. Nozzles such as these cannot be obtained from any other source at any price, and illustrate the value that Bosch places on this research. In total, Bosch made approximately $62,000 of in-kind contributions to the project in FY 2008. All of this has been done based on a handshake agreement with Bosch researchers, and the work has been freely publishable and available to our Memorandum of Understanding partners.

- In July 2008 we made a series of measurements of the time-resolved motion of the internal components of several different diesel fuel injectors. These measurements show the operation of the valve inside the injectors in real-time and in three dimensions. These measurements are crucial for accurate computational modeling of in-nozzle flow, as they are the only data available that capture the dynamic motion of the needle valve. These data are currently being analyzed and will be published in 2009.
- For the first time, it has been demonstrated that X-ray imaging can be used to image fuel droplet sizes and velocity. Droplet size and motion is a

common validation technique for spray models, but the instruments used to measure these properties have severe limitations and the results are easy to misinterpret. In August 2008 we were able to capture clear high-speed X-ray images of droplets in fuel sprays that allow unambiguous measurement of size and velocity. These measurements are still under analysis, but in the future, publication of these results will allow the laser droplet sizing instrumentation that is relied on as the industry standard to be thoroughly tested.

Conclusions

- The X-ray technique can be used to observe subtle changes in the spray structure resulting from different nozzle geometries. These changes are not apparent using other imaging techniques. This is a very useful diagnostic tool to fuel system manufacturers when designing and testing new injection systems.
- The time-dependent mass measurements provide unique information to spray modelers, and allow them to test their models in the near-nozzle region of the spray, something that was impossible previously. This data is crucial for the development of accurate spray models and for the detailed understanding of spray behavior. The quantitative measurements that we have provided may help to elucidate the mechanisms of spray atomization. This could ultimately lead to the design of cleaner, more efficient engines.
- The impact of our work on the engine community is shown by the expanding list of collaborators and by the significant in-kind contributions to our work that are being made by fuel system and engine manufacturers.

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FY 2008 Publications/Presentations

1. "Study of Diesel Jet Variability Using Single-Shot X-ray Radiography", A.L. Kastengren, C.F. Powell, Y.-J. Wang, J. Wang. Proceedings of the ASME Internal Combustion Engine Division 2007 Fall Technical Conference, Charleston, South Carolina, USA, Paper ICEF2007-1663. October 2007.

2. "Study Of Diesel Jet Variability Using Single-Shot X-ray Radiography", A. Kastengren, C.F. Powell, K.-S. Im, Y. Wang, J. Wang, Presentation to the USCAR Tech Team and MOU partners, Southfield, Michigan, October 2007.

3. "Ultra-Fast X-ray Radiography for the Study of Fuel Sprays" C.F. Powell, Presentation to Bosch Corporate Research, Stuttgart, Germany, October 2007.

4. "Fuel Spray Research Using X-ray Radiography", C.F. Powell, E. El-Hannouny, A. Kastengren, D. Longman, J. Wang, OVT Merit Review, Bethesda, MD, February 2008.

5. "X-ray Radiography Measurements Of Diesel Sprays And The Effects Of Ambient Pressure", A. Kastengren, C.F. Powell, Y. Wang, K.-S. Im, J. Wang, Presentation to the Combustion MOU Partners, Sandia National Laboratory, March 2008.

6. "Nozzle Geometry and Injection Duration Effects on Diesel Sprays Measured by X-ray Radiography", A.L. Kastengren, C.F. Powell, T. Riedel, S.-K. Cheong, K.-S. Im, X. Liu, Y. Wang, J. Wang, Journal of Fluids Engineering, Vol.130, Iss.4, April 2008.

7. "Measurement of Biodiesel Blend and Conventional Diesel Spray Structure Using X-ray Radiography", A.L. Kastengren, C.F. Powell, K. -S. Im, Y.-J. Wang, J. Wang. ASME Paper ICES 2008-1646, ASME Internal Combustion Engines Division Spring Technical Conference, Chicago, IL, April 2008.

8. "Fuel Spray Characterization Using Ultra-Fast X-ray Radiography", C.F. Powell, Advanced Photon Source User Science Seminar, Argonne, IL, April 2008.

9. "Study of Diesel Jet Variability Using Single-Shot X-ray Radiography", A.L. Kastengren, C.F. Powell, Y.-J. Wang, J. Wang. Journal of Engineering for Gas Turbines and Power GTP-07-1195 May 2008.

10. "X-ray Radiography Measurements of Diesel Spray Structure at Engine-Like Ambient Density", A.L. Kastengren, C.F. Powell, K. -S. Im, Y.-J. Wang, J. Wang. 21st Annual Conference on Liquid Atomization and Spray Systems, Orlando, FL, May 2008.

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II.A.2 Low-Temperature Automotive Diesel Combustion

Paul Miles
Sandia National Laboratories
PO Box 969
Livermore, CA 94551-0969

DOE Technology Development Manager:
Gurpreet Singh

Subcontractor:
University of Wisconsin Engine Research Center,
Madison, WI

Objectives

- Provide the physical understanding of the in-cylinder combustion processes needed to minimize the fuel consumption and the carbon footprint of automotive diesel engines while maintaining compliance with emissions standards.
- Develop efficient, accurate computational models that enable numerical optimization and design of fuel-efficient, clean engines.
- Provide accurate data obtained under well-controlled and characterized conditions to validate new models and to guide optimization efforts.

Accomplishments

- Performed a detailed emissions and combustion performance-based study to clarify the impact of boost on fuel economy and emissions of carbon monoxide (CO), unburned hydrocarbons (UHC), soot, and oxides of nitrogen (NOx).
- Developed new diagnostic technique for measuring the in-cylinder spatial distributions of CO and UHC using 2-photon, planar laser-induced fluorescence.
- Developed image distortion correction techniques that enable acquisition of spatially-accurate images within the highly curved combustion chamber–a capability that is critical for both scalar and velocity measurements within the bowl.
- Performed extensive simulations of CO and UHC yield from homogeneous mixtures to better understand the dependence of these emissions on mixture equivalence ratio and temperature.
- Measured the spatial distributions of CO and UHC in an early-injection, partially-premixed combustion regime for various loads, injection timings, and charge gas oxygen concentrations. Established the importance of the squish volume and partially-burned mixture near the cylinder centerline to both CO and UHC emissions. Demonstrated the importance of UHC stemming from the ring-land crevice.
- Established particle image velocimetry measurement capability and developed techniques to correct clearance volume velocity data for bias due to out-of-plane motion. Measured the velocity fields throughout the combustion chamber for various injection timings in a partially-premixed combustion system.
- Computed CO, UHC, and velocity distributions for several operating conditions and performed a detailed comparison with experimental data.
- Examined the impact of a non-linear turbulent stress model on predicted in-cylinder velocity fields, and identified its significant impact on entrainment into the fuel spray.

Future Directions

- Develop and apply additional diagnostic techniques that yield information characterizing the stoichiometry and temperature of regions where UHC is observed.
- Develop and apply diagnostics to identify the presence of liquid fuel in the cylinder, stemming from both the main injection event as well as inadvertent secondary injections and injector sac dribble.
- Further quantify and develop correction techniques to compensate for out-of-plane velocity biasing effects on velocity data obtained within the piston bowl.
- Apply both planar fluorescence imaging and particle image velocimetry techniques to measure UHC, CO, and velocity fields in late-injection low-temperature combustion systems.
- Investigate the impact of squish height and spray targeting on CO and UHC emissions from low-temperature combustion systems.
- Assess the impact of strain and rotation dependent model coefficients on the modeling of the turbulent kinetic energy dissipation in flows with bulk compression.

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Introduction

Direct-injection diesel engines have the highest fuel conversion efficiency and the lowest carbon dioxide (CO_2) emissions of any reciprocating internal combustion engine technology. However, conventional diesel engines produce elevated emissions of both soot and NOx. To address this shortcoming, low-temperature combustion techniques are being developed that prevent the formation of these pollutants within the engine. These techniques generally rely on high levels of charge dilution with recirculated exhaust gases to keep in-cylinder temperatures low. High dilution levels with attendant low charge oxygen concentrations make it difficult to mix the fuel with sufficient oxygen to achieve complete combustion, and the low combustion temperatures also slow the kinetic rates of oxidation. Hence, incomplete combustion–characterized by high UHC and CO emissions–can lead to a significant fuel economy penalty. A major focus of this work is to understand the main causes of combustion inefficiency through examination of the in-cylinder sources of UHC and CO emissions. Identifying these sources is insufficient, however: an ability to accurately predict these sources and how they vary with different engine design parameters is required to enable the design of clean, more efficient engines. Consequently, we also focus on careful comparison of the experimentally measured CO and UHC fields with the results of numerical simulations, including the predicted in-cylinder flows that strongly impact these fields.

Approach

The research approach involves carefully coordinated experimental, modeling, and simulation efforts. An optical engine facility with geometric and thermodynamic characteristics that allow it to closely match the combustion and engine-out emissions behavior of a traditional, all-metal test engine is established. Detailed measurements of in-cylinder flows, fuel and pollutant spatial distributions, and other thermo-chemical properties are subsequently obtained. These measurements are closely coordinated and compared with the predictions of numerical simulations.

The experimental and numerical efforts are mutually complementary. Detailed measurements of the in-cylinder variables permit the evaluation and refinement of the computer models, while the model results can be used to clarify the in-cylinder flow and combustion physics–a process that is difficult if only limited measurements are employed. Jointly, these approaches address the principal goals of this project: development of the physical understanding to guide and the modeling tools to refine the design of optimal, clean, high-efficiency combustion systems.

Results

Our research has followed a natural progression, starting with establishing that the emissions and performance behavior of the optical engine could match the behavior of a traditional metal test engine. Because the optical engine was operated in a skip-fired mode, simulated exhaust gas recirculation (EGR) was required to achieve the required charge dilution. Consequently, our tests have also included an evaluation of the effect of diluent gas composition on emissions and performance, including assessment of the impact of high levels of UHC and CO within real engine EGR. To perform this evaluation, the specific heat ratio and total mass flow rate was held constant as the simulated EGR gas composition was varied. Typically, the combustion behavior was similar for all EGR gas combinations tested, although small variations (typically about 1° crank angle [CA]) in ignition delay were observed. More importantly, for a wide variety of EGR gas compositions, both the magnitude and the trends with injection timing of CO and UHC emissions observed in a metal test engine with real EGR were well-captured [1].

With this reassurance that the physical processes impacting the combustion and emissions formation processes could be faithfully reproduced in the optical engine, the optical engine performance and emissions was evaluated over a matrix of low-temperature operating conditions, encompassing a wide range of charge oxygen (O_2) concentrations, injection timings, engine loads, and boost levels [2]. The results of this evaluation were used to select appropriate operating conditions at which to conduct more detailed optical investigations and numerical simulations. An example of the measured CO and UHC emissions behavior as charge dilution is varied is shown in Figure 1. Also indicated on the figure is one of the operating points selected for further investigation, characterized by a 10% O_2 concentration. At this level of dilution, the CO and UHC emissions are clearly rising rapidly, yet combustion efficiency has not yet suffered dramatically.

To aid in the identification of potential UHC and CO emissions sources, we have also undertaken extensive simulations of the yield of these species predicted by homogeneous reactor simulations employing detailed chemical kinetic mechanisms. The results of constant temperature and pressure simulations are shown in Figure 2, where they are overlaid with the well-known soot and NOx production regions [3]. Note that both UHC and CO can stem from fuel-rich as well as fuel-lean regions, while UHC additionally is found at all mixture stoichiometries where the local temperatures are too cool to permit fast reaction. Figure 2 also shows that significantly higher temperatures are required to rapidly oxidize lean mixture CO than UHC (approximately 1,500 K vs. 1,200 K), and that at higher temperatures considerable CO will be produced from mixtures which produce very little UHC ($1.0 < \phi < \approx 1.3$). Jointly, these observations indicate that it will be more difficult to eliminate CO emissions than UHC emissions, whether these emissions stem from fuel-lean or fuel-rich sources. In this context, it is interesting to note from

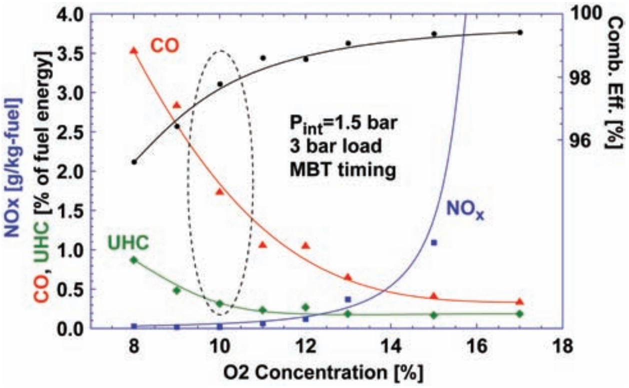

FIGURE 1. Variation in CO, UHC, and combustion efficiency with intake charge O_2 concentration. At the selected operating point, denoted by the dashed ellipse, the global equivalence ratio is about 0.36.

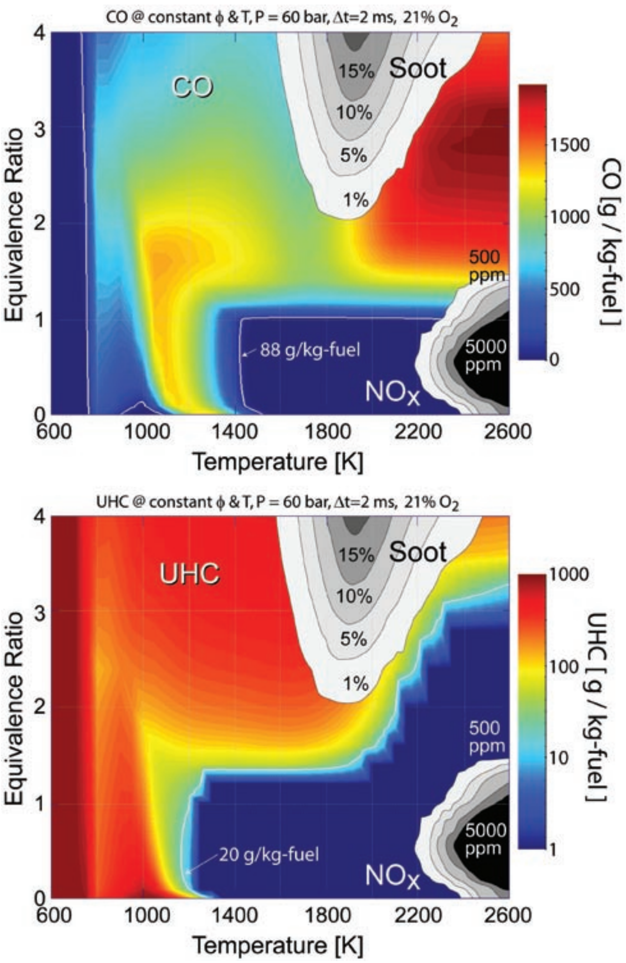

FIGURE 2. CO and UHC yield at 2.0 ms obtained from a homogeneous reactor simulation of the combustion of n-heptane. The 88 g/kg-fuel and 20 g/kg-fuel isopleths represent 2% of the fuel energy embodied in CO or UHC, respectively. Similar behavior is observed when the pressure is constrained to follow the measured cylinder pressure and the temperature is obtained by solving the energy equation.

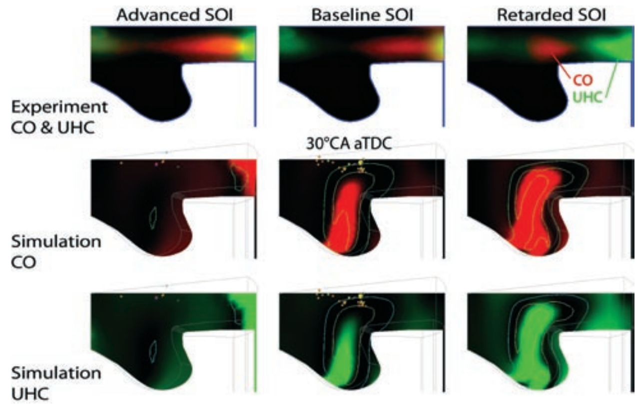

FIGURE 3. Comparison of measured and predicted spatial distributions of CO and UHC. The measurements are restricted to the clearance volume, as the high laser fluence required will damage the optical piston. (SOI - start of injection, aTDC - after top-dead center)

Figure 1 that the measured CO emissions account for the majority of the loss in combustion efficiency.

Cycle-averaged spatial distributions of CO and UHC measured within the clearance volume, at the operating condition identified in Figure 1, are shown in Figure 3 for optimal (maximum brake torque, MBT) injection timing as well as advanced and retarded injection timings. Two distinct differences can be observed between the measured and predicted CO distributions: first, at the advanced and baseline injection timings, the measurements indicate a greater amount of CO within the squish volume than is indicated by the simulations; second, with advanced injection, CO is predicted to be found close to the cylinder wall, while the measurements imply that it is displaced out a few millimeters. These observations suggest that the impact of heat losses to combustion chamber surfaces on the reaction kinetics may not be accurately captured by the combustion model employed. Conversely, with retarded injection timing, the CO cloud predicted to be exiting the bowl agrees well with the measured CO locations.

The predicted spatial distributions of UHC are generally similar to CO. However, significant amounts of UHC are predicted within the ring-land crevice only for advanced injection timing, and a UHC cloud leaving the bowl when injection timing is retarded is not observed. The failure to observe this cloud in the experiments could be due to two factors: a inability to detect UHC arising from hot, moderately rich mixture due to low concentrations of fluorescing compounds, or inaccurate predictions of UHC oxidation to CO by the reduced kinetic mechanism employed for the multi-dimensional simulations.

In addition to the UHC and CO fields, we have also compared the measured mean flow structures with the predictions of the simulations. Figure 4 shows the

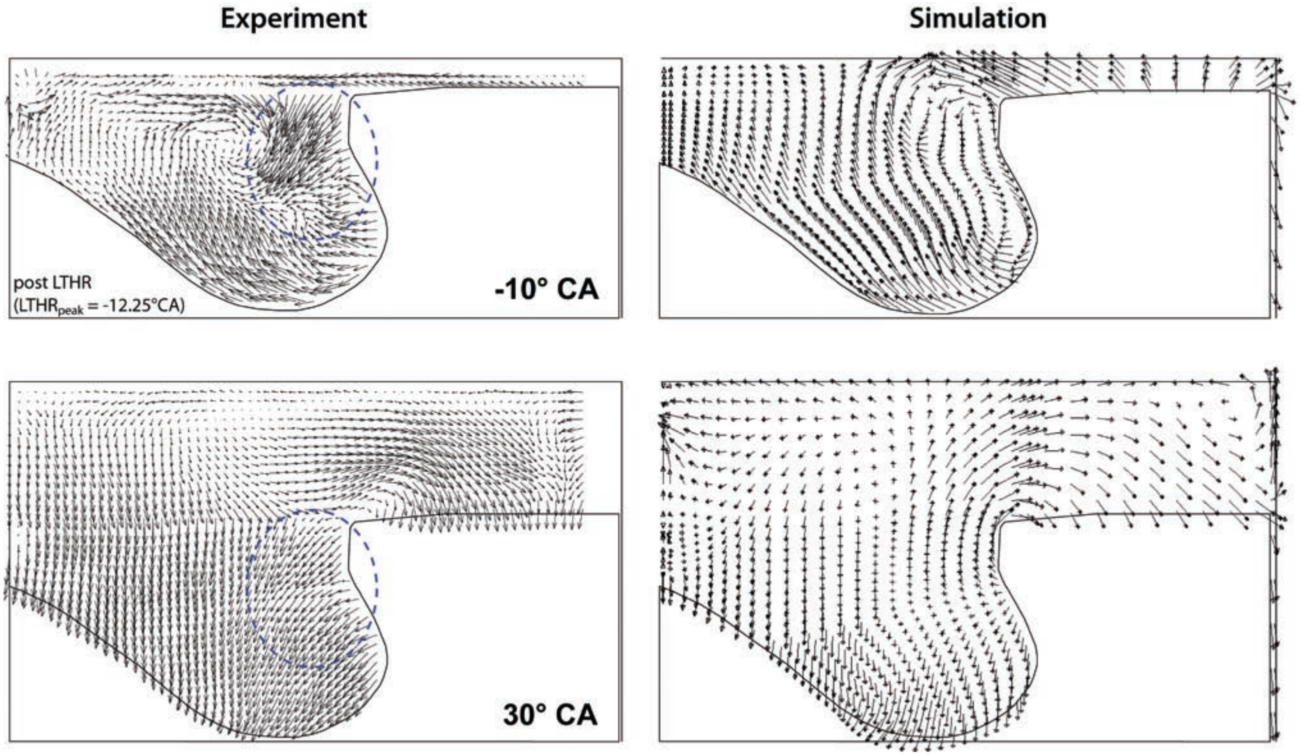

FIGURE 4. Measured mean velocity fields (left) are contrasted with the predictions of multi-dimensional simulations (right). The ellipses denote areas where the experimental measurements within the bowl will be influenced by out-of-plane fluid motion to the greatest extent.

mean velocity fields measured at two different crank angles, corresponding to the low-temperature heat release period and near the end of mixing-controlled combustion. Although the simulations capture many features of the bulk flow structures, there are important differences. During the low-temperature heat release, there are significant differences observed in the flow structures near the bowl lip–a region were significant fuel is expected. A large part of this difference may be associated with the influence of out-of-plane motion on the measured flow, which will introduce an inward, downward bias to the measured velocities in this region. Resolving and quantifying the impact of out-of-plane motion on the measured velocities will be critical to our ability to reliably assess the accuracy of the model predictions. On the other hand, significant differences are observed between the measured and predicted velocity fields within the clearance volume. In this region, errors induced by the out-of-plane velocity are small, and have moreover been partially corrected. Here, the differences observed are clearly associated with inaccuracies in the prediction of the flows during the combustion event.

Conclusions

- Combustion performance and emissions behavior has been examined over a wide range of operating conditions representative of low-temperature combustion regimes. Based on the results of this exploration, specific operating conditions have been selected for detailed study employing both optical experiments and numerical simulations.
- Homogeneous reactor simulations employing detailed chemical kinetic mechanisms have been used to clarify the impact of mixture equivalence ratio and temperature on CO and UHC yield. The results show that CO emissions will be more difficult to eliminate than UHC emissions in both mixing- and kinetically-controlled combustion regimes.
- Planar laser-induced fluorescence has been used to observe the spatial distributions of CO and UHC within the cylinder. The results have been compared with the predictions of multi-dimensional simulations. The comparison has identified specific aspects of the models that should be examined and possibly modified to improve the simulation accuracy.
- Measurement of in-cylinder flow structures provides the means for a detailed validation of model predictions. Additional work to quantify and correct for the impact of out-of-plane motion on the measured velocity fields is required to extract the full benefit of these measurements.

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3. Ekoto IW, Colban WF, Miles PC (2008) In-cylinder unburned hydrocarbon development for light-duty diesel engines operating under low-temperature combustion schemes, ***US DOE OVT Advanced Engine Combustion Working Group Meeting**, Aug 19-20.*

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Special Recognitions & Awards

1. Invited Lecture: 3rd Int. Symp. on Clean High-Efficiency Combustion in Engines, June 19–22, Tianjin, China.

II.A.3 Heavy-Duty Low-Temperature and Diesel Combustion Research (8748) and Heavy-Duty Combustion Modeling (12349)

Mark P. B. Musculus
Combustion Research Facility
Sandia National Laboratories
P.O. Box 969, MS9053
Livermore, CA 94551-0969

DOE Technology Development Manager:
Gurpreet Singh

Objectives

The overall Office of Vehicle Technologies goal for this project is to develop fundamental understanding of advanced low-temperature combustion (LTC) technologies. The project includes diesel combustion research (8748) at Sandia National Laboratories (SNL) and combustion modeling (12349) at the University of Wisconsin (UW). The specific goals for Fiscal Year 2008 include:

- Understand how engine design affects in-cylinder processes (SNL and UW)
  - This responds to requests from industry and suggestions from previous annual reviews of this project to study parametric variations in engine hardware to understand how engine design can control combustion and pollutant formation processes in LTC engines.
- Continue to improve LTC models (SNL and UW)
  - Validate/improve modeling of LTC mixing, combustion, and pollutant formation processes.
- Understand fluid mechanics of unsteady sprays (SNL)
  - Improve understanding of rapid leaning near the injector after the end of injection that causes unburned hydrocarbon (UHC) emissions for LTC.
  - Improve predictions of penetration for unsteady injection rates.
- Continue to refine conceptual model for LTC conditions (SNL)
  - This is a long-term goal with continuous effort to update our understanding of in-cylinder LTC processes as more data becomes available.

Accomplishments

- Optical data reveal how engine design affects jet-jet interactions
  - (1) Jet-jet interactions create fuel-rich regions, which lead to soot formation, and (2) fuel-lean regions near the injector do not burn to completion, leading to UHC emissions.
  - Jet-jet interaction increases with a smaller bowl, pushing hot combustion farther into the center of the combustion chamber, thus displacing the fuel-lean regions of UHC into the hot combustion zones, which may help to consume unburned fuel.
  - Similar observations for jet-bowl interaction with different spray angles.
- Initial KIVA mixing predictions agree well with experiments
  - Effects of jet-jet interactions on fuel-air mixing are well captured.
- One-dimensional model reveals why mixtures rapidly become lean after injection
  - Lean mixtures come from (1) low velocity, fuel-lean mixtures in the wings of the jet that lag behind and (2) increased entrainment, as model shows is required by conservation of mass.
- New unsteady spray model improves KIVA spray prediction
  - Dramatically reduces grid dependency, improving KIVA simulations of sprays and LTC combustion.

Future Directions

- Apply optical diagnostics for other LTC conditions
  - Compare single and split/pilot injection schemes for conventional and LTC combustion using multiple imaging diagnostics.
    - Survey industrial partners to define relevant operating conditions.
  - Acquire and process in-cylinder soot data to understand the influence of end-of-injection mixing on soot formation and oxidation.
- Maintain modeling collaboration with UW to improve computer model performance for LTC conditions
  - Use experimental data to validate and improve computer models.

  - Plan future experiments to continue to provide relevant data for computer model development and validation.
- Continue to extend the conceptual model of diesel combustion to LTC conditions
  - In addition to journal/conference publications, disseminate results in comprehensive textbook chapters, review articles, etc.

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Introduction

LTC strategies for diesel engines are of increasing interest because of their potential to significantly reduce particulate matter (PM) and nitrogen oxide (NOx) emissions. LTC with late fuel-injection offers the benefit of combustion phasing control, because ignition is closely coupled to the fuel injection event [1]. But with a short ignition-delay, fuel-jet mixing processes must be rapid to achieve adequate premixing before ignition. In the 2006 annual report for this project, we used laser-induced soot incandescence imaging to show that mixtures near the head of the diesel jets have inadequate mixing, so they are fuel-rich at ignition and they go on to form soot [2]. Furthermore, in the 2007 annual report, we used laser-induced fluorescence of hydroxyl radical (OH), formaldehyde (H_2CO), and toluene fuel-tracer to show that very fuel-lean regions can form near the injector, and that these regions lead to UHC emissions [3]. These data show that formation of mixtures that are either too fuel-lean or too fuel-rich at ignition can lead to significant pollutant formation in LTC engines.

In-cylinder mixture preparation and pollutant-formation processes may be controlled to some degree by engine design. The primary objective of this project for FY 2008 is to gain a better understanding of mixing and combustion processes for an exhaust gas recirculation (EGR)-diluted late-injection LTC strategy and to assess the potential impact of combustion chamber design on these processes. Other objectives include continuation of improvements to LTC diesel computer models and developing better understanding of diesel jet mixing processes after the end of injection.

Approach

This project uses an optically-accessible, heavy-duty, direct-injection diesel engine (Figure 1). Imaging access is through a window in the bowl of an extended piston. Windows in the cylinder wall and in the piston bowl-wall are for the laser diagnostics. Figure 1 also shows the setup of the optical diagnostics, which use three cameras. Direct measurements of fuel-vapor concentration by toluene fuel-tracer fluorescence are compared to simultaneous OH planar laser-induced fluorescence (PLIF) imaging and combined H_2CO and polycyclic aromatic hydrocarbon (PAH) PLIF imaging to evaluate mixing, combustion, and pollutant formation. The optical diagnostics are applied in a low-swirl, heavy-duty optical engine with three different piston designs having bowl diameters of 60%, 70%, and 80% of the cylinder bore. The horizontal laser sheets for the optical diagnostics are adjusted to three different heights for each of the piston bowls, as shown in Figure 2. By examining images at each of the three laser-sheet elevations, the mixing and combustion behavior throughout the bowl can be studied. The engine load is near 4 bar indicated mean effective pressure, with injection near top-dead center and using simulated EGR with 12.7% intake oxygen (O_2).

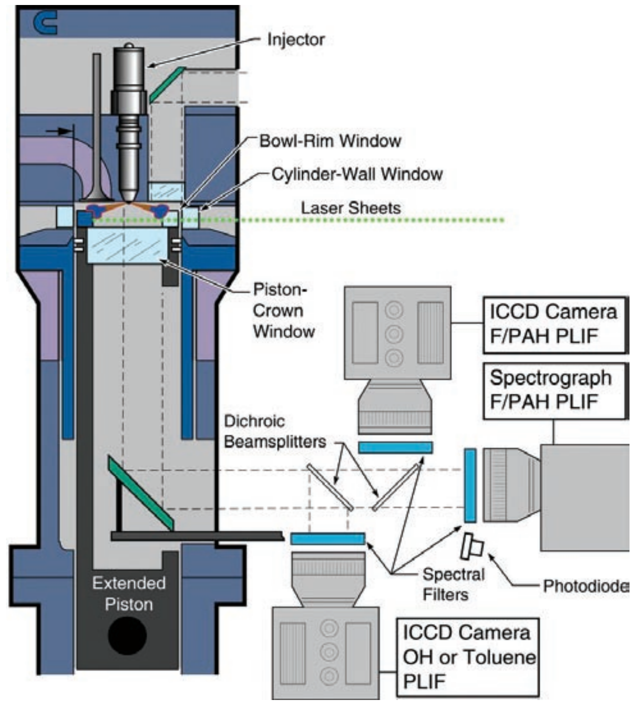

FIGURE 1. Schematic diagram of the optically accessible direct injection diesel engine and optical setup. (ICCD - intensified charged-coupled device)

The modeling work uses a version of the Los Alamos KIVA computer code that has been improved at the UW. Instead of using full detailed chemistry, the model uses a reduced kinetic mechanism for n-heptane ignition and combustion so that solutions can be completed in a reasonable time [4]. As described in the FY 2007 report for this project, a multi-objective genetic algorithm [5] using the KIVA computer model predicted an optimal set of piston bowl designs and spray geometries, which were studied and validated experimentally this year.

Results

Simultaneous images of OH PLIF (green) and combined formaldehyde and PAH PLIF (F/PAH PLIF, red) are shown in Figure 3 for the baseline 70% piston bowl, shortly after the start of combustion (ignition occurs near 9° after top-dead-center [ATDC] for this condition). The colorbars at the bottom of the images indicate the source of the F/PAH fluorescence from left to right – bright red indicates formaldehyde PLIF, while darker colors in the colorbar indicate PAH PLIF. Images of equivalence ratio, measured using the toluene fuel-tracer diagnostic under non-combusting conditions are also shown at 12° ATDC.

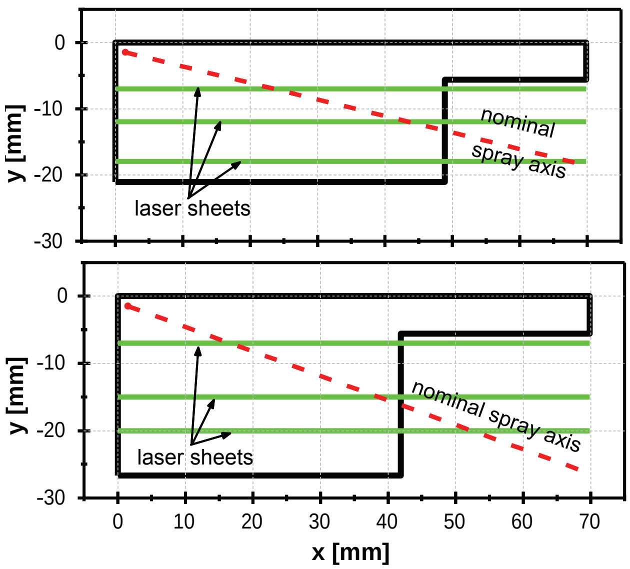

FIGURE 2. Diagram of relationship between piston bowl geometry, nominal spray axis and laser sheet heights for the baseline 70% (top) and 60% (bottom) piston bowls.

The 11° ATDC image in Figure 3 shows that first-stage ignition, marked by formaldehyde (bright red in image with red colorbar below), occurs simultaneously throughout the jet, in both fuel-rich and fuel-lean regions (see corresponding equivalence ratio contours at 12° ATDC). Second-stage ignition, marked by OH (green), occurs downstream, in regions of intermediate stoichiometry somewhere near an equivalence ratio of unity (regions with yellow equivalence ratio contours at 12° ATDC). At 12 and 14° ATDC, PAH soot-precursors (bright red with dark colorbar) appear downstream, in the fuel-rich regions (red equivalence ratio contours) between jets, where the jets interact with each other after impinging on the piston bowl-wall.

Figure 4 shows similar images later in the cycle, where the PAH and soot (bright red in image, dark colorbar) is pushed toward the center of the combustion chamber by the jet-jet interaction (especially in the lower laser-sheet planes at 12 and 18 mm), where it gradually oxidizes (decreasing red intensity at 24 and 40° ATDC). Late in the cycle (40° ATDC), significant formaldehyde

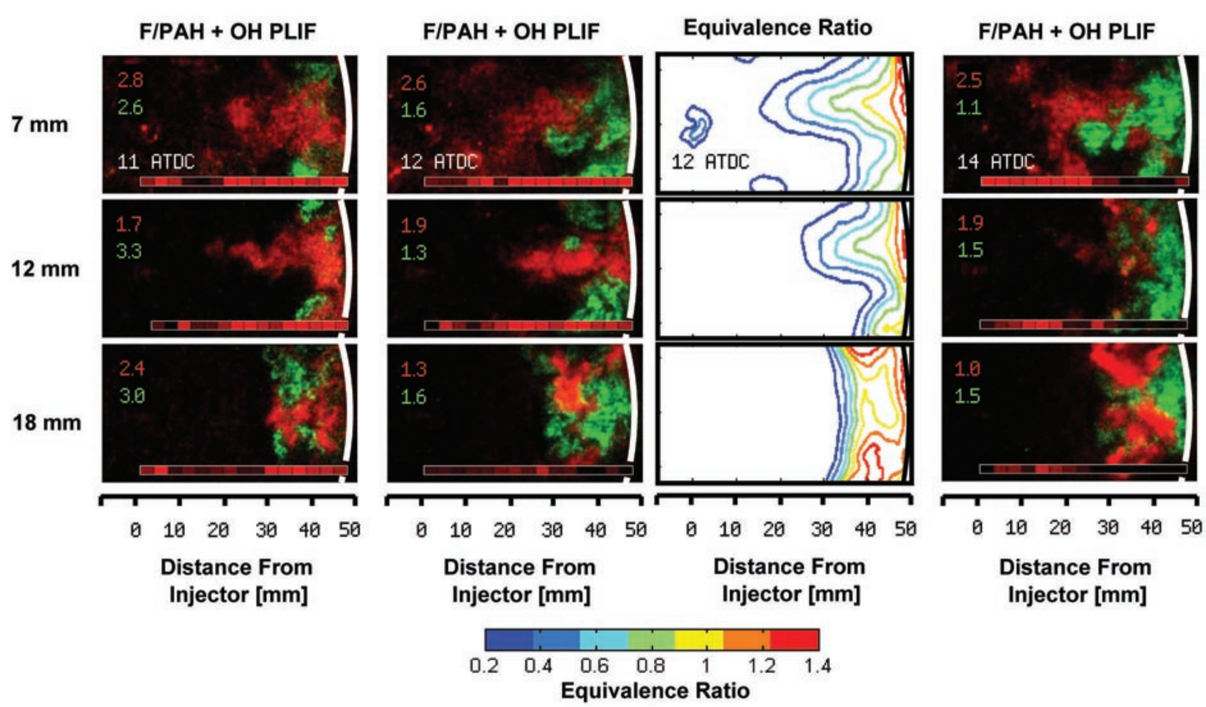

FIGURE 3. Single-shot simultaneous images of OH-PLIF (green), F/PAH-PLIF (red), and ensemble-averaged equivalence ratio (contours) during the premixed burn in vertical planes at 7 mm (top row) 12 mm (middle) and 18 mm (bottom) below the firedeck for the 70% bowl.

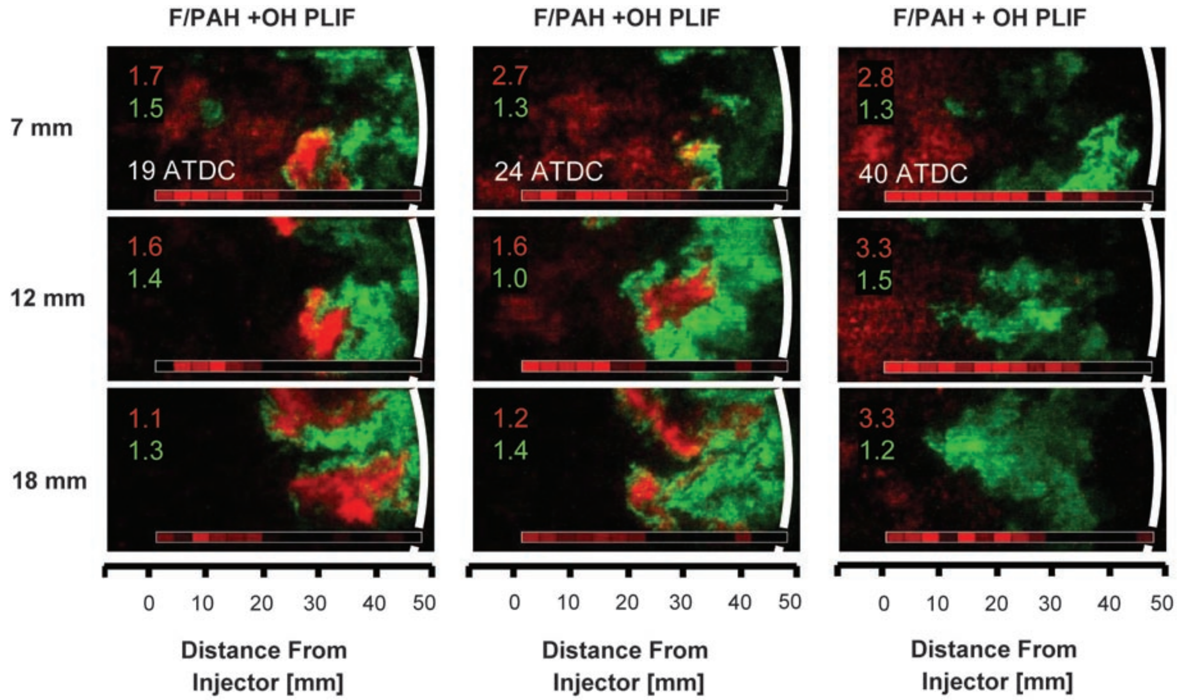

FIGURE 4. Single-shot simultaneous images of OH-PLIF (green) and F/PAH-PLIF (red) during mixing-controlled combustion in vertical planes at 7 mm (top row) 12 mm (middle) and 18 mm (bottom) below the firedeck for the baseline 70% bowl.

(dim red in image, with bright red colorbar) remains in the upper laser sheet plane (7 mm), near the injector, where very lean equivalence ratios occur (see equivalence ratio contours at 12° ATDC), indicating UHCs that arise from mixtures that are too fuel-lean to burn completely.

For the 60% bowl, where the perimeter of the bowl is closer to the injector, the jet-jet interaction is stronger, and the late-cycle combustion is pushed back away from the bowl-wall, closer to the injector. As shown for the 60% bowl in Figure 5, late in the cycle, the PAH and soot (bright red, in 15 and 20 mm planes) are pushed by jet-jet interaction farther into the center of the combustion chamber, where they oxidize. The increased jet-jet interaction with the smaller 60% bowl also pushes OH (green) back away from the bowl perimeter, so that it fills much more of the combustion chamber in all three planes. This movement of the hot combustion, marked by OH, also affects formaldehyde, and thus UHCs. Compared to the 70% bowl in Figure 4, the formaldehyde fluorescence (dim red, bright colorbar) for the 60% bowl in Figure 5 is significantly weaker late in the cycle (40° ATDC), especially in the upper measuring plane (7 mm), indicating more complete combustion.

Finally, Figure 6 shows the results of a simple one-dimensional LTC diesel jet model for understanding the cause of over-mixing that creates the near-injector fuel-lean regions. The red curve in the upper plot shows the predicted average equivalence ratio along the jet axis after the end of injection, and the lower plot shows a visualization of predicted equivalence contours in the jet. These equivalence ratio predictions, which show fuel-lean mixtures near the injector forming rapidly after the end of injection (left side of plots) are consistent with the equivalence ratio measurements from both this year's report and the FY 2007 report. The blue curves in the upper part of the figure show the entrainment rate relative to that of a steady jet. The predictions show that after the end of injection, a wave of increased entrainment travels downstream through the jet after the end of injection, consistent with mass and momentum conservation. This "entrainment wave" is responsible for the rapid mixing after the end of injection that is observed experimentally, and it helps to explain many observations of in-cylinder combustion and pollutant formation for both conventional and LTC diesel combustion. Recognition of the effects and of the importance of this entrainment wave will be useful for designing and optimizing future LTC and multiple-injection strategies.

Conclusions

- This project uses an optical engine to study in-cylinder phenomena coupled with modeling collaborations to improve simulation capabilities for LTC conditions.
- Multiple imaging diagnostics showed that bowl design and spray targeting can change jet-jet

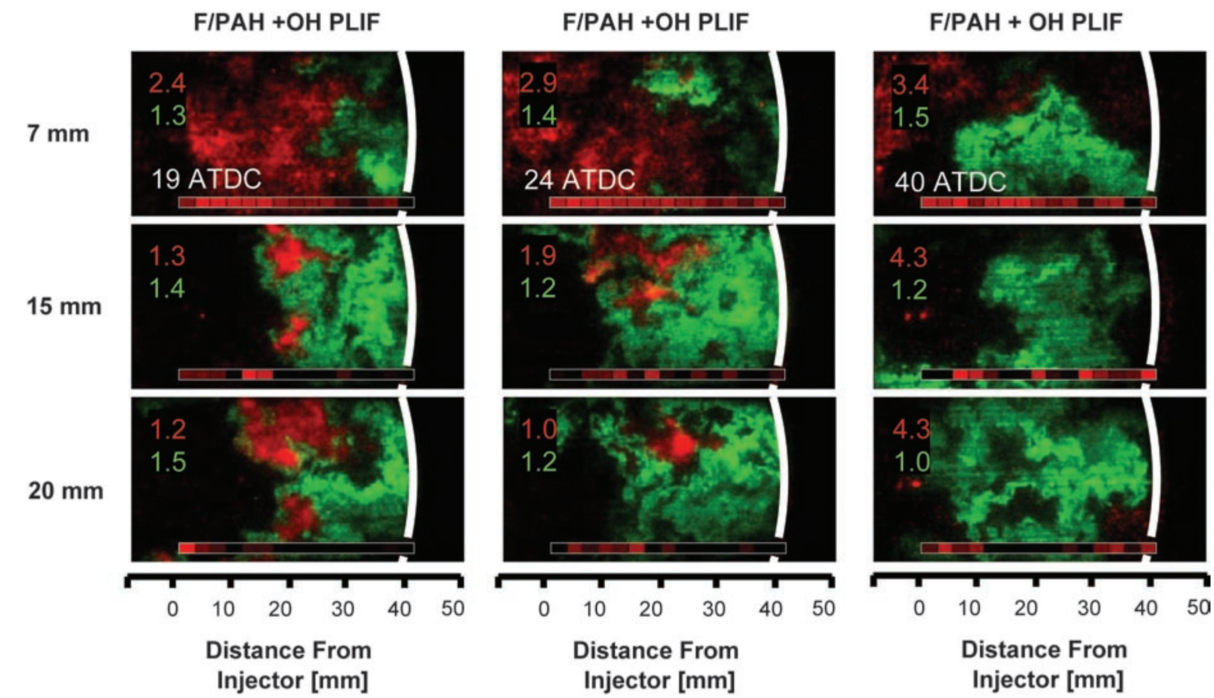

FIGURE 5. Single-shot simultaneous images of OH-PLIF (green) and F/PAH-PLIF (red) during mixing-controlled combustion in vertical planes at 7 mm (top row) 15 mm (middle) and 20 mm (bottom) below the firedeck for the baseline 60% bowl.

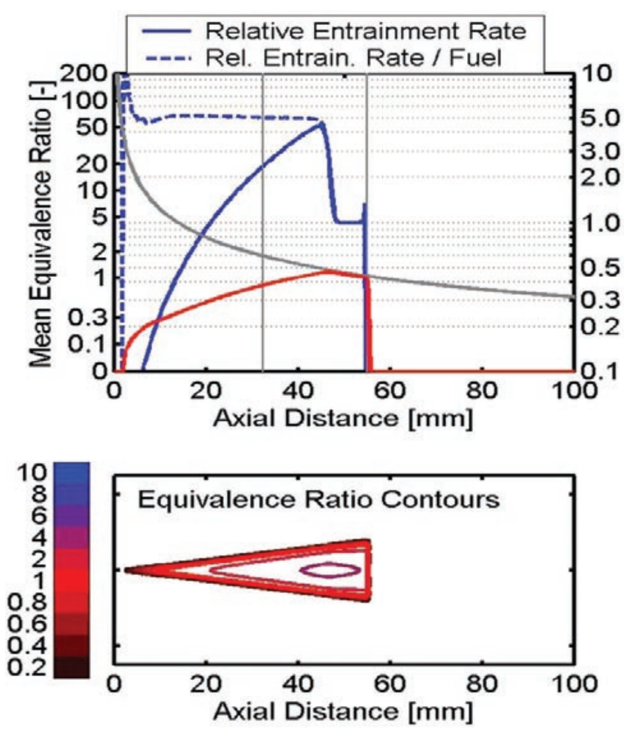

FIGURE 6. Predictions of one-dimensional diesel jet model after the end of injection. Top: cross-sectionally averaged equivalence ratio (red) and entrainment rate (blue) relative to a steady jet. Bottom: equivalence ratio contours.

interactions, which affect soot formation and mixing after the end of injection.

- New computer models explain why fuel-lean UHCs arise from near-injector LTC jets, and other model improvements help to reduce the grid dependency of KIVA.
- FY 2007 activity transfers understanding of the effects of engine design on in-cylinder combustion and pollutant formation processes.
- Future experimental work will explore multiple-injection strategies, and future modeling work will focus on improving model simulation of effects of engine design on in-cylinder combustion and pollutant-formation processes.

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Publications:

1. "Optical Diagnostics of a Late Injection Low-Temperature Combustion in a Heavy Duty Diesel Engine," T. Lachaux, M. Musculus, S. Singh and R. Reitz, ASME Internal Combustion Engine Division 2007 Fall Technical Conference, October, 2007.

2. "In-Cylinder and Exhaust Soot in Low-Temperature Combustion Using a Wide-Range of EGR in a Heavy-Duty Diesel Engine," E. Huestis, P. Erickson, and M. Musculus, SAE paper 2007-01-4017, 2007 SAE Powertrain and Fluid Systems Conf., October 2007.

3. Book chapter for "Direct Injection Combustion Engines and Their Fuels for Automotive Applications in 21st Century," Woodhead Publishing of Cambridge, in preparation.

4. "Gradient Effects on Two-Color Soot Optical Pyrometry in a Heavy-Duty DI Diesel Engine," M. Musculus, S. Singh, and R. Reitz, Combustion and Flame, accepted October 2007.

5. "Optical Diagnostics Of a Late Injection Low-Temperature Combustion In a Heavy Duty Diesel Engine," T. Lachaux, M. Musculus, S. Singh and R. Reitz, Gas Turbines and Power, accepted October, 2007.

6. "Simultaneous Optical Diagnostic Imaging of Low-Temperature, Double-Injection Combustion in a Heavy-Duty DI Diesel Engine," S. Singh, R. Reitz, and M. Musculus, Combustion Science and Technology 179 (11), 349-70, November 2007.

7. "Effects of Piston Bowl Geometry on Mixture Development and Late-Injection Low-Temperature Combustion in a Heavy-Duty Diesel Engine," C. Genzale, R. Reitz, and M. Musculus, SAE paper 2008-01-1330, SAE International Congress and Exposition, accepted December 2007.

8. "Unsteady Turbulent Round Jets and Vortex Motion," N. Abani and R. Reitz, Physics of Fluids 19, December 2007 "Effects of Spray Targeting on Mixture Development and Emissions in Late-Injection Low-Temperature Heavy-Duty Diesel Combustion," Proceedings of the Combustion Institute, *In Press*, 2009.

9. "Effects of Jet-Bowl and Jet-Jet Interactions on Late-Injection Low-Temperature Heavy-Duty Diesel Combustion," C. Genzale, R. Reitz, and M. Musculus, Proceedings of Conference on Thermo-and Fluid Dynamic Processes in Diesel Engines (THIESEL), Valencia, Spain, September 9–12, 2008.

Presentations:

1. "Discrete Control-Volume Analysis of Post-Injection Diesel Jet Entrainment," Kyle Kattke, Mark P.B. Musculus, Lyle M. Pickett, Chuck Mueller, and Krishna "LK" Lakshminarasimhan, Advanced Engine Combustion Working Group Meeting, USCAR, October 2007.

2. "Optical Diagnostics Of a Late Injection Low-Temperature Combustion In a Heavy Duty Diesel Engine," T. Lachaux, M. Musculus, S. Singh and R. Reitz, ASME Internal Combustion Engine Division 2007 Fall Technical Conference, October, 2007.

3. "In-Cylinder and Exhaust Soot in Low-Temperature Combustion Using a Wide-Range of EGR in a Heavy-Duty Diesel Engine," E. Huestis, P. Erickson, and M. Musculus, SAE paper 2007-01-4017, 2007 SAE Powertrain and Fluid Systems Conference, October 2007.

4. "What's New in Engine Research," M. Musculus, University of Southern California School of Engineering, December 2007.

II.A.4 Low-Temperature Diesel Combustion Cross-Cut Research

Lyle M. Pickett
MS 9053
Sandia National Laboratories
P.O. Box 969
Livermore, CA 94551-9053

DOE Program Manager: Gurpreet Singh

Objectives

- Determine methods for reducing liquid penetration at conditions typical of early-injection low-temperature combustion (LTC).
- Develop better understanding of spray vaporization processes after the end of injection.
- Distinguish between flame propagation and ignition mechanisms for lift-off stabilization at LTC conditions.

Accomplishments

- Demonstrated that shortening the injection duration to one-half of the quasi-steady liquid length time reduces the liquid-phase penetration of the spray. Provides an understanding needed to prevent liquid wall impingement and its negative impacts on emissions and combustion efficiency.
- Discovered that the maximum liquid penetration recedes towards the injector after the end of injection. The cause of the liquid length recession is an entrainment wave of enhanced fuel-ambient mixing that occurs during the injection-rate ramp down.
- Provided new insight into diesel lift-off stabilization by using laser-ignition upstream of the natural lift-off length. Ignition stabilizes lift-off upstream for a substantial period of time, effectively controlling lift-off length for LTC.

Future Directions

- Determine how multiple injections can be used to affect ignition timing and minimize unburned hydrocarbons at LTC conditions.
- Perform direct measurements of mixing (equivalence ratio) at the time of the premixed burn in constant-injection-duration diesel fuel jets for various exhaust gas recirculation levels and multiple injection strategies. This investigation will show how mixing between injections affects the equivalence ratio and location of the premixed burn.
- Investigate jet-jet interaction effects on flame lift-off.

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Introduction

LTC strategies have shown promise in reducing nitrogen oxide (NOx) and particulate matter emissions. However, these combustion modes have also been shown to produce higher unburned hydrocarbon (UHC) and carbon monoxide (CO) emissions. As a result, the combustion efficiency may decrease for LTC compared to traditional diesel combustion. We have studied the fundamental causes of UHC and CO formation in LTC with several phases of research over the past year, including (1) early-injection liquid spray penetration, (2) transient liquid vaporization after the end of injection, and (3) flame lift-off stabilization mechanisms for LTC. This research encompasses several different areas that can be important for UHC minimization for LTC. Early-injection timing can cause liquid impingement upon the cylinder liner and piston bowl thereby contributing to UHC emissions. As LTC usually occurs with positive ignition dwell (ignition occurs after the end of injection), the spray vaporization processes after the end of injection affect the type of mixture that burns during LTC. Finally, the region separating high-temperature combustion and unburned fuel-air mixtures upstream is the lift-off length. Therefore, understanding the causes of lift-off stabilization for LTC is fundamental to understanding sources of UHC emissions (as well as soot and NOx formation).

Approach

We used a constant-volume vessel for this research because of the ability to carefully control the charge-gas temperature and density within the chamber, as well as full optical access (100-mm access from multiple angles) for advanced diagnostics. Figure 1 shows the vessel and common-rail injector (Bosch CRIP 2.2) used for these studies. Single-hole nozzles of the same shape (KS1.5/86) but different diameter were included in the study. A more detailed description of the facility may be found in [1].

Mie-scattering and shadowgraph images were simultaneously acquired using high-speed cameras to define the spray liquid and vapor phases, respectively. Experimental conditions were chosen to simulate early-injection conditions, as well as top-dead-center (TDC) conditions. Particular focus was paid to the period of the spray after the end of injection.

We used high-speed chemiluminescence imaging to develop an understanding of the mechanisms for lift-off stabilization. This work is expected to benefit the diesel modeling community, as many different modeling approaches have been proposed to mimic the flame lift-off behavior. Some believe that diesel flame lift-off is a flame propagation process while others hold that it is controlled entirely by self-ignition or by recirculation of hot combustion products. However, for diesel sprays it is difficult to separate the timing and position of the premixed burn (autoignition) region from the lift-off stabilization region. For this research, we intentionally decouple the self-ignition/premixed-burn region and the quasi-steady lift-off by igniting the fuel jet in a region upstream of the naturally occurring lift-off length. A high-energy laser is focused to form a plasma at specific spatial locations and times after the start of injection (ASI), thereby igniting the fuel spray as shown in Figure 1. By monitoring the response of the reacting jet, we can gain insights into the fundamental mechanisms affecting lift-off stabilization at diesel conditions, thereby providing guidance for further combustion model development at these conditions.

Results

Figure 2 shows the liquid penetration time history as the injection duration, or the injection mass, is increased. The maximum liquid penetration distance rapidly increases as the injection duration is increased. Longer injection durations produce sprays with a quasi-steady liquid length [2], shown as the dashed line after about 0.8 ms ASI. The experimental condition of Figure 2 simulates injection near -20 crank angle degree (CAD) timing. The steady liquid length is about 65 mm. For an engine, this length may result in liquid impingement upon in-cylinder surfaces. However, shortening the injection duration limits the maximum liquid penetration.

Summarizing many different experimental conditions in Figure 3, we show the maximum liquid distance during any period of injection, normalized by the quasi-steady liquid length, and plot this against the injection duration time, normalized by the time (t_{ss}) that long-injection sprays require to reach a quasi-

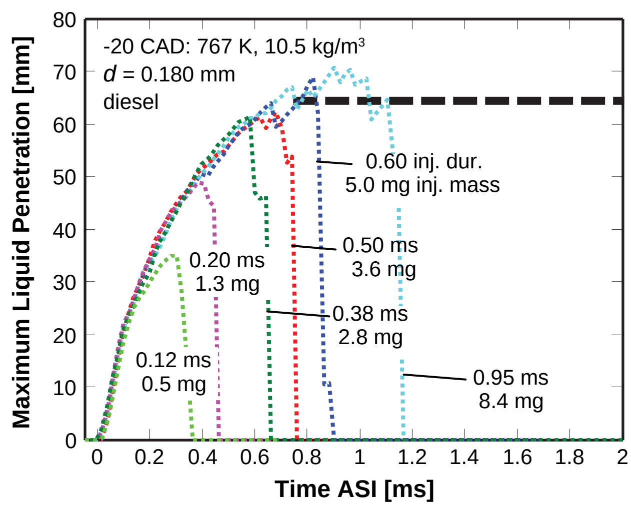

FIGURE 2. Effect of increasing injection duration on liquid penetration at -20 CAD simulated ambient conditions. Injector conditions: 0.180 mm nozzle, 110 MPa, #2 diesel.

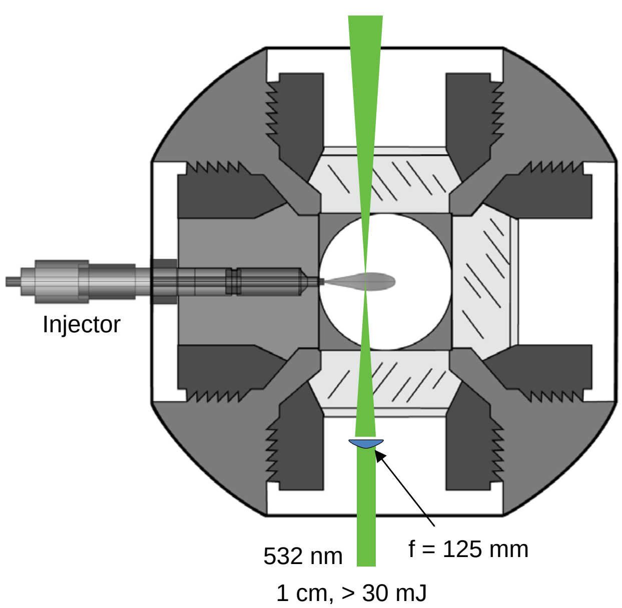

FIGURE 1. Combustion Vessel And High-Speed Imaging Setup (Mirror spacing not to scale.)

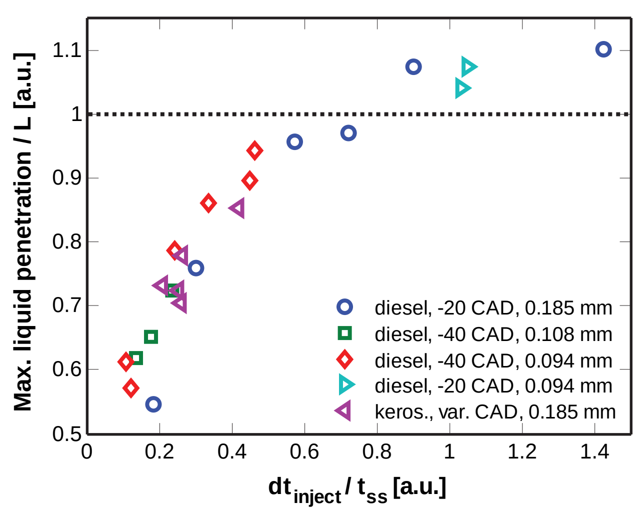

FIGURE 3. Effect of injection duration on liquid penetration. Injection duration is normalized by the time for a spray to reach a steady liquid length at a given condition. The maximum liquid penetration during injection is normalized by the steady liquid length. Various experimental conditions are given in the legend.

steady liquid length. When plotted in these normalized coordinates, there is a general collapse of data.

A major finding shown in Figure 3 is that it is necessary to make the injection duration (dt_{inject}) approximately 50% of t_{ss}, or less, in order to achieve liquid penetration distances that are lower than the steady liquid length. Clearly, some delay after the end of injection (AEI) is needed for the end of injection "effect" to be "transmitted" to the liquid near the head of the jet, which explains why the injection duration cannot be close to t_{ss}. Current research on the jet mixing processes that occur AEI shows that an "entrainment wave", indicative of enhanced relative fuel-ambient mixing, travels from the injector approximately twice as fast as the initial jet penetration rate [3]. Consequently, increased mixing AEI is expected to affect the head of the jet in only one-half of the time that it took for a steady jet to penetrate to that location. As a result, the entrainment wave reaches the head of the jet at double the injection duration of a finite injection [3]. This is essentially the dt_{inject} / t_{ss} = 0.5 condition given in Figure 2.

An entrainment wave AEI also causes other interesting effects on spray mixing and vaporization, even if the spray reaches a quasi-steady liquid length during injection. Figure 4 shows that the spray recedes back toward the nozzle from the quasi-steady liquid length, opposite to the general convective direction of the spray. From a Lagrangian perspective, if all liquid fuel leaving the injector experienced the same mixing with the ambient, we might have expected that liquid fuel leaving the nozzle after end of injection (EOI) would vaporize at the same quasi-steady liquid length. However, with enhanced fuel-ambient mixing (an entrainment wave) occurring after the injection-rate ramp down, the liquid can vaporize progressively closer to the injector, causing a liquid length recession.

The above results were achieved using a hot, inert ambient gas, to focus on only spray vaporization processes. In Figure 5, we show a chemiluminescence image sequence demonstrating the transient lift-off of a reacting fuel jet with laser ignition. The sequence corresponds to a condition where natural autoignition begins at approximately 1.3 ms ASI and lift-off stabilization occurs shortly thereafter at 40-50 mm from the injector. At 3.9 ms ASI, a laser is fired at 20 mm from the injector, forming a plasma upstream of the natural lift-off length. A light border line is provided on selected images to indicate the low-level (100/4096 counts) detection limit of a chemiluminescence region. The minimum axial distance from the injector to this border line is defined as the lift-off distance.

At the time of laser-induced plasma ignition (3.9 ms ASI), a chemiluminescence kernel is formed. The kernel remains small for about 0.1 ms before the kernel intensity and size begins to increase significantly. The kernel grows in a connected reaction zone before it merges with the downstream flame body (the original lift-off) after only 0.25 ms after the time of plasma

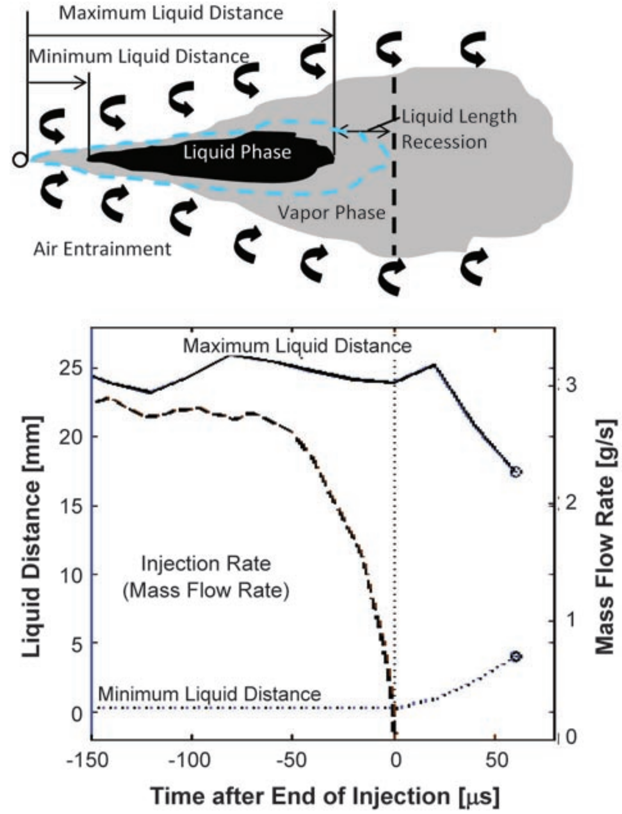

FIGURE 4. Maximum and minimum liquid penetration distances along with a fuel mass flow rate before and after EOI. Schematic of liquid length recession after the end of injection. Ambient conditions: 850 K, 14.8 kg/m^3 0% O_2. Injector conditions: 0.090 mm nozzle, 150 MPa, #2 diesel.

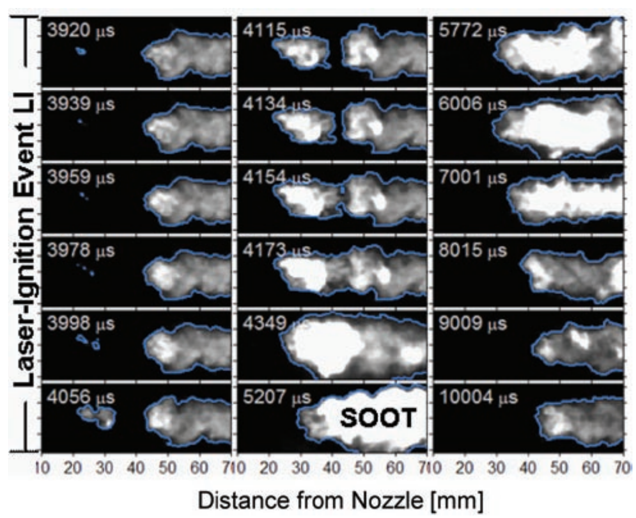

FIGURE 5. Chemiluminescence image sequence with laser ignition at 3.9 ms ASI. Conditions the same as Figure 4, except 21% O_2.

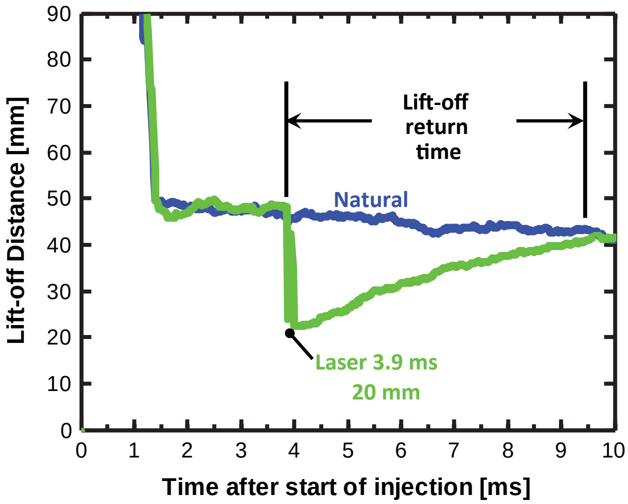

FIGURE 6. Lift-off distance with and without laser ignition for the conditions of Figure 5.

formation–an average speed of 100 m/s, which is similar to jet convective speed estimates. The original lifted flame appears largely unaffected by the upstream kernel's growth as there is little change in its axial position during this time.

Although the downstream portion of the laser-ignition region moves quickly downstream, the upstream reaction zone does not. The average lift-off distance from multiple injections, with and without laser ignition, is shown in Figure 6. The calculated lift-off distance remains close to the original plasma location by the time that the flame merges downstream. Afterwards, the laser-affected lift-off gradually increases to the natural lift-off distance, but over a period of 5 ms. This time is significantly longer than practical injection durations in an engine and the eventual merge back to the natural lift-off distance could be discovered only by resorting to a long injection duration (10.8 ms) in the experiment.

An immediate observation from these results is that ignition events have a stabilizing effect on flame lift-off that persists for a long time relative to jet convective times. While not discounting the role of flame propagation downstream of the ignition event, these results show that upstream ignition sites can start a chain of events that effectively controls lift-off.

Conclusions

Our results show that short injection durations are less likely to experience wall impingement, and therefore could be used for successful LTC operation. Also, new guidance about the critical injection duration to shorten the liquid penetration from the quasi-steady liquid length is provided. Reducing the injection duration to one-half of the time for steady-liquid length development is necessary to limit liquid penetration.

A detailed understanding of the spray vaporization and mixing processes after EOI has also been provided. Because of an "entrainment wave" produced during the injection-rate ramp down, the maximum liquid distance may recede towards the injector. This information provides additional understanding about mixing and production of UHC emissions from the near-nozzle region.

Laser ignition is found to have a strongly stabilizing influence as lift-off persists upstream near the ignition site for a substantial period of time. Lift-off eventually returns to its natural position, but only after injection times that are too long for practical engines. These results provide guidance for the development of new combustion models for LTC diesel sprays.

References

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2. Siebers, D.L., "Liquid-Phase Fuel Penetration in Diesel Sprays," SAE Paper 980809, 1998.

3. Musculus, M.P.B. and Kattke, K., "Entrainment Waves in Diesel Jets," SAE Paper 09PFL-0538, 2009.

FY 2008 Publications/Presentations

1. Pickett L.M. and Hoogterp L., "Fundamental Spray and Combustion Measurements of JP-8 at Diesel Conditions", SAE Paper 2008-01-1083, 2008.

2. Pickett, L.M. and Kook, S., "Diesel Fuel Jet Lift-off Stabilization in the Presence of Laser-Induced Plasma Ignition," Proc. Combust Inst. doi:10.1016/j.proci.2008.06.082, 2008.

3. Kook S., Pickett L.M., Musculus M.P.B., Kattke K., and Gemlich R.K., "Liquid-Phase Diesel Spray Penetration during End-of-Injection Transient", Proceedings of the International Symposium on Diagnostics and Modeling of Combustion in Internal Combustion Engines (COMODIA), Hokkaido, Japan, 2008.

4. Kook, S. and Pickett, L.M., "Effect of Ambient Temperature and Density on Diesel-Spray-Generated Shock Waves," ILASS Americas, 21st Annual Conference on Liquid Atomization and Spray Systems, 2008.

II.A.5 High Efficiency Clean Combustion in Light-Duty Multi-Cylinder Diesel Engines

Robert M. Wagner (Primary Contact), Kukwon Cho, Manbae Han, C. Scott Sluder
Oak Ridge National Laboratory (ORNL)
2360 Cherahala Boulevard
Knoxville, TN 37932

DOE Technology Development Manager: Gurpreet Singh

Objectives

- Support demonstration of DOE FreedomCAR emissions milestones for light-duty diesel engines.
- Explore potential pathways for expanding robust high efficiency clean combustion (HECC) operation for improving system thermal efficiency.
- Characterize HECC from a thermodynamics perspective and integration with thermal energy recovery.
- Complete transition from the Mercedes-Benz (MB) 1.7-L engine to the General Motors (GM) 1.9-L engine.

Accomplishments

- Completed mixed-source exhaust gas recirculation (EGR) experiments and the effect of intake charge temperature on emissions and efficiency.
- Evaluated three low-temperature combustion (LTC) strategies on multi-cylinder engine for emissions, brake thermal efficiency (BTE), and stability.
- Characterized thermodynamic availability of conventional diesel combustion and LTC operation.
- Explored LTC operation on the GM 1.9-L engine and compared/contrasted with the MB 1.7-L engine operation, which has a significantly higher compression ratio.
- Supplied HECC performance map of MB engine and non-proprietary performance map of GM engine for inclusion in the Powertrain Systems Analysis Toolkit (PSAT).
- Completed transition to the GM 1.9-L engine.

Future Directions

- Further explore HECC strategies on the GM engine for comparison of technologies and compression ratio effects on the MB engine.
- Characterize cylinder/cyclic dispersion sensitivity to HECC method and EGR/air maldistribution.
- Continue development of acoustic/vibration phenomenological model for combustion characterization and insight into the potential of noise damping.
- Continue to support efficiency and emission controls activities to ensure collaborative path toward Fiscal Year 2010 DOE FreedomCAR milestones.

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Introduction

Advanced combustion modes such as premixed charge compression ignition (PCCI) have shown promise as potential paths for meeting 2010 and beyond efficiency and emissions goals. ORNL as well as others have shown success in achieving reduced emissions and acceptable efficiency using high charge dilution for a somewhat limited speed-load range. This activity builds on many years of HECC experience at ORNL, including the demonstration of HECC operation in a multi-cylinder engine, characterization of cylinder-to-cylinder stability issues, detailed speciation of hydrocarbons (HCs) in HECC modes, description of the effect of particulate matter (PM) precursors on engine-out emissions, and the demonstration of transitions to, from, and within HECC modes. The primary objective of this study is to investigate potential near-term technologies for expanding the usable speed-load range and to evaluate the potential benefits and limitations of these technologies for achieving HECC in light-duty diesel engines.

For further clarification, the term HECC was first introduced in the FreedomCAR Advanced Combustion and Emissions Control Tech Team and Diesel Crosscut Team in 2003. The intent was to convey the objectives of advanced combustion research in a fresh, all-encompassing name in a time when LTC, PCCI, HCCI (homogeneous compression ignition), MK (modulated kinetics), and many more acronyms were in use, but conveyed nothing about the advantages and were aligned with certain companies. DOE adopted HECC as the subject of a large request for proposals in 2004. ORNL adopted the term in 2004.

Approach

Significant progress in expanding the useful speed-load range and robustness of HECC operation will require an improved understanding of near- and long-term enabling technologies (e.g., EGR composition, injector design, etc.) on multi-cylinder engine efficiency, stability, and emissions. A combination of thermodynamic and detailed exhaust chemistry information will be used to improve the understanding of and issues related to achieving HECC operation, which is expected to contribute to more efficient and cleaner diesel engine operation. This information will be considered in other ORNL light-duty diesel engine activities as well as shared with other institutions for the development and validation of improved combustion models and aftertreatment systems.

HECC operation is being investigated at ORNL on a modified MB 1.7-L and a GM 1.9-L common rail four-cylinder diesel engine. These engines are equipped with microprocessor-based dSpace control systems which permit unconstrained access to engine hardware including the integration of custom control algorithms. The GM engine also has an electronic control unit donated by GM which allows for the monitoring and manipulation of the base engine calibration. The GM engine will be the focus for HECC experiments for FY 2009.

Five speed-load conditions which were originally defined by an industry working group to be representative of light-duty diesel engine operation were selected for use in this study. While this approach does not take into account cold-start or other transient phenomena, the metric has been successfully used by others for comparison purposes and to demonstrate potential improvements from one technology to another. The five modes used in this study are summarized in Table 1. ORNL is also working with the Advanced Combustion & Emissions Control Technical Team to propose a new set of operating conditions for use in characterizing efficiency and emissions improvements from advanced engine technologies. A well-defined set of operating conditions would allow improved comparisons across the DOE light-duty diesel activities. The modal conditions are used extensively at ORNL for combustion, aftertreatment, and efficiency activities in support of DOE FreedomCAR efficiency and emissions milestones.

TABLE 1. Representative Light-Duty Modal Conditions for Drive-Cycle Emissions Estimation

Mode	Speed / Load	Weight Factor	Description
1	1,500 rpm / 1.0 bar	400	Catalyst transition temperature
2	1,500 rpm / 2.6 bar	600	Low speed cruise
3	2,000 rpm / 2.0 bar	200	Low speed cruise with slight acceleration
4	2,300 rpm / 4.2 bar	200	Moderate acceleration
5	2,600 rpm / 8.8 bar	75	Hard acceleration

Results

The effect of intake charge temperature on efficiency, emissions, and cylinder/cyclic dispersion was investigated on the MB engine using mixed-source EGR. Mixed-source EGR makes use of high-pressure loop and low-pressure loop EGR for manipulating the intake/EGR mixture temperature. The mixed-source EGR study has been documented in the literature (Cho et al., SAE 2008-01-0645) and will not be repeated here due to the concise nature of this report. Mixed-source EGR will be further investigated on the GM 1.9-L engine as an HECC enabler (as was done on the MB engine) as well as for improving the low-load efficiency of HECC operation through improved matching of intake and exhaust mass flow rate with the turbo-machinery.

Final experiments on the MB engine consisted of the exploration of several HECC strategies for future comparison with the GM engine to characterize differences in engine technologies and compression ratio. A PCCI combustion approach to HECC is most compatible with near-term engine technologies. Three approaches were investigated on the MB engine: (1) early PCCI with a single-injection event, (2) late PCCI with a delayed single-injection event, and (3) split-injection PCCI which makes use of two injection events. Example injection strategies are illustrated in Figure 1. All three approaches are driven by intake charge dilution and high fuel injection pressures to expand the premixed combustion event as compared to conventional diesel combustion. Intake charge dilution, fuel injection pressure, and fuel mass delivery was the same for each approach for a specific speed/load combination.

The optimal combination of charge dilution and injection parameters was determined for each method through a systematic investigation of engine parameters. As an example, the effect of engine parameters on brake specific fuel consumption (BSFC), NOx, and PM are

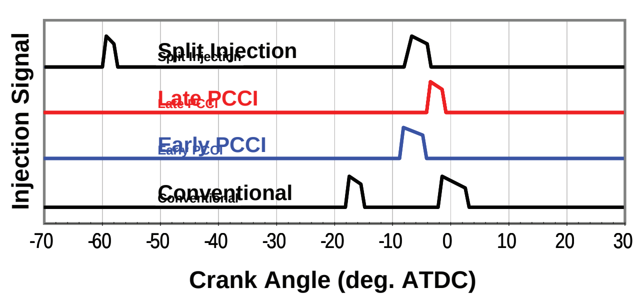

FIGURE 1. Fuel injection strategy for three HECC strategies investigated in this activity. Fuel injection pressure and mass delivery was maintained constant for comparison of the three approaches.

summarized in Table 2 for the split-injection method. The optimal combination for all three methods was chosen for conditions which simultaneously minimize performance metrics BSFC, NOx, and PM. While there are other metrics which are perhaps equally important (*e.g.*, combustion noise), these metrics were the focus of this investigation. Figure 2 shows the optimal results

TABLE 2. Parameter Effect on Achieving HECC Operation for Split-Injection PCCI Strategy (2,300 rpm/4.2 bar BMEP)

Engine Parameter	BSFC	NOx	PM
Increase charge dilution	↑	↓	↑
Advance pilot start of injection (SOI)	↓	–	↓
Advance main SOI	↓	↑	–
Increase pilot pulse width	↑	–	↑

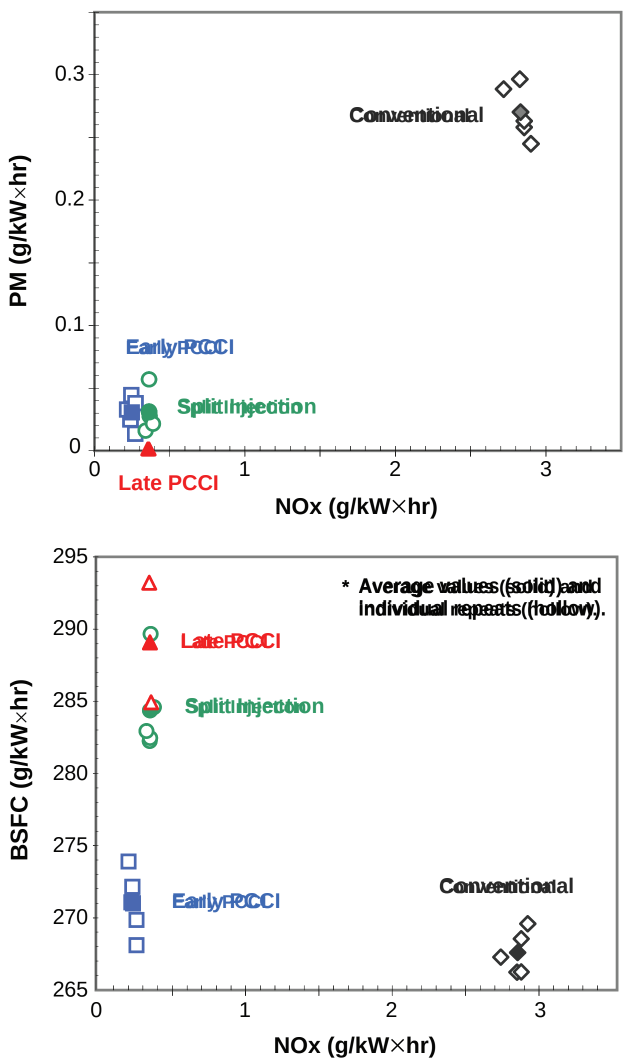

FIGURE 2. Example efficiency and emissions comparison for three HECC strategies and conventional combustion (1,500 rpm/2.6 bar BMEP).

for all three methods as well as the spread in the data (hollow symbols) as compared to the average values (solid symbols) for the 2,300 rpm/4.2 bar condition. Early PCCI appeared to be the most effective for this condition as well as the other conditions evaluated in this study and summarized in Table 1. The combustion process was characterized with in-cylinder pressure data to better understand the differences observed in performance data for these approaches. Average heat release rate is shown in Figure 3 for the 1,500 rpm/2.6 bar condition for all three approaches, with corresponding emissions and efficiency data in Table 3. Combustion phasing for the early PCCI and conventional mode were very similar and most likely explains the similarity in BSFC for the two cases. The combustion phasing for the other two approaches was significantly different and appeared to be the cause of an increase in BSFC (reduction in BTE). The split-injection and late PCCI cases also showed a substantial increase in HC emissions further supporting the observation of suboptimal combustion phasing and possibly over mixing and/or incomplete combustion.

HECC operation was also explored for the five modal conditions on the GM 1.9-L engine for comparison with the MB engine. Preliminary data for comparison is summarized in Table 4 with an early PCCI approach used for both engines. Note that the base calibration for the GM engine is not a production calibration but rather a development calibration which GM supplied to ORNL. This is important when comparing results between the base calibrations for the two engines. A comparison of the performance data for the two engines indicates a lower BSFC for the MB engine. This was not completely unexpected due to the higher compression ratio of the MB (19.0) as

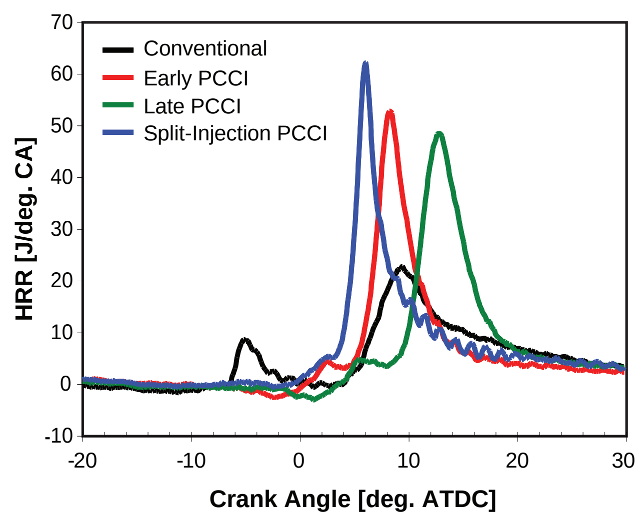

FIGURE 3. Average heat release rate profiles for three HECC strategies and conventional combustion (1,500 rpm/2.6 bar BMEP).

TABLE 3. Comparison of Performance and Emissions Data for Three HECC Strategies (1,500 rpm/2.6 bar BMEP)

Mode	NOx (g/kW·hr)	PM (g/kW·hr)	CO (g/kW·hr)	THC (g/kW·hr)	BSFC (g/kW·hr)	Noise (dB)
Conventional	2.70	0.29	4.12	1.75	268	81.2
Late PCCI	0.35	0.00	15.12	3.44	285	86.0
Split-Injection	0.37	0.02	8.16	4.29	285	88.9
Early PCCI	0.26	0.02	7.36	2.02	268	87.8

TABLE 4. Initial Comparison of Conventional and HECC Operation on the MB and GM Engines for Five Modal Conditions

Speed / Load	Mode	MB Engine				GM Engine			
		EGR [%]	BSNOx [g/kW·hr]	BSFC [g/kW·hr]	Noise [dB]	EGR [%]	BSNOx [g/kW·hr]	BSFC [g/kW·hr]	Noise [dB]
1,500 rpm 1.0 bar	Base	16.3	3.43	419	81.5	42.1	0.68	476	80.2
	HECC	40.6	0.99	436	88.8	43.9	0.53	475	83.3
1,500 rpm 2.6 bar	Base	14.0	2.68	270	83.4	38.9	0.71	311	82.3
	HECC	38.0	0.03	274	89.3	42.6	0.25	312	88.3
2,000 rpm 2.0 bar	Base	21.7	1.92	310	85.1	32.0	0.76	353	81.7
	HECC	43.3	0.38	318	90.6	50.7	0.47	363	88.1
2,300 rpm 4.2 bar	Base	12.6	2.12	253	86.5	21.1	1.23	287	89.9
	HECC	32.4	0.65	257	96.8	32.4	0.81	292	96.0
2,600 rpm 8.8 bar	Base	0.4	4.94	228	88.6	16.2	2.16	236	93.8
	HECC	NA	NA	NA	NA	17.7	2.30	238	97.9

compared to the GM engine (16.5). HECC experiments will continue on the GM engine to further develop an appropriate strategy which makes use of the advanced technologies of the engine as well as to understand the robustness of the engine to PCCI operation and intake/exhaust boundary conditions.

Due to the concise nature of this report, we were not able to discuss all of the research performed during this activity in FY 2008. Please see the publications/presentations list for more information.

Conclusions

This activity has been successful at providing new insight into the implementation of advanced combustion operation on multi-cylinder engines and is an important component to demonstrating 2010 FreedomCAR efficiency and emissions milestones on light-duty diesel engines. Specific accomplishments are as follows:

- Completed mixed-source EGR experiments and the effect of intake charge temperature on emissions and efficiency.
- Evaluated three LTC strategies on multi-cylinder engine for emissions, BTE, and stability.
- Characterized thermodynamic availability of conventional diesel combustion and LTC operation (not shown).
- Explored LTC operation on the GM 1.9-L engine and compared/contrasted with the MB 1.7-L engine operation, which has a significantly higher compression ratio.
- Supplied HECC performance map of the MB engine and non-proprietary performance map of GM engine for inclusion in PSAT (not shown).
- Completed transition to the GM 1.9-L engine.

FY 2008 Publications/Presentations

1. R.M. Wagner, K. Cho, M. Han, C.S. Sluder, "Overview of engine efficiency activities at ORNL" and "Overview of High Efficiency Clean Combustion (HECC) activities at ORNL", DOE Vehicle Technologies program mid-year review (Knoxville, TN; October 2008).

2. R.M. Wagner, "Review of ongoing combustion & aftertreatment R&D activities at ORNL", DOE Vehicle Systems Analysis Tech Team meeting at Argonne National Laboratory (Argonne, IL; May 2008).

3. M. Han, K. Cho, C.S. Sluder, R.M. Wagner, "Soybean and coconut biodiesel fuel effects on combustion characteristics in a light-duty diesel engine", SAE 2008-01-2501 (Detroit, MI USA; April 2008).

4. K. Cho, M. Han, R.M. Wagner, C.S. Sluder, "Mixed-source EGR for enabling high efficiency clean combustion modes in light-duty diesel engines", SAE Paper 2008-01-0645 (Detroit, MI USA; April 2008).

5. R.M. Wagner, K. Cho, M. Han, C.S. Sluder, "Achieving high-efficiency clean combustion in multi-cylinder light-duty engines (Agreement 15936)", 2008 DOE Office of Vehicle Technologies Annual Merit Review (Bethesda, MD; February 2008).

6. R.M. Wagner, "Update on ORNL efficiency and advanced combustion activities for LD diesel engines", 2007 AEC Working Group Meeting at USCAR (Southfield, MI; September 2007).

Special Recognitions & Awards/Patents Issued

Activity contributed to 2008 Advanced Combustion & Emissions Control Technical Accomplishment in report to USCAR Board of Directors; "Demonstrated 2008 FreedomCAR engine efficiency milestones of 43% peak BTE and 27% road-load BTE on a light-duty engine" and "2nd Law thermodynamics perspective helps to define path to 45% peak BTE in light-duty internal combustion engines".

II.A.6 Large Eddy Simulation Applied to Low-Temperature and Hydrogen Engine Combustion Research

Joseph C. Oefelein
Sandia National Laboratories
7011 East Avenue, Mail Stop 9051
Livermore, CA 94550

DOE Technology Development Manager:
Gurpreet Singh

Objectives

- Combine unique state-of-the-art simulation capability based on the Large Eddy Simulation (LES) technique with Advanced Engine Combustion research and development (R&D) activities.
- Perform companion simulations that directly complement optical engine experiments being conducted at the Combustion Research Facility (CRF).
- Focus initially on optical hydrogen-fueled internal combustion engine (H_2-ICE) experiment and systematically extend to low-temperature combustion (LTC) applications.

Accomplishments

- Awarded grand-challenge grant for central processing unit time on DOE "capability-class" computers based on this project's objectives.
  - Multiyear INCITE award (2008 – 2010) at National Center for Computational Sciences, Oak Ridge National Laboratory (see www.nccs.gov).
    - 18-million hours in 2008 (CRAY XT4, 32,000 cores).
    - 30-million hours in 2009.
    - To be determined in 2010.
    - Developed new tabulation approach for treatment of complex hydrocarbon fuels based on the Linear Eddy Model (LEM).
    - Developed high-fidelity model for high-pressure direct injection processes and completed validation studies in collaboration with Ghandhi et al., University of Wisconsin.
    - Performed comparisons between LES and particle image velocimetry (PIV) data in the CRF H_2-ICE in collaboration with S. Kaiser (see related annual report).
    - Systematically extended effort toward treatment of LTC engine processes.
  - Simulation of the effect of spatial fuel distribution using the LEM.
  - LES of direct injection processes for diesel and LTC engine applications (see Pickett et al., www.ca.sandia.gov/ecn).

Future Directions

- Continue high-fidelity simulations of the optical H_2-ICE.
  - Direct-injection with new (Ford) head, match experimental activities.
  - Validation through comparison of measured, modeled results.
    - Chemiluminescence imaging and PIV.
    - Planar laser induced fluorescence.
  - Joint analysis of data extracted from validated simulations.
    - Enhance basic understanding.
    - Improve engineering models.
    - H_2-injector pattern optimization.
    - Systematically extend to homogeneous charge compression ignition (HCCI) engine experiments.
  - Perform detailed studies of LTC processes.
  - Work toward treatment of complex hydrocarbon processes.
- Continue leveraging between DOE Office of Science and Energy Efficiency and Renewable Energy activities.
  - Detailed validation, analysis of key combustion phenomena.
  - Access to high-performance "leadership-class" computers.

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Introduction

The objective of this research is to combine a unique high-fidelity simulation capability based on the LES technique with the Advanced Engine Combustion R&D activities at Sandia National Laboratories. The goal is to perform a series of benchmark simulations that identically match the geometry and operating conditions of select optical engine experiments. The investment in time and resources will provide two significant benefits. After systematic validation of key processes using available experimental data, quantitative information can be extracted from the simulations that are not otherwise available. This information will provide 1) a detailed and complementary description of intricately coupled processes not measurable by experimental diagnostics, and 2) the information required to understand and develop improved predictive models. The combination of detailed experiments, complementary simulations, and the joint analysis of data will provide the basic science foundation required to systematically address the targeted research areas identified for Clean and Efficient Combustion of 21st Century Transportation Fuels.

Approach

In addition to providing a comprehensive multiscale modeling framework based on LES, we have established direct collaborations with two of the "flagship" experimental efforts at the CRF. A scientific foundation for advanced development of subgrid-scale models for LES has been established in collaboration with Barlow et al. as a direct extension of the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (i.e., the "TNF Workshop," www.ca.sandia.gov/TNF). Similarly, we have established collaborative research activities that focus on key optical engine experiments and the Engine Combustion Network (i.e., ECN, as established by Pickett, www.ca.sandia.gov/ECN). The ECN has analogous objectives to those of the TNF workshop. The novelty our approach is that it provides direct one-to-one correspondence between measured and modeled results at conditions unattainable using direct numerical simulation (DNS) by providing detailed simulations that incorporate the fully coupled dynamic behavior of a given configuration in the full experimental or device-scale geometry without canonical approximations. As part of our long-term operating plan under the Advanced Engine Combustion program, needs and milestones in three critical areas have been established: 1) to continue a progression of LES studies focused on the CRF optically accessible H_2-ICE, 2) to establish a parallel task focused on HCCI engines, and 3) to begin a series of supporting studies focused on the development and validation of multiphase combustion models with emphasis placed on direct-injection processes.

Results

Calculations in Fiscal Year 2008 were carried out in a manner consistent with our proposed milestones. As a prerequisite for detailed simulations of the CRF H_2-ICE, we have performed a series of high-fidelity LES calculations of the transient behavior of high-pressure injection processes that identically match the topology of actual original equipment manufacturer (OEM) hardware. Results have been published in a paper entitled "Large Eddy Simulation of Direct Injection Processes for Hydrogen and Low-Temperature-Combustion Engine Applications" by T.G. Drozda and J.C. Oefelein [1]. These studies focus on transient expansion of high-pressure hydrogen through the injector using the experimental data of Petersen and Ghandhi [2, 3] to validate our models. We have focused on three cases that match the range of conditions observed in the CRF H_2-ICE. For all three cases the hydrogen is injected at 10.4 MPa (103 atm). Chamber pressures were fixed at atmospheric, 340 kPa, and 720 kPa, respectively. The high-pressure injection process places the system in the thermodynamically supercritical regime. This is typical in modern state-of-the-art systems and requires advanced treatment of the equation of state, thermodynamics, and transport processes. In particular, real-gas/liquid effects must be considered.

Figure 1 shows an example calculation of the three orifice injector used in the actual engine. On the left is a

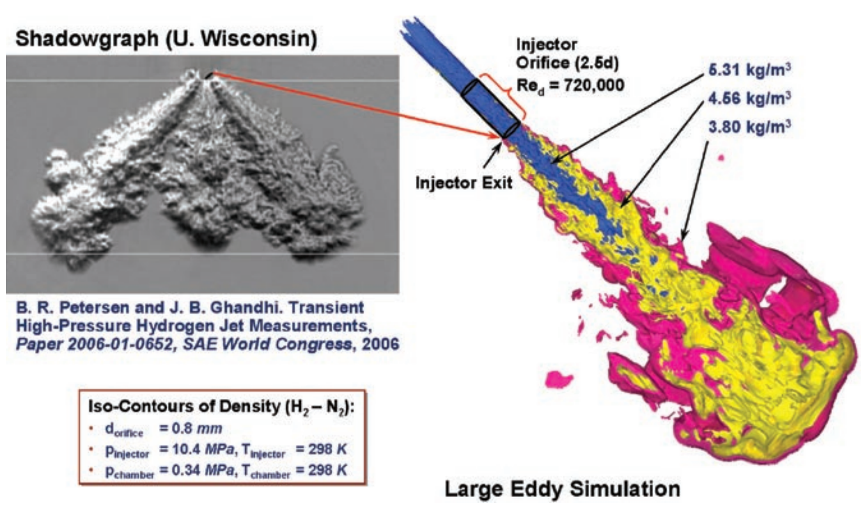

FIGURE 1. Shadowgraph showing high Reynolds number, high-pressure injection of supercritical hydrogen into nitrogen (left) compared with corresponding iso-contours of density from LES (right).

shadowgraph obtained experimentally from Petersen and Ghandhi [2, 3] that shows the turbulent flow structure at an instant in time. On the right is the corresponding LES result (i.e., one of the three jets), which shows qualitative agreement with the experimental data. The grid used for the calculations is stretched to provide appropriate resolution in the jet region where the shear-layer interactions are the strongest. Note that the jet Reynolds number for this case is 720,000, which is a direct consequence of the high-pressure conditions. This has a profound impact on the range of turbulence scales that must be considered and significantly increases the cost of the calculation.

A cross-section of the computational domain is shown in Figure 2, which includes a plenum chamber upstream of the injector (shown in black), an actual multi-orifice OEM injector in the middle, and the main chamber downstream (shown in red). Calculations were performed in a domain that was 100 injector body diameters long and 50 diameters wide. The total grid density required for the LES is approximately 10-million cells (4-million cells in the plenum, 2-million cells in the injector, and 4-million in the main chamber). This resolution criteria allowed us to fully resolve the boundary layer dynamics in each orifice. Calculations were performed using the solver developed by Oefelein, which is designed for LES or DNS of turbulent, chemically reacting, multiphase flows. It solves the fully coupled conservation equations of mass, momentum, total-energy, and species for a chemically reacting flow system (gas or liquid) in complex geometries, using a structured hexahedral formulation in generalized coordinates. Details related to the theoretical formulation and related subgrid-scale models are given by Oefelein [4]. This framework accounts for detailed chemistry, thermodynamics, and transport processes at the molecular level, and is sophisticated in its ability to handle a generalized subgrid-scale model framework. It also employs a general treatment of the equation of state, thermodynamics, and transport properties that accommodates real gas or liquid mixtures. Thus, it is not constrained to ideal gas applications and well suited to study high-pressure phenomena.

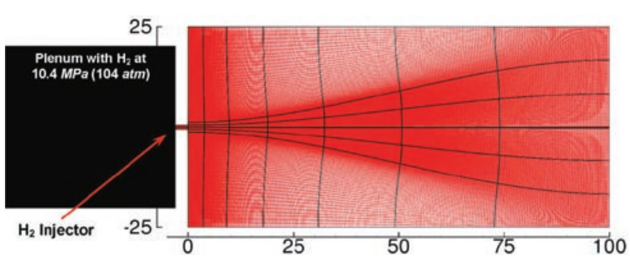

FIGURE 2. Cross-section of the three-dimensional computational domain showing how the grid was optimized.

Simulations performed to-date have allowed us to identify various loss mechanisms that hinder the flow of hydrogen through the injector. Examples are shown in Figure 3. By identifying the various loss mechanisms, we are able to develop appropriate inflow boundary conditions for the in-cylinder calculations and provide valuable data for development of advanced engineering models. This analysis has provided a reliable way to reproduce the turbulent structure and penetration dynamics from these injectors. Figure 4 shows the predictive accuracy with which we can now reproduce the experimentally measured trends. These plots show jet penetration predictions from LES compared to the experimental measurements of Petersen and Ghandhi [2, 3]. Note that all of these calculations are performed with no tuned constants in the models (as enabled by the dynamic modeling procedure for LES). Thus, the only adjustable parameters are the boundary conditions, grid resolution and integration time step.

Having validated a theoretical-numerical framework for treatment of high-pressure direct injection processes in internal combustion engines, we have now begun production level simulations in the full CRF optically

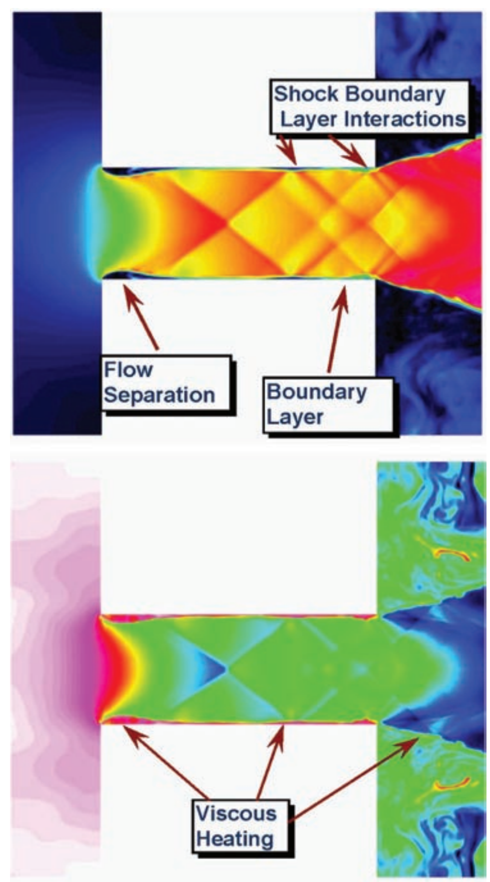

FIGURE 3. Orifice flow velocity (top) and temperature (bottom) after start of injection showing various loss mechanisms.

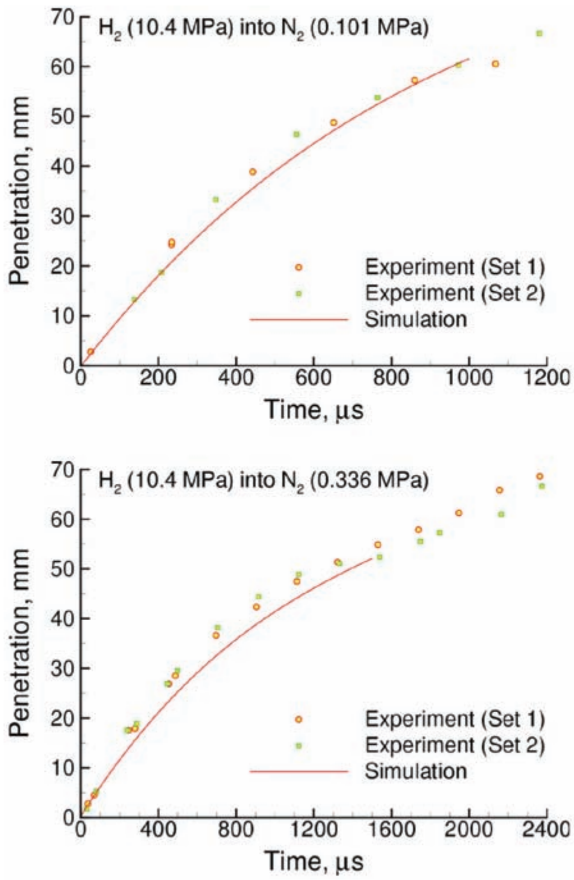

FIGURE 4. Jet penetration data compared to experimental measurements of Petersen and Ghandhi [2, 3].

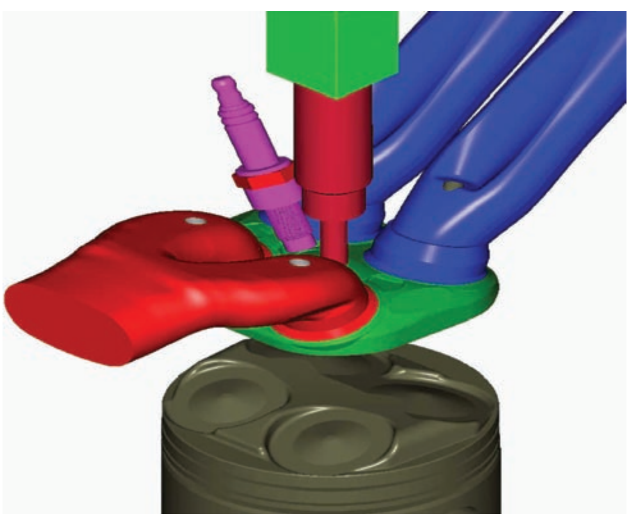

FIGURE 5. Grid surface topology generated for simulation of the CRF optically accessible H_2-ICE.

accessible H_2-ICE. The surface topology associated with the grid is shown in Figure 5. Here, the high-pressure injector is centrally mounted next to the spark plug between the (blue) intake ports and (red) exhaust ports. Calculations of the turbulent combustion processes associated with this geometry are currently in progress in a manner consistent with our original milestones.

Conclusions

Calculations performed to date have provided a systematic way toward detailed simulations of in-cylinder processes. Future analysis will focus on multidimensional turbulence-chemistry interactions and related cycle-to-cycle variations in the actual engine geometry. The simulations will be coordinated with the experimental campaign at the CRF. In addition, we will begin to focus on high-pressure injection of liquid hydrocarbon fuels at thermodynamically near-critical and supercritical conditions. The multiphase injection dynamics associated with these conditions are common to state-of-the-art engines and dominate all subsequent modes of combustion. We will focus on the transient evolution of the injection process with different fuels to determine the mixture state and flow topology just prior to, and during, combustion. In addition, we will perform a series of simulations that identically match the hierarchy of direct injection experiments of Pickett (see www.ca.sandia.gov/ECN) using n-heptane as our initial fuel. This work will be complemented by extending our subgrid-scale model development efforts in combustion to high-pressure regimes in collaboration with Barlow et al. as an extension of the flames studies as part of the TNF workshop (www.ca.sandia.gov/TNF).

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1. R.C. Knaus, C. Pantano and J.C. Oefelein (2009). Statistical analysis and modeling of scalar dissipation and its relation to the filtered mixture fraction. *Physics of Fluids*. **Submitted** (8/08).

2. J.C. Oefelein (2008). Toward high-fidelity simulations for clean and efficient combustion of alternative fuels. *LES for*

Internal Combustion Engine Flows, December 1-2, Ruell-Malmalson, France. **Invited**.

3. T.G. Drozda, G. Wang, V. Sankaran, J.R. Mayo, J.C. Oefelein and R.S. Barlow (2008). Scalar filtered mass density functions in nonpremixed turbulent jet flames. *Combustion & Flame*. **Accepted**.

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5. P.K. Tucker, S. Menon, C.L. Merkle, J.C. Oefelein and V. Yang (2008). Validation of high-fidelity CFD simulations for rocket injector design. *44th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit*, *Paper 2008-5526,* July 21–23, Hartford, CT.

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II.A.7 Modeling of High Efficiency Clean Combustion Engines

Salvador Aceves (Primary Contact), Francisco Espinosa-Loza, Mark Havstad, Nick Killingsworth, Matt McNenly, Tom Piggott, Randy Hessel
Lawrence Livermore National Laboratory (LLNL)
7000 East Ave. L-645
Livermore, CA 94550

DOE Technology Development Manager: Gurpreet Singh

Subcontractor:
University of Wisconsin, Madison, WI

Objectives

- Obtain low emissions, high efficiency, high load operation with homogeneous charge compression ignition (HCCI), premixed charge compression ignition (PCCI), and other low-temperature clean combustion regimes.
- Advance analysis techniques to learn the fundamentals of HCCI and PCCI combustion and make accurate predictions of combustion and emissions.
- Provide analytical support for experimental projects within the Advanced Combustion in Engines program.

Accomplishments

- Developed and tested detailed 3-dimensional meshes for analysis of partially stratified combustion in experimental engines at Sandia Livermore (John Dec, Dick Steeper).
- Conducted detailed analysis of HCCI combustion in Sandia engine (Dick Steeper).
- Migrated homogeneous and partially stratified analysis methodologies to KIVA4 – the new KIVA platform allowing parallelization and unstructured meshes.
- Developed a new analysis tool for modeling of spark ignition (SI)-HCCI transition experiments being conducted at Oak Ridge National Laboratory (ORNL).

Future Directions

- Validate analysis tools under partially stratified conditions: we are working with engine researchers at Sandia Livermore (John Dec and Dick Steeper) to validate KIVA multi-zone code at partially stratified conditions.
- Demonstrate fast modeling of partially stratified combustion with an artificial neural network-based chemical kinetics model: we have previously demonstrated applicability of artificial neural networks for fast and accurate HCCI modeling. We see no limitations in using the same approach to model the more challenging problem of partially stratified combustion.
- Demonstrate analysis tool for modeling unstable SI-HCCI transition experiments: transitioning between SI and HCCI by advancing exhaust valve closing produces oscillatory behavior for intermediate residual gas fraction (30-50%). We are working with ORNL in developing chemical kinetics-based models that help in understanding this complex phenomenon.
- Release and license LLNL analysis tools to collaborators: there is continuous interest in industry and academia in using our analysis tools. We will carefully document them and make them available to our collaborators.

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Introduction

Modeling high efficiency clean engine concepts such as partially stratified combustion requires a balanced approach that captures both fluid motion as well as low- and high-temperature fuel oxidation. A fully integrated computational fluid dynamics (CFD) and chemistry scheme (i.e. detailed chemical kinetics solved in every cell of the CFD grid) would be the ideal modeling approach for partially stratified combustion, but is computationally very expensive. As a result, modeling assumptions are required to develop computationally efficient tools that maintain an acceptable degree of accuracy. Multi-zone models have been previously shown by the authors to capture HCCI processes with enough fidelity to make accurate predictions. We have been testing methodologies for multi-zone analysis of partially stratified combustion that show promise for delivering accurate results within a reasonable computational time. We are also developing new tools of analysis for fast modeling of partially stratified combustion based on artificial neural networks, and multiple reactor models for analysis of SI/HCCI transition experiments.

Approach

LLNL collaborates with other national laboratories, universities, and private industry by providing analytical support that complements the very high quality experimental work being conducted at institutions that participate in the DOE's Advanced Combustion in Engines program. Our research topics to date include homogenous and partially stratified combustion, low-temperature diesel combustion, hydrogen engines, and HCCI/SI transition.

Results

In our continuous effort to demonstrate efficient analysis tools for partially stratified combustion, we have developed and tested detailed 3-dimensional meshes for the Sandia engines currently experimenting with homogeneous and partially stratified combustion (John Dec, Dick Steeper). These meshes are currently being refined, and we anticipate detailed results for partially stratified combustion in the near future.

In preparation for the challenge of analyzing partially stratified combustion, we have tested the "Steeper" mesh under HCCI combustion by conducting a comprehensive fluid mechanics-chemical kinetics analysis [1]. This analysis applied LLNL's multi-zone code KIVA3V-MZ to conduct a Lagrangian analysis where different air-fuel packets are tracked during the full engine cycle (including gas exchange as well as compression and expansion) to reveal details about the flow and combustion. The engine mesh includes all details of the intake and exhaust ports (Figure 1), and therefore can capture gas exchange processes and the resulting velocity and turbulence fields inside the cylinder at intake valve closing.

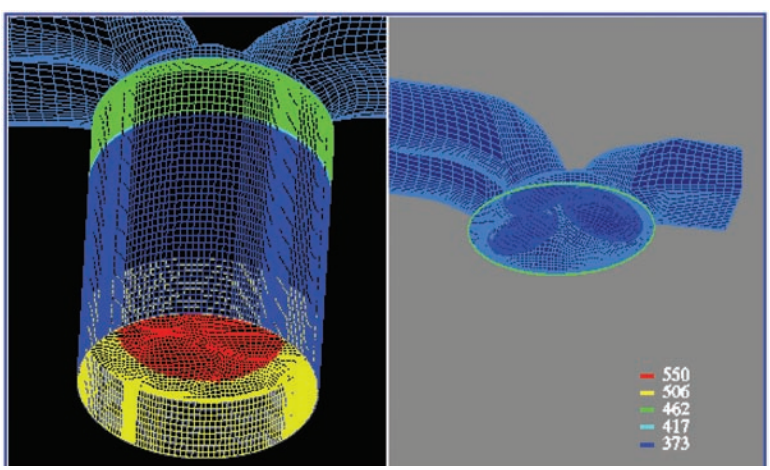

FIGURE 1. Three-dimensional mesh modeling Sandia Livermore (Steeper) engine. The mesh includes the two intake ports, the exhaust port and the valves in addition to the cylinder. Left: mesh at bottom-dead center. Right: mesh at top-dead center. Colors indicate wall temperature boundary conditions according to the scale in the lower right.

Previous modeling work at LLNL has applied customized versions of KIVA3V to problems of interest to the Advanced Combustion in Engines program. LLNL's code KIVA3V-MZ accurately predicts HCCI combustion with a very efficient chemistry solver that groups KIVA's computational cells into a few (10-100) zones that have similar temperature and pressure histories, reducing the computational effort by 2-3 orders of magnitude when compared to methodologies that solve for chemical kinetics in every computational cell, assuming a typical problem involving a fine mesh (~50,000 elements) and a detailed chemical kinetic mechanism (~200 species).

While KIVA3V-MZ has demonstrated high accuracy for homogeneous and partially stratified combustion, it maintains the limitations of its parent code KIVA3V: it is restricted to structured grids and it does not allow parallelization in the fluid mechanics routines (chemical kinetics is parallelized in KIVA3V-MZ). We have therefore migrated the kinetic multi-zone solver to the new KIVA4 code. The new code has been titled KIVA4-MZ and has been developed in collaboration with David Torres from Los Alamos National Laboratory. KIVA4-MZ offers the same computational efficiency of KIVA3V-MZ, with the additional advantage of potential for massive parallelization and the use of unstructured grids that are easier to make and more accurate to compute.

KIVA4-MZ has been benchmarked against numerical results previously calculated with KIVA3V-MZ. The results (Figure 2) show excellent agreement, opening the possibility for fast and accurate computation of homogeneous and partially stratified combustion with parallelization and unstructured grids.

We are also analyzing engine experiments conducted at ORNL for evaluating transition strategies between SI and HCCI modes. In the ORNL experiments, SI-HCCI transition is accomplished by increasing the residual gas fraction through early exhaust valve closing. The experiments show steady SI combustion at low residual gas fraction (<20%) and steady HCCI combustion at very high residual gas fraction (>50%). At intermediate residual gas fractions (20-50%) combustion becomes unsteady, often alternating between SI and HCCI in bimodal, trimodal, or more chaotic patterns.

It is often considered that HCCI engines need to transition to SI for high load operation. Modeling SI-HCCI transition experiments will enhance the understanding of the process leading to improved engine operation through smoother, cleaner and faster transitions.

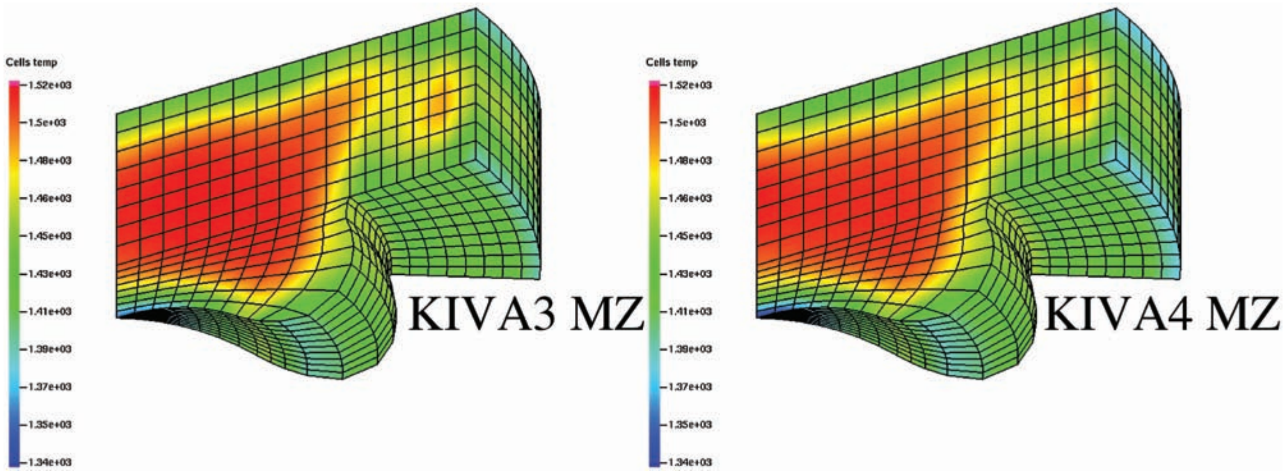

FIGURE 2. Comparison of cell temperatures during HCCI combustion for benchmarking of KIVA3V-MZ and KIVA4-MZ.

Today's engine modeling tools (e.g. KIVA) are well suited for stable SI combustion and stable HCCI combustion, but may have difficulty modeling unstable conditions. Propagation of weak flames followed by autoignition (soft knock) may be better modeled with a detailed chemical kinetics model that uses simplified mixing models instead of detailed fluid mechanics.

We have developed a model for SI-HCCI transition that uses a detailed chemical kinetic model with multiple (20) independent reactors based on the CHEMKIN platform [2]. Flame propagation is modeled through diffusion of mass and heat between the reactors, and autoignition is modeled with detailed chemical kinetics. The reactors may be considered as annular, extending from the center of the cylinder (reactor 1) to the cylinder wall (reactor 20). Spark ignition is modeled by raising the temperature of zone 1 to ~1,500 K, enough to combust fuel. The total mass in the cylinder is divided among the 20 reactors. The mass distribution considered here uses small reactors in the center of the cylinder (reactors 1-5) to accurately model the spark ignition process, and small reactors at the cylinder wall (reactors 16-20) to accurately model crevices and boundary layer effects. Therefore, most of the mass is allocated to the intermediate reactors (6-15). The model uses Woschni correlation [3] to estimate wall heat transfer and a reduced iso-octane chemical kinetic mechanism with 63 species [4] to predict ignition and heat release.

The model has successfully predicted pressure traces for stable SI combustion conditions at relatively low (<20%) residual gas fraction and for stable HCCI conditions at high (>50%) residual gas fraction (Figure 3). Unstable SI-HCCI transition obtained at intermediate residual gas fraction (20-50%) is now being analyzed. Future work in this topic includes

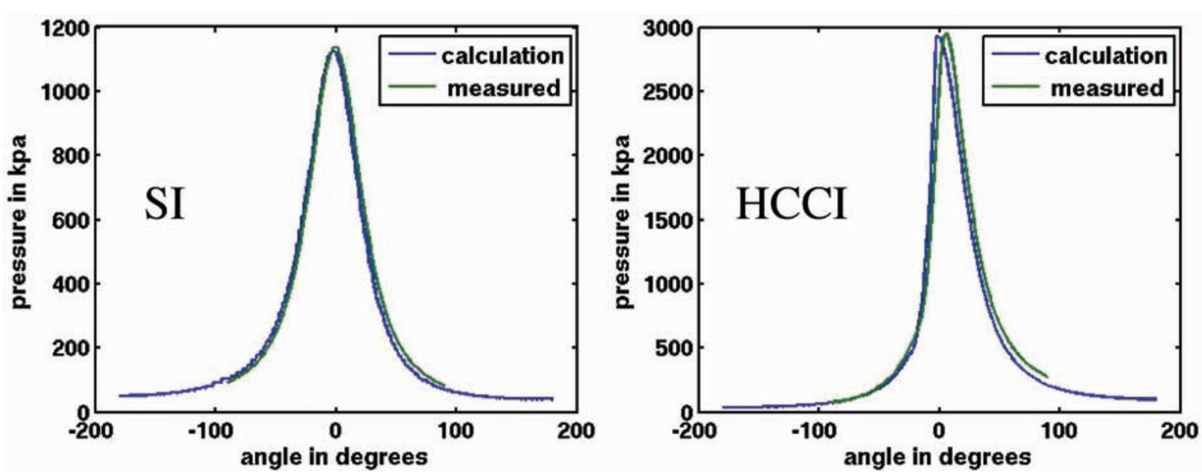

FIGURE 3. Comparison between ORNL experimental results and LLNL numerical results for SI combustion at low residual gas fraction (20%, left) and HCCI combustion at high residual gas fraction (60%, right).

parallelization, where each of the reactors is assigned to an individual processor for fast execution. We also plan linking the code with GT-POWER for detailed analysis of the gas exchange process.

Conclusions

- We have developed and tested detailed 3-dimensional meshes for analysis of partially stratified combustion in experimental engines at Sandia Livermore (Dec, Steeper).
- We conducted detailed analysis of HCCI combustion in the Sandia engine (Steeper).
- Our multi-zone model has been migrated to KIVA4 enabling parallelization and unstructured meshes.
- We have developed a new analysis tool for modeling of SI-HCCI transition experiments being conducted at ORNL.

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2. **Improving Ethanol Life Cycle Energy Efficiency by Direct Utilization of Wet Ethanol in HCCI Engines,** Joel Martinez-Frias, Salvador M. Aceves, Daniel L. Flowers, JSAE Paper 20077037, SAE Paper 2007-01-1867.

3. **Effect of Laser-induced Excitation of Oxygen on Ignition in HCCI Engines Analyzed by Numerical Simulations,** Daniel L. Flowers, Salvador M. Aceves and Robert W. Dibble, Combustion Theory and Modelling, Vol. 11, No. 3, pp. 455-468, 2007.

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8. **Liquid penetration Length in Direct Diesel Fuel Injection,** S. Martínez-Martínez, F.A. Sánchez-Cruz, J.M. Riesco-Ávila, A. Gallegos-Muñoz and S.M. Aceves, Applied Thermal Engineering, Vol. 28, pp. 1756-1762, 2008.

9. **Pathline Analysis of Full-cycle Four-stroke HCCI Engine Combustion Using CFD and Multi-Zone Modeling,** Randy P. Hessel, David E. Foster, Richard R. Steeper, Salvador M. Aceves, Daniel L. Flowers, SAE Paper 2008-01-0048, SAE Transactions, 2008.

10. **Modeling Iso-octane HCCI using CFD with Multi-Zone Detailed Chemistry; Comparison to Detailed Speciation Data over a Range of Lean Equivalence Ratios,** Randy P. Hessel, David E. Foster, Salvador M. Aceves, M. Lee Davisson, Francisco Espinosa-Loza, Daniel L. Flowers, William J. Pitz, John E. Dec, Magnus Sjöberg, Aristotelis Babajimopoulos, SAE Paper 2008-01-0047.

11. **Demonstrating Optimum HCCI Combustion with Advanced Control Technology**, Daniel Flowers, Nick Killingsworth, Francisco Espinoza-Loza, Joel Martinez-Frias, Salvador Aceves, Miroslav Krstic, Robert Dibble, SAE Paper 2008-01-2458, 2008.

Special Recognitions & Awards/Patents Issued

1. Salvador M. Aceves invited to deliver a seminar at the SAE 2007 symposium on HCCI, September 2007, Lund, Sweden.

2. Daniel Flowers invited to deliver a seminar at the SAE 2007 symposium on HCCI, September 2007, Lund, Sweden.

3. Salvador Aceves invited to serve as an opponent in Ph.D. exam, Chalmers University, Gothenburg, Sweden, September 2008.

4. Nick Killingsworth invited to deliver a seminar at the "Advanced Engine Control Symposium," Tianjin, China, November 2008.

II.A.8 HCCI and Stratified-Charge CI Engine Combustion Research

John E. Dec
Sandia National Laboratories
MS 9053, P.O. Box 969
Livermore, CA 94551-0969

DOE Technology Development Manager:
Gurpreet Singh

Objectives

Project Objective:

- Provide the fundamental understanding of homogeneous charge compression ignition (HCCI) combustion required to overcome the technical barriers to the development of practical HCCI engines by industry.

Fiscal Year 2008 Objectives:

- Investigate the potential of exhaust gas recirculation (EGR) or retained residuals for reducing heat-release rates to allow higher loads without knock, and determine their effect on NOx for well-mixed HCCI.
- Determine the high-load limits for representative single- and two-stage ignition fuels, and investigate the reasons for these limits.
- Complete detailed exhaust-speciation analysis for well-mixed operation and for mixture-stratified operation at low load, using iso-octane fueling.
- Complete setup of a variable valve actuation (VVA) system and on-engine testing.
- Support chemical-kinetics and computational fluid dynamics (CFD) modeling work at Lawrence Livermore National Laboratory (LLNL) to help develop improved kinetic mechanisms and to advance the understanding of in-cylinder processes.

Accomplishments

- Determined the effect of EGR/residuals on HCCI heat-release rates and NOx formation for well-mixed HCCI by isolating these effects from the other effects of EGR.
  - Showed that EGR offers little direct benefit for extending the high-load limit.
- Determined the high-load limits for single- and two-stage fuels, and identified three different mechanisms for these limits, depending on fuel type.
- Completed detailed exhaust-speciation analysis for well-mixed operation at a variety of loads and for stratified operation at low loads with iso-octane fueling (with LLNL).
  - Expanded this study to include initial work on exhaust-speciation for gasoline fueling.
- Completed setup and testing of VVA system. Demonstrated negative valve overlap (NVO) and late intake valve closure (IVC) operation.
- Initiated development of a planar temperature-measurement technique to determine the evolution of thermal stratification in an HCCI engine.
- Provided data, analysis, and discussions to support: 1) chemical-kinetic mechanism development at LLNL (improved pressure dependence and additional species), and 2) CFD/kinetic modeling of HCCI performance and emissions at LLNL and the University of Wisconsin (UW).

Future Directions

- Determine how natural thermal stratification develops in an HCCI engine (including its magnitude and distribution), which is critical for high-load operation.
  - Complete development of an appropriate planar temperature-imaging diagnostic.
- Determine the potential of pressure-boost to extend the high-load range of HCCI by using EGR to control the pressure-induced combustion-phasing advance.
- Investigate the behavior of ethanol as an HCCI fuel over a range of loads, speeds, and intake-pressure boost conditions. Conduct work jointly with researchers from the Advanced Light-Duty Engine Fuels Research Laboratory.
- Conduct detailed exhaust-speciation study over a range of loads for a representative two-stage ignition fuel and compare with previous data for single-stage fuels (with LLNL).
- Determine the traces species that affect autoignition recovery from near misfire for single- and two-stage ignition fuels, by using detailed exhaust-speciation analysis under these conditions.
- Continue to work cooperatively with LLNL on improving chemical-kinetic mechanisms for fuel constituents and surrogate fuels, and to support their CFD modeling work with data and analysis.

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Introduction

HCCI engines have significant efficiency and emissions advantages over conventional spark-ignition and diesel engines, respectively. However, several technical barriers must be addressed before it is practical to implement HCCI combustion in production engines. One of the most important of these barriers is extending HCCI operation to higher loads, and three studies conducted during FY 2008 addressed this barrier. These studies included: 1) the potential of EGR/residuals for reducing the heat-release rate (HRR) to allow higher loads without knock, 2) determining the high-load limits for representative single- and two-stage ignition fuels and the mechanisms responsible for these limits, and 3) initiating the development of a planar temperature-measurement technique to investigate natural thermal stratification, which is critical for high-load HCCI operation.

In addition, a detailed exhaust-speciation analysis was completed for both well-mixed and mixture-stratified operation, and an electro-hydraulic VVA system was completed and tested on the engine. These efforts are related to technical barriers of poor combustion efficiency (and high hydrocarbon [HC] and carbon monoxide [CO] emissions) at low loads and combustion-phasing control, respectively.

Approach

These studies were conducted in our dual-engine HCCI laboratory using a combination of experiments in both the all-metal and optically accessible HCCI research engines. This facility allows operation over a wide range of conditions, and can provide precise control of operating parameters such as combustion phasing, injection timing, intake temperature and pressure, and mass flow rates of supplied fuel and air. The facility is also set up to allow the use of cooled EGR, or to meter nitrogen (N_2), carbon dioxide (CO_2), and water vapor into the intake stream to simulate the addition of complete combustion products (*i.e.* EGR with no trace species). Additionally, the laboratory is equipped with a full emissions bench (HC, CO, CO_2, oxygen, NOx, and smoke), and a sample port on the exhaust runner of the metal engine allows collection of exhaust gases for detailed exhaust speciation.

To study the potential of EGR for reducing the HRR to improve high-load operation, cooled real EGR was used. For this study, it was necessary to control combustion phasing since it is well known that EGR retards the combustion phasing [1], and that retarded phasing will reduce the HRR, whether it is caused by EGR addition or other means [2]. To prevent this indirect effect of EGR on the HRR from masking any direct effect that EGR might have, the intake temperature was increased as EGR was added to maintain the 50% burn point (CA50) at 370° crank angle (CA) (10° after top-dead center [TDC]).

Determining the high-load limits for various fuels also required combustion-phasing control. This is because, as the fueling rate is increased, the heat release becomes more rapid and the total pressure rise with combustion becomes greater. These act together to increase the maximum pressure-rise rate (PRR), eventually causing knock. To overcome this, the combustion phasing was systematically retarded as fueling was increased to maintain a constant PRR. For single-stage ignition fuels this was accomplished by reducing the intake temperature. However, for the two-stage fuels, intake temperatures were already near ambient even for low loads, so combustion-phasing retard was accomplished by EGR addition.

For the detailed exhaust speciation analysis, samples were extracted from the exhaust-runner port and analyzed by three techniques in cooperation with an analytical-chemistry group at LLNL. Most species were measured with a gas chromatograph combined with a mass spectrometer, while high-performance liquid chromatography was used for formaldehyde and acetaldehyde, and light HC species were measured using a gas chromatograph combined with a flame ionization detector. Combustion phasing was held constant at CA50 = TDC, since variations in phasing can strongly affect combustion efficiency and emissions.

Results

High-load HCCI operation is typically limited by the HRR becoming so rapid that the associated PRR causes the engine to knock. It is often stated in the literature that adding EGR can slow the PRR to allow higher loads without knock, and it is generally accepted that this EGR is also beneficial for reducing NOx. However, in previous works, the effect of EGR on the PRR was convolved with its effect on combustion phasing, so it was not possible to determine specific cause-and-effect relationships. In the current study, combustion-phasing was held constant, as discussed above, so the direct effect of EGR on the PRR could be determined.

Figure 1a shows the effect of EGR on the maximum PRR, and Figure 2 shows the power output as measured by the gross indicated mean effective pressure ($IMEP_g$). As can be seen, when constant fueling is maintained, the PRR decreases with EGR addition, but the $IMEP_g$ also falls. Therefore, fueling must be increased as EGR is added to maintain a constant engine power output ($IMEP_g$), as shown in Figure 2. The reason for this behavior is that EGR reduces the thermal efficiency of the engine, as shown in Figure 1b. This drop in thermal efficiency occurs because the higher specific heat of the EGR gases reduces the γ (c_p/c_v) of the gas mixture, so less pressure work can be extracted for a given

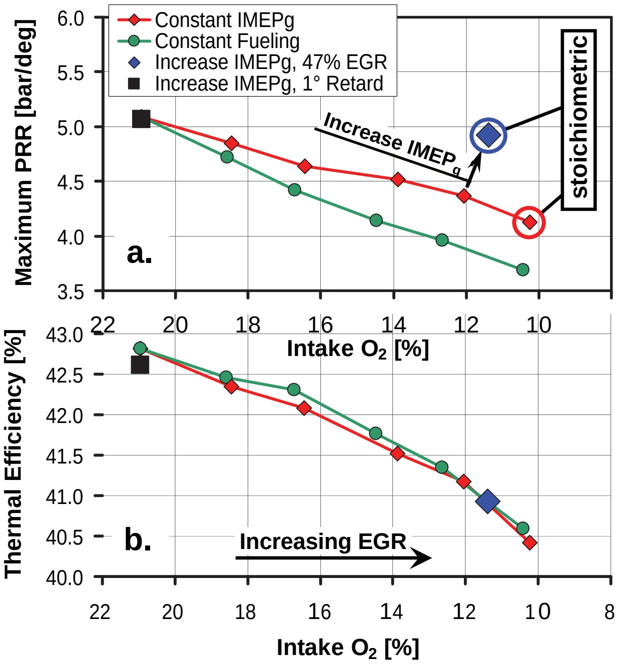

FIGURE 1. The effect of EGR addition on (a) PRR, and (b) thermal efficiency. The amount of EGR is shown by the decrease in intake oxygen.

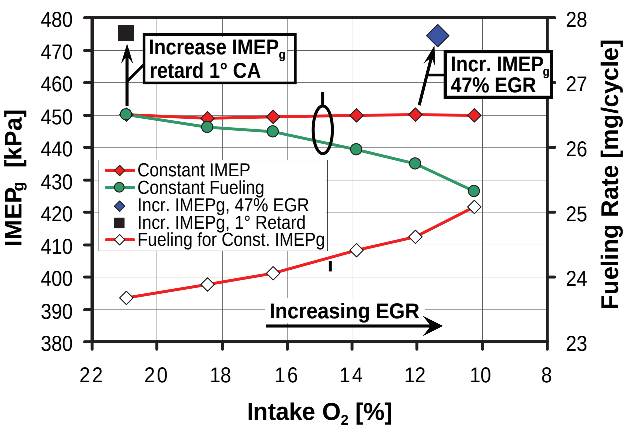

FIGURE 2. The effect of EGR on the $IMEP_g$ and fueling rate, for constant fueling and for constant $IMEP_g$.

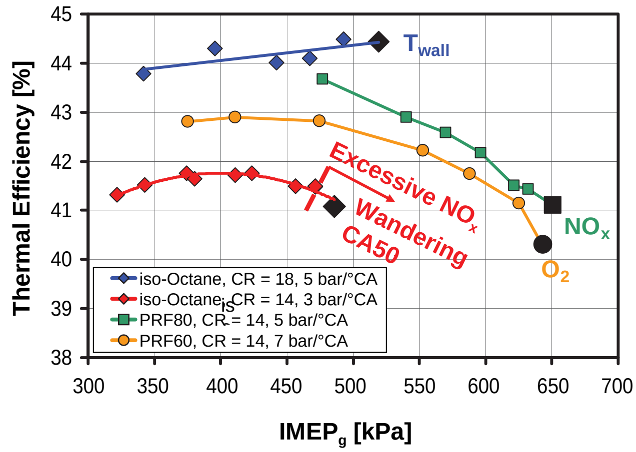

FIGURE 3. Thermal efficiency vs. $IMEP_g$ for iso-octane, PRF80, and PRF60. The large black symbols indicated the maximum load of each fuel. The load-limiting factor is indicated for each fuel (see text).

expansion ratio. The net effect is that fuel consumption increases by nearly 6% from the zero-EGR condition (20.9% oxygen) to the maximum-EGR condition (10.2% O_2) shown, for a constant $IMEP_g = 450$ kPa.

Despite this drawback, Figure 1 shows that EGR addition does decrease the maximum PRR, even when fueling is increased to maintain a constant $IMEP_g$. As a result, the $IMEP_g$ can be increased from 450 to 475 kPa without exceeding the maximum PRR of 5 bar/°CA obtained for $IMEP_g = 450$ kPa without EGR addition (*i.e.*, for the same knocking propensity, more power can be obtained), as indicated by the large blue diamond symbols in Figures 1-2. However, this increase in $IMEP_g$ is modest, and it can be achieved without EGR addition by retarding the combustion timing by only 1°CA, as shown by the large black square symbols in Figures 1-2. This small amount of additional timing retard has almost no effect on the thermal efficiency, so the thermal efficiency is 1.7% greater than that of the high-EGR case, for a 4% fuel savings. Another drawback of using EGR is that, contrary to intuition, NOx emissions actually increase when the $IMEP_g$ is held constant, for well-mixed HCCI. This increase in NOx is due to the higher temperatures resulting from the increased fueling required to maintain $IMEP_g$ with EGR addition. This finding contrasts with the benefit of EGR for reducing local peak temperatures for partially stratified HCCI and low-temperature diesel combustion (or in flame zones for conventional spark ignition or diesel combustion). These findings show that, although EGR may be required for combustion-phasing control, it offers little direct benefit for reducing the PRR in HCCI engines, and it can be detrimental to NOx emissions.

The high-load limits for single- and two-stage ignition fuels were explored, using combustion-phasing retard to maintain a constant PRR as fueling was increased. Iso-octane (a good surrogate for gasoline) was chosen as the single-stage fuel, and tests were performed for compression ratios (CR) of both 14 and 18. PRF80[1] and PRF60[2] were chosen as the two-stage fuels. Because of their relatively high autoignition reactivity, tests were performed with only the lower CR = 14. Figure 3 summarizes the results in terms of the $IMEP_g$ and thermal efficiencies obtained. As can be seen, the maximum load for the single-stage

[1] Primary Reference Fuel blend, 80% iso-octane and 20% n-heptane
[2] Primary Reference Fuel blend, 60% iso-octane and 40% n-heptane

fuel is limited to an $IMEP_g$ ~500 kPa, while the two-stage fuels reach an $IMEP_g$ ~650 kPa. Two factors contribute to this increased $IMEP_g$. First, because they are more reactive, the two-stage fuels require lower intake temperatures, which results in a higher intake-charge density and therefore, more mass inducted. Second, more retarded combustion phasing can be used with two-stage fuels due their greater autoignition stability [3]; this allows higher fueling without engine knock. However, thermal efficiency drops somewhat for the two-stage fuels as load is increased. This results from both the more retarded combustion phasing and the increased amounts of EGR required to retard the phasing. For iso-octane, increasing the CR from 14 to 18 increases the thermal efficiency almost 3%. Additionally, the maximum $IMEP_g$ is increased with CR = 18, in part because the lower required intake temperatures result in a greater inducted charge mass.

The reasons for these high-load limits were also examined, and a different mechanism was found to be responsible for the limit of each fuel, as noted on Figure 3. For iso-octane, combustion phasing becomes very sensitive to small changes in the charge temperature. This results in an inability to adequately control combustion phasing (wandering CA50) for CR = 14, or for CR = 18, small changes in the wall temperature can cause CA50 to advance to runaway knock or retard to misfire (designated T_{wall} on Figure 3). The two-stage primary reference fuels are less sensitive to changes in temperature and are load-limited by other factors. For PRF80, the load can be increased until the combustion becomes sufficiently hot to produce small amounts of NOx. Although emissions are still well below the US-2010 (or Tier 2, Bin 5) limits, very low concentrations of NOx (a few ppm) transferred to the incoming charge through the residuals or EGR enhance the autoignition, rapidly advancing the combustion phasing to runaway knock [4]. For PRF60, at the conditions studied, the high load was limited by the available oxygen. This is because PRF60 has a high autoignition reactivity, so substantial amounts of EGR must be used to retard the combustion phasing to maintain an acceptable PRR. A full discussion of this study may be found in Ref. [4].

HCCI engines can produce significant emissions of HC and oxygenated HC (OHC), particularly at low loads. Detailed-speciation of these emissions is important for understanding the in-cylinder processes responsible for their formation, and to understand how their production can be reduced by mixture stratification. Speciation data also provides a database for validation of models and for the development of appropriate catalytic aftertreatment. Accordingly, detailed HC and OHC speciation measurements were made over a range of fuel loadings for well-mixed HCCI, and for varying amounts of mixture stratification at an idle fueling rate. Data were first acquired using iso-octane fueling since the formation of the various species is more easily understood for a fuel of known composition. A follow-on study for gasoline fueling is underway.

For all conditions studied, the largest contributor to the HC and OHC emissions is unreacted fuel (iso-octane). However, the data show that its proportion of the total emissions decreases from 71% to 36% as fueling is decreased from an equivalence ratio (ϕ) = 0.28 to 0.08. Thus, the large increase in HC and OHC emissions at low loads come from the production of smaller species (fuel-breakdown and partial-oxidation products). These species fall into three categories based on the relationship of their molecular structure to the parent fuel molecule. As shown in Figure 4, as fueling (ϕ) is reduced, the relative increase in the amounts of these species correlates with their molecular structure and shows a clear progression from fuel (iso-octane) → break-down products → small species → CO. Analysis shows that this trend can be explained by the variation in the in-cylinder temperature from the ring-land crevice through the boundary layer to the bulk gas, and the locations along this temperature gradient where the various species form. Analysis of the speciation data for various amounts of fuel stratification (obtained by varying the injection timing) shows that two separate mechanisms contribute to the improvement in low-load combustion efficiency with stratification. A complete discussion of these findings is given in Ref. [5]. Finally, in cooperation with LLNL and UW, these data have been used as a basis for validating the results of a combined CFD/chemical-kinetic modeling study [6].

Naturally occurring thermal stratification is critical for high-load HCCI operation because it causes the charge to autoignite sequentially, which decreases the HRR, reducing the propensity for engine-knock.

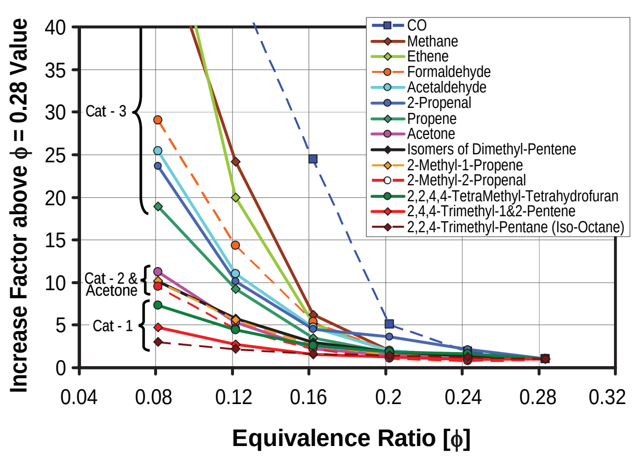

FIGURE 4. Normalized emissions of HC, OHC, and CO as a function ϕ. For each curve, the data have been normalized by the value of that species at ϕ = 0.28, thus providing the "increase factor" above this value.

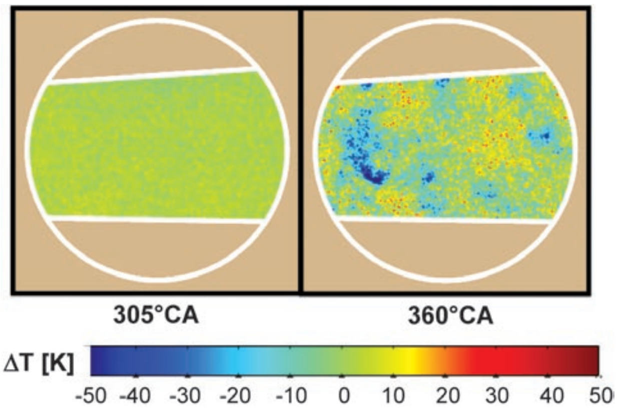

FIGURE 5. Preliminary temperature-map images showing the ability of the diagnostic to measure differences in thermal stratification between 305°CA and TDC (360°CA). The white circle shows the field of view through the piston-crown window of the optical engine, and the white lines mark the edges of the laser sheet, which is positioned at the mid-plane of the pancake combustion chamber.

However, little is known about the development of this stratification or its distribution. Investigation of the thermal stratification first requires the development of a planar temperature-imaging diagnostic. A tracer-based single-line planar laser-induced fluorescence (PLIF) technique was selected for its good precision and simplicity. The principle of the technique relies on the temperature sensitivity of the PLIF signal of toluene, added as a 2% tracer in the fuel. Preliminary results, presented in Figure 5, verify the capability of this diagnostic to measure the thermal inhomogeneities that develop throughout the bulk gas in the latter part of the compression stroke. Based on these promising results, an expanded study is planned.

Conclusions

- EGR provides only a small potential for slowing the HRR to extend the knock limit, and it reduces the thermal efficiency of the engine by approximately 2%.
  - Therefore, the use of EGR/residuals should be minimized to the extent possible.
- Two-stage-ignition fuels (PRF60 and PRF 80) allowed higher loads without knock than the single-stage fuel (iso-octane). Two factors contribute to this: 1) two-stage fuels require a lower intake temperature, which results in more charge-mass inducted, and 2) two-stage fuels allow greater combustion phasing retard with good stability, which reduces the knocking propensity.
- For the single-stage fuel, increasing the compression ratio from 14 to 18 offers advantages of increased thermal efficiency, increased maximum load ($IMEP_g$), and reduced NOx for a given load.
- Three different mechanisms were identified that limit high-load HCCI operation for the various fuels studied: 1) excessive sensitivity of autoignition to small changes in temperature, 2) enhancement of autoignition by small amounts of NOx, and 3) lack of oxygen when high levels of EGR are required.
- Unreacted fuel is the main HC emission from HCCI engines, but as fueling is decreased, smaller HC and OHC species become increasingly prevalent. The various HC and OHC species show different trends as fueling is reduced, which can be related to the in-cylinder locations where they form.
- Fuel stratification improves combustion efficiency at low loads for two reasons: 1) it produces local regions that are less lean, so they burn hotter and more completely, and 2) the reduced mixing time prevents fuel from reaching the crevices where low temperatures prevent combustion.
- Preliminary results indicate that the single-line, PLIF-based, temperature-imaging diagnostic examined has good potential for investigating the naturally occurring thermal stratification in HCCI engines.

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FY 2008 Publications/Presentations

1. Hwang, W., Dec, J.E. and Sjöberg, M., "Fuel Stratification for Low-Load Combustion: Performance & Fuel-PLIF Measurements," SAE paper 2007-01-4130, SAE Powertrains, Fuels and Lubricants Meeting, October 2007.

2. Silke, E., Pitz, W.J., Westbrook, C.K., Sjöberg, M., and Dec, J.E., "Understanding the Chemical Effects of Increased Boost Pressure under HCCI Conditions," presented at and published in the proceedings, AIChE Annual Meeting, Salt Lake City, UT, November 2007.

3. Hwang, W., Dec, J.E., and Sjöberg, M., "Spectroscopic and Chemical-Kinetic Analysis of the Phases of HCCI Autoignition and Combustion for Single- and Two-Stage Ignition Fuels," *Combustion and Flame*, Vol. 154(3), pp. 387-409, 2008.

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9. Hwang, W., Dec, J.E., and Sjöberg, M., "Spectroscopic and Chemical-Kinetic Analysis of the Phases of HCCI Autoignition and Combustion for Single- and Two-Stage Ignition Fuels," oral-only presentation at the 2008 SAE Congress.

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11. Dec, J.E., "Advanced Compression-Ignition Engines – Understanding the In-Cylinder Processes," topical review for the 32nd International Combustion Symposium, to be published in the *Proceedings of the Combustion Institute*, 2009.

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Special Recognitions & Awards/Patents

1. Invited topical review paper and lecture at the 32nd International Combustion Symposium, Montreal, Canada, August 2008.

2. Invited presentation at the 3rd International Symposium on Clean and High-Efficiency Combustion in Engines, Tianjin, China, June 2008.

3. Invited presentation for the Coordinating Research Council, Advanced Vehicle/Fuels/Lubricants Meeting, September 2008.

II.A.9 Automotive HCCI Combustion Research

Richard Steeper
Sandia National Laboratories, MS 9053
P.O. Box 969
Livermore, CA 94551-0969

DOE Technology Development Manager:
Gurpreet Singh

Objectives

This project comprises optical-engine investigations designed to enhance our understanding of in-cylinder processes in automotive-scale homogeneous charge compression ignition (HCCI) engines. Objectives for Fiscal Year 2008 include:

- Expand our capability to operate in advanced HCCI operating modes, specifically recompression or negative-valve-overlap (NVO) mode.
- Continue the development of laser-based diagnostics, and conduct tests of the diagnostics in Sandia HCCI research engines.
- Continue our investigation of the correlation between fuel-air mixture preparation and combustion/emission processes in HCCI engines.
- Continue development and application of collaborative HCCI engine-simulation tools.

Accomplishments

- Characterized HCCI-NVO operation in our optical engine, comparing performance with one-dimensional engine model predictions (motored) and with industry all-metal engine data (fired).
- Optimized performance of Stanford's two-wavelength planar laser-induced fluorescence (PLIF) diagnostic for use during conventional HCCI and NVO-HCCI operation. Acquired simultaneous composition and temperature measurements during the NVO recompression period.
- Performed bench-top tests of a carbon monoxide (CO) laser-absorption diagnostic for characterizing the extent of reactions during NVO reformation.
- Completed an experimental examination of combustion effects of common laser-induced fluorescence (LIF) tracers on single- and two-stage-fuel combustion in engines.
- Continued collaboration with the University of Wisconsin (UW), Lawrence Livermore National Laboratory (LLNL), and Sandia's Reacting Flow department to develop modeling tools for automotive HCCI application.
- Developed a facility upgrade plan to enable more flexible valve timing, wider operating range, and multiple combustion modes. Began acquisition of engine hardware.

Future Directions

- Validate the UW computational fluid dynamics (CFD) model of our automotive HCCI engine using optical and conventional measurements over a range of NVO operating conditions.
- Apply optical diagnostics to characterize reforming reactions during NVO period and correlate to main combustion.
- Expand tunable diode laser absorption diagnostic to permit in-cylinder measurement of water (H_2O) and carbon dioxide (CO_2).
- Perform facility upgrade. Install new spray-guided direct injection (DI) head.

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Introduction

Major challenges to the implementation of HCCI combustion–including phasing control, operating-range extension, and emissions control–will require advanced charge-preparation strategies. Alternative strategies such as retarded injection and variable valve timing can be used to modify local charge composition and temperatures, thereby affecting, and possibly controlling, ignition phasing, rate of heat release, combustion efficiency, and engine-out emissions. This project is focused on understanding the in-cylinder processes characteristic of automotive HCCI engine combustion. Optical engine experiments employ in-cylinder diagnostics to quantify mixture preparation, ignition, combustion, and emission processes. Computational models help interpret the results and guide further research. The knowledge gained supports DOE's goal of facilitating the development of energy-efficient, low-emission engine combustion.

Approach

A variety of optical and mechanical diagnostics are applied to obtain information about HCCI in-cylinder processes. In-cylinder spray imaging allows assessment of spray evolution, penetration, and wall-wetting. LIF imaging produces fuel vapor and temperature distribution data, and statistics derived from the images quantify the state of mixing just prior to heat release. Chemiluminescence imaging provides information about combustion that can be related to the LIF fuel-distribution images. Finally, engine-out emission measurements help correlate mixture-preparation strategies with combustion/emission performance. Development of new diagnostics for in-cylinder temperature measurements, a critical need for HCCI research, continues at Stanford University, with testing taking place in Sandia's optical engines. Work on a KIVA simulation of our automotive HCCI engine continues at UW and LLNL. Technical exchanges with original equipment manufacturers, national labs, and academia provide feedback and guidance for the research program.

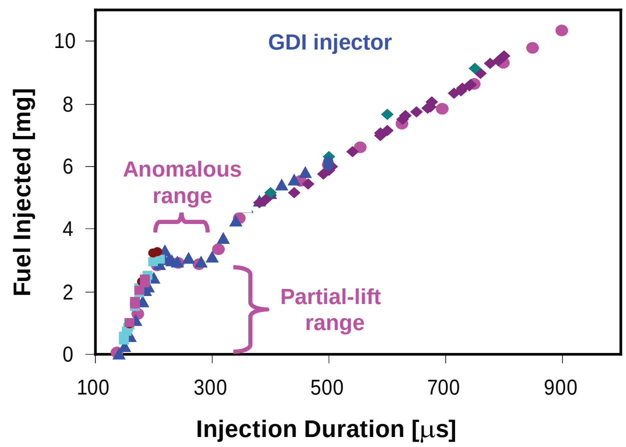

FIGURE 1. Injector fuel delivery for a fuel pressure of 100 bar measured for a range of motored operating conditions.

Results

A main focus of our current research is understanding recompression–or NVO–strategy for HCCI combustion. The strategy has shown a potential to achieve and control low-load HCCI operation, but the thermal and chemical details of the process remain uncertain. Select results of our research this year are summarized below in three subsections.

NVO Operation:

In the absence of variable valve control, we have developed a two-fuel technique (dimethyl ether plus iso-octane) for initiating NVO combustion and quickly warming the engine to steady conditions. The ever-present possibility of misfire followed by over-fueling and over-pressurization of the optical cylinder led us to incorporate a real-time indicated mean effective pressure (IMEP) monitor into our safety system this year. Once fueling is begun, any significant drop in IMEP (caused by misfire) now triggers an immediate fuel shut-off. Since NVO operation is usually coupled with multiple fuel injections of widely varying duration, we have quantified the performance of our multi-hole gasoline direct injection (GDI) injector. The results shown in Figure 1 clearly identify an anomalous range of injection times for which delivery actually declines with increasing duration–behavior attributed to needle bounce. Fueling during the NVO period typically requires very short injections (a few mg or less), forcing us to operate in the partial-needle-lift range identified in Figure 1.

Our characterization of baseline engine performance during NVO operation included an optimization of valve timing. We found that setting exhaust valve closure (EVC) to 75 crank angle degrees (CAD) before top-dead center (bTDC) and intake valve opening (IVO) to 75 CAD after top-dead center (aTDC) retained sufficient hot residuals to allow fired iso-octane operation with modest intake air heating. The relatively wide operating range allowed us to conduct sweeps of load, NVO fuel fraction (during split injection), and NVO injection timing.

Figure 2 shows the results during sweeps of NVO fuel fraction (top) and NVO injection timing (bottom). For the fuel-fraction sweep, total fuel was held constant, with the NVO injection at 100 CAD bTDC of exhaust and the main fuel injection at 90 CAD aTDC of intake. Fuel injected during NVO recompression can react, and the positive values of NVO (i.e., pumping) IMEP seen in the top graph are due to heat release during this period. Following the IMEP curve from *right to left*, we see little change in NVO IMEP as the fraction of fuel injected during NVO is reduced from 50% to 30%. Extent of reaction is likely dictated by available oxygen at this high residual-gas-fraction operating point. Below 30% however, NVO IMEP drops precipitously, causing a significant retardation of main combustion phasing (CA50 in Figure 2). These observations suggest a means of controlling main combustion phasing that is a focus of current investigations.

The bottom graph in Figure 2 represents the results of sweeping NVO fuel injection timing. For this test, the total fuel injected and the NVO fuel fraction are held constant. Starting at 100 CAD bTDC of exhaust, retarding start of NVO injection (moving *left to right* on the graph) causes NVO IMEP to decrease (while the main IMEP rises steadily), indicating diminishing NVO heat release. The trends in NVO and main IMEP offset one another, causing net IMEP to remain constant. During this period, however, phasing of the main combustion reactions undergoes a sharp trend reversal. For SOI timings up to about 40 CAD bTDC, there is a steady advance in CA50 that counters the retarding effect expected from decreasing NVO heat release. A possible cause of the phasing advance is a change in the composition of NVO reformation products carried over to the main combustion event. For injections after

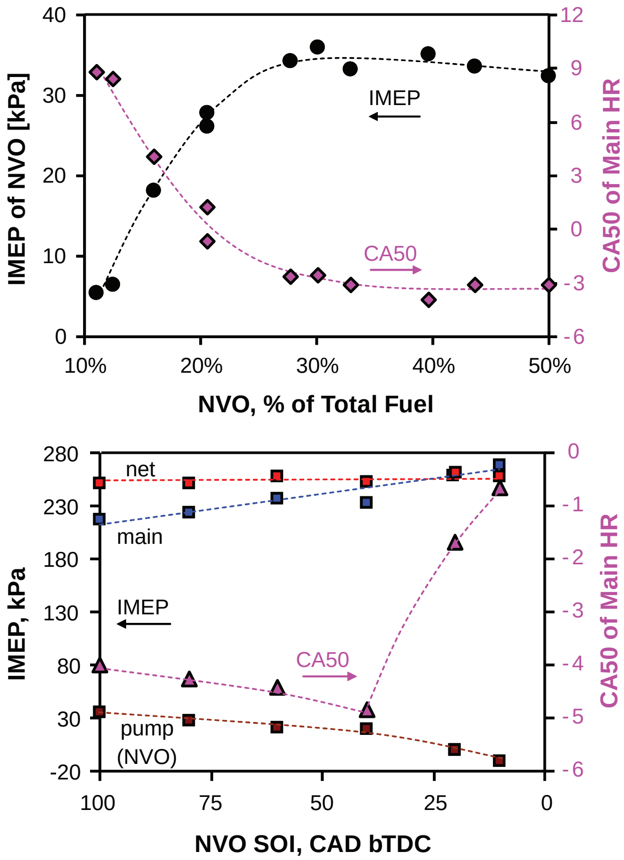

FIGURE 2. Engine performance during sweeps of NVO fuel-injection parameters. **Top:** Sweep of NVO fuel fraction. Total fuel injected = 10.9 mg per cycle, with constant NVO start of injection (SOI) timing of 100 CAD bTDC of exhaust. **Bottom:** Sweep of NVO SOI timing. Total fuel injected = 10.9 mg per cycle and constant NVO fuel fraction of 50%.

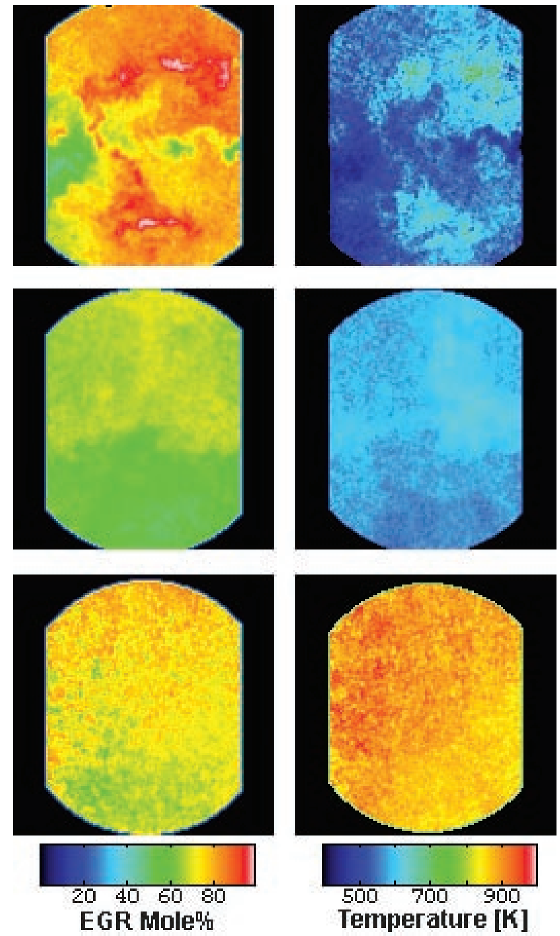

FIGURE 3. Simultaneous single-shot EGR and temperature images recorded during NVO operation. **Top row:** Images captured mid-intake stroke (135 CAD aTDC intake); **Middle row:** Images captured mid-compression stroke (80 CAD bTDC compression); **Bottom row:** Images captured late in compression stroke (24 CAD bTDC compression).

40 CAD, main combustion phasing rapidly retards as injected NVO fuel no longer reacts sufficiently to assist main combustion.

Two-Wavelength PLIF Diagnostic:

We have continued our work with Stanford on the refinement and application of a two-wavelength PLIF diagnostic for simultaneous, in-cylinder imaging of temperature and composition. Two Stanford students worked in our lab to apply the diagnostic over a range of operating conditions. Tests included both air-seeded and fuel-seeded variations of the diagnostic and application during both conventional HCCI and NVO-HCCI operation.

Figure 3 provides sample exhaust gas recirculation (EGR) and temperature images from the air-seeded PLIF experiments. Results shown here represent fired NVO-HCCI operation, although the technique works equally well for conventional HCCI operation. For these tests, we selected a light load with 30% of the fuel injected at the start of NVO recompression, and the remainder injected just prior to the main compression stroke. Other conditions are similar to those described in the previous section.

The three rows of image pairs in Figure 3 represent three different crank-angle positions. The top image pair was recorded during the intake stroke, prior to the main fuel injection, and shows the incomplete mixing of hot residuals with cooler intake air. Areas of high EGR concentration (left image) correspond to areas of elevated temperature (right image). The middle pair of images was recorded after the main fuel injection, about half-way through the compression stroke. Mixing has homogenized the charge to some extent, but significant non-uniformities in concentration and temperature remain. The bottom pair of images was recorded just prior to the start of heat release–the mixture is much more uniform although some variation is still evident. This type of measurement can be used to quantify charge conditions at a reference crank angle position in order to assess the effects of varying operating parameters.

The above air-seeded PLIF technique is restricted to the period beginning when tracer enters the cylinder during intake and ending when it disappears due to reaction. The fuel-seeded technique expands the measurement period, and has enabled us to obtain images during the NVO portion of the cycle. We began these tests by assessing potential interferences caused by fluorescence from droplets and from non-tracer combustion products. The short NVO re-compression period means that the time between injection and reactions is brief. Nonetheless, we found that temperatures are high enough to evaporate fuel droplets within 15-20 CAD of injection, leaving a droplet-free period needed for LIF imaging. A second potential interference during this period is fluorescence from non-tracer species. Such molecules potentially could be formed during incomplete main combustion and be carried over to recompression along with residual gases. Tests described below showed that this source of interference is minor for a range of operating conditions.

The three rows of Figure 4 represent three different experiments designed to measure the extent of interferences for PLIF measurements recorded during the NVO period. In this figure, the image pairs represent signal from our two laser sheets before being processed into composition/temperature data. In the first experiment (top row), we operated with no tracer added to the fuel. The images were captured near the start of recompression, and the low counts recorded indicate that there is little interference from non-tracer fluorescence. In the next experiment, tracer was added to the fuel, but since the images were recorded *prior* to NVO fuel injection, the signal is attributed to unburned tracer sequestered in the crevices and carried over to recompression. This signal is nearly an order of magnitude larger than the non-tracer interference. Interestingly, this signal does not represent a source of error since it can be interpreted in the same fashion as the signal in the following experiment. In the final experiment (bottom row), the images were captured *following* NVO fuel/tracer injection, and the signal has increased by another order of magnitude. For both of the last two experiments, there is sufficient signal to provide useful temperature measurements.

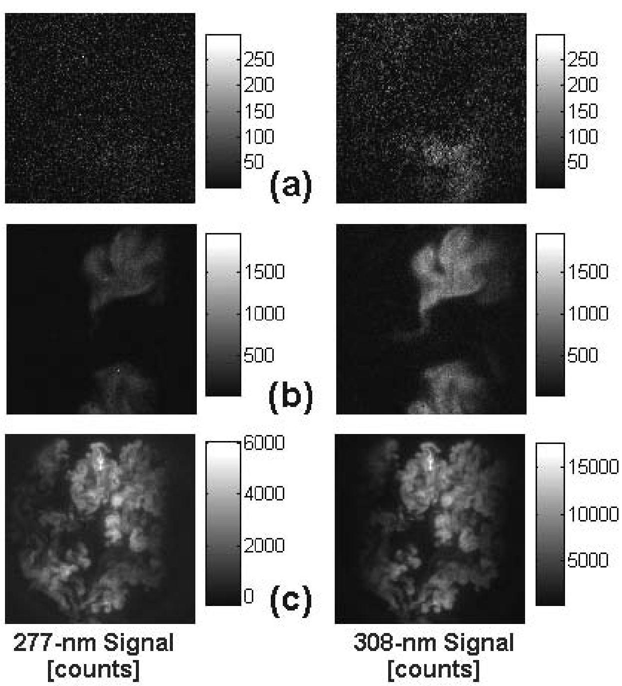

FIGURE 4. Single-shot 277-nm and 308-nm LIF images of **(a):** Residual gas recorded at +260 CAD (no tracer); **(b):** Carry-over 3P recorded at +260 CAD (prior to NVO fuel injection); and **(c):** 3P recorded at +285 CAD (following NVO fuel injection).

LIF Tracer Effect on Combustion:

This year we addressed a significant question associated with LIF imaging: do the tracers used for the diagnostic influence the combustion processes being examined? We conducted fired NVO tests using the two common ketones, acetone and 3-pentanone, as tracers for the air-seeded PLIF technique. Two common surrogate fuels, iso-octane and n-heptane, were used in the tests. Our results revealed complex effects of the tracers on combustion as summarized in Figures 5 and 6.

The apparent heat-release rate (AHRR) curves in Figure 5a sort out several details of the 3-pentanone/iso-octane experiments. The blue curve is the reference case with no tracer added and all fuel directly injected. The green curve also has no tracer added, but 20% of the fuel is premixed into the intake air to mimic the air-seeding process. The effect of premixing some of the fuel is a visible advancement of phasing due to the reduction in DI evaporative cooling. In the final case, tracer is substituted for the premixed fuel, and the resulting red curve shows that 3-pentanone enhances heat release in both phasing and magnitude. Figure 5b presents the same three cases for the tracer acetone. Here the effect of acetone addition is a retardation of heat release. This retardation is actually greater than the red curve indicates: intake temperature had to be raised by several degrees to avoid the frequent misfires that occurred without this temperature boost.

Figure 6 represents the same experiments using the two-stage fuel n-heptane–the low-temperature and main heat release periods are obvious in these graphs. Contrary to its promotion of iso-octane combustion, 3-pentanone has a dramatic retarding effect on both the low-temperature and main heat release curves for n-heptane in Figure 6a. However, in Figure 6b, the effect of acetone is to retard n-heptane combustion as it did for iso-octane in Figure 5b. As a final observation, we found

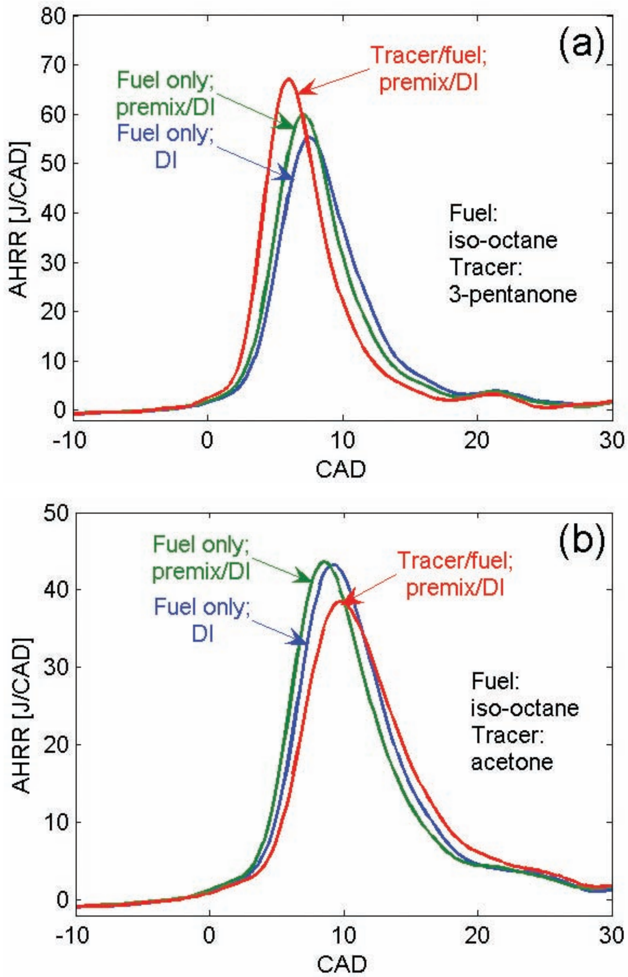

FIGURE 5. Effect of tracers on the AHRR of iso-octane combustion. Each plot shows three different experimental cases: (i) fuel only, with all of it direct injected; (ii) fuel only, with 80% direct injected and 20% premixed upstream; and (iii) same as previous, but with tracer substituted for the premixed fuel. **(a):** 3-pentanone tracer; **(b):** acetone tracer.

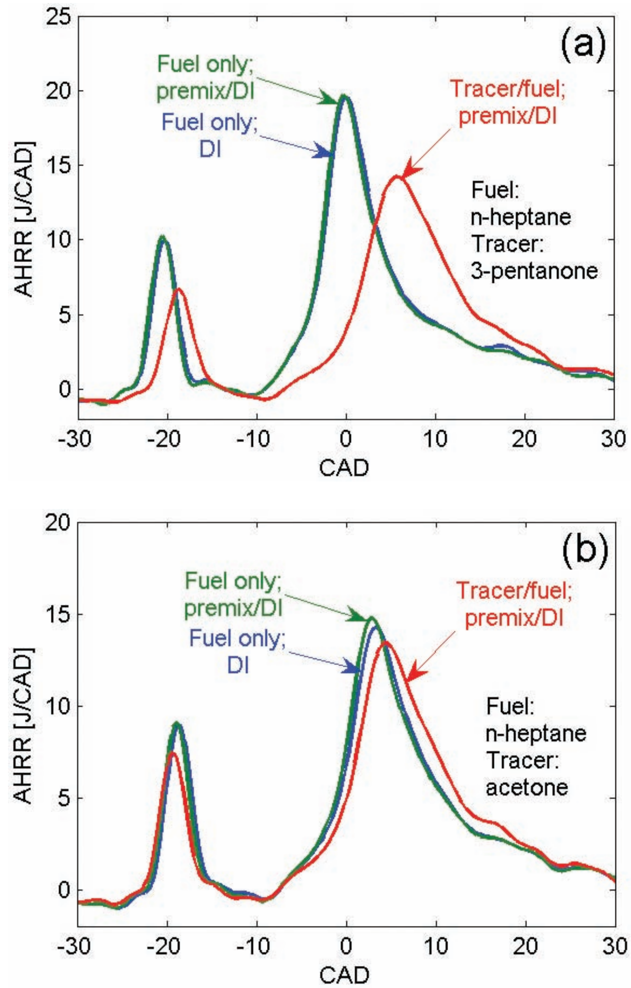

FIGURE 6. The effect of tracers on the AHRR of n-heptane fuel. **(a):** 3-pentanone tracer; **(b):** acetone tracer. To run continuously, the tracer/fuel case in (b) required a 5°C-hotter intake temperature.

that we could compensate for these tracer effects through appropriate adjustments of intake air temperatures.

Conclusions

- Operation of our automotive HCCI optical engine has been expanded to include the NVO-HCCI strategy for low loads, and a useful range of operating conditions has been mapped. An operating procedure has been developed to quickly attain steady operating conditions and enable optical measurements.
- Continued development and application of Stanford's two-wavelength PLIF diagnostic has produced viable in-cylinder measurements of temperature and composition during fired operation. In addition to air-seeded EGR measurements, the fuel-seeded LIF technique was used to obtain measurements during the difficult NVO period. Spatially averaged temperatures obtained with the diagnostic will be useful for validating models of our HCCI engine.
- We began development of a laser-absorption diagnostic for providing further details of the NVO reformation process. Bench-top experiments demonstrated the capability of measuring CO using a multi-pass beam arrangement that could provide spatially averaged concentration measurements during NVO re-expansion.
- The effects of LIF tracer addition on engine combustion were quantified. The tracer 3-pentanone was shown to advance iso-octane, and retard n-heptane, combustion. The effect of acetone was to uniformly retard iso-octane and n-heptane fuels. A CHEMKIN model using LLNL reaction mechanisms correctly predicted these trends and assisted interpretation.

FY 2008 Publications/Presentations

1. Steeper, R.R., "Automotive HCCI Engine Research," Proc. of DOE Advanced Engine Combustion and Fuels Program Review, DOE/OFCVT Annual Report, 2007.

2. Hessel, R.P., Foster, D.E., Aceves, S.M., Flowers, D.L., Pitz, W., and Steeper, R.R., "Pathline Analysis of Full-cycle Four-stroke HCCI Engine Combustion Using CFD and Multi-zone Modeling," SAE Paper 2008-01-0048, 2008.

3. Rothamer, D.A., Snyder, J., Hanson, R.K., and Steeper, R.R., "Two-Wavelength PLIF Diagnostic for Temperature and Composition," SAE Paper 2008-01-1067, 2008.

4. Fitzgerald, R.P., Steeper, R.R., and Snyder, J., "Effects of LIF Tracers on Combustion in a DI HCCI Engine," SAE Paper 2008-01-2407, 2008.

5. Rothamer, D.A., Snyder, J.A., Hanson, R.K., Steeper, R.R., and Fitzgerald, R.P., "Simultaneous Imaging of Exhaust Gas Residuals and Temperature During HCCI Combustion," Proceedings of the Combustion Institute, doi:10.1016/j.proci.2008.07.018, 2009.

6. Steeper, R.R., "Simultaneous PLIF Temperature/Composition Measurements in an HCCI Engine," DOE AEC Working Group Meeting, USCAR, Detroit, October 2, 2007.

7. Rothamer, D.A., "Optimized Two-Line Tracer PLIF Measurements of Temperature and Composition in an IC Engine," Fall Meeting of the Western States Section of the Combustion Institute, Sandia, October 17, 2007.

8. Steeper, R.R., "Simulation of the Effect of Spatial Fuel Distribution Using a Linear-Eddy Model," SAE Powertrain and Fluid Systems Conference, Chicago, October 31, 2007.

9. Steeper, R.R., "Sandia Automotive HCCI Engine Research," DOE Advanced Combustion Engine Program Review, Bethesda, MD, February 25, 2008.

10. Fitzgerald, R.P., "Establishing NVO Operation in an Optical HCCI Engine," DOE Advanced Combustion Engine Working Group Meeting, Sandia, March 20, 2008.

11. Rothamer, D.A., "Two-Wavelength PLIF Diagnostic for Temperature and Composition," SAE 2008 World Congress, Detroit, April 16, 2008.

12. Rothamer, D.A., "Simultaneous Imaging of Exhaust Gas Residuals and Temperature During HCCI Combustion,". 32nd International Symposium on Combustion, Montreal, August 4, 2008.

13. Fitzgerald, R.P., "Effects of LIF Tracers on Combustion in a DI HCCI Engine," DOE Advanced Combustion Engine Working Group Meeting, Auburn Hills, MI, August 19, 2008.

II.A.10 Spark-Assisted HCCI Combustion

Robert M. Wagner (Primary Contact), K. Dean Edwards, C. Stuart Daw, Charles E.A. Finney
Oak Ridge National Laboratory
2360 Cherahala Boulevard
Knoxville, TN 37932

Keith Confer (Primary Contact), Matthew Foster
Delphi Automotive Systems
Auburn Hills, MI 48326

DOE Technology Development Manager: Gurpreet Singh

Objectives

- Improve understanding of dynamic combustion instability in SI-HCCI (spark-ignition assisted homogeneous charge compression ignition) transition.
- Make use of engine-based, dynamic combustion measurements to quantify effective global kinetic rates.
- Develop simplified cyclic combustion models for rapid simulation, diagnostics, and controls.

Accomplishments

- A low-order dynamic model has been developed to predict the complex cycle-to-cycle interactions of SI-HCCI which have been observed in experiments.
- A new combustion metric has been developed for use with feedback control to provide rapid characterization of the SI-HCCI combustion event.
- Delphi Automotive Systems has modified a four-cylinder gasoline engine with advanced powertrain components and controls for use in this activity. The engine is installed and operational at the Delphi Technical Center (Rochester, NY) with HCCI experiments underway.
- Patent issued to ORNL team on HCCI combustion mode transition control concepts (US 7,431,011).

Future Directions

- Continue to map HCCI and SI-HCCI regions of operation on multi-cylinder engine.
- Refine low-order combustion model with data from multi-cylinder engine experiments to facilitate the development of real-time predictive controls.
- Continue simulations of SI-to-HCCI transition to improve fundamental understanding of combustion modes and transitions. Simulations will be performed in-house as well as in collaboration with Lawrence Livermore National Laboratory.

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Introduction

An improvement in the fuel efficiency of gasoline engines is necessary to realize a significant reduction in U.S. energy usage. HCCI in internal combustion engines is of considerable interest because of the potential reductions in flame temperature and nitrogen oxide (NOx) emissions as well as potential fuel economy improvements resulting from un-throttled operation, faster heat release, and reduced heat transfer losses. Unfortunately for many transportation applications, HCCI may not be possible or practical under the full range of speed and load conditions. Thus, the most important technical developments needed to achieve wide-spread HCCI utilization are expansion of the operational range and the ability to switch between HCCI and traditional propagating flame (e.g., SI) combustion as power and speed change. Several recent publications and presentations have begun to address the control issues but have not focused on the fundamental nature of the transition dynamics associated with switching from SI to HCCI combustion. The development of both combustion-mode switching and stabilization technologies requires that the fundamental nature of the transition be well understood, especially in the context of realistic engine conditions.

Delphi Automotive Systems and ORNL have established a Cooperative Research and Development Agreement on the control of advanced mixed-mode combustion for gasoline engines. ORNL has extensive experience in the analysis, interpretation, and control of dynamic engine phenomena, and Delphi has extensive knowledge and experience in powertrain components and subsystems. The partnership of these knowledge bases is critical to overcoming the critical barriers associated with the realistic implementation of HCCI and enabling clean, efficient operation in the next generation of transportation engines.

Approach

Significant progress in expanding the usefulness of advanced combustion modes of operation in gasoline engines will require an improved understanding of the potential of control methods to stabilize the transition between SI and HCCI combustion modes as well as to stabilize intermediate hybrid (mixed-combustion) modes which exhibit characteristics and benefits of SI and HCCI combustion. This improved understanding will be used to develop control strategies for improved utilization of hybrid combustion modes as well as for the development of physical models which will be useful for linking global combustion characteristics with fuel chemistry.

A single-cylinder research engine was used in the preliminary phase of this activity to improve the fundamental understanding of SI-HCCI combustion dynamics. The engine was a 0.5-L single-cylinder AVL research engine with an 11.34:1 compression ratio. To achieve the transition from SI to HCCI combustion, this engine was fitted with a full-authority hydraulic variable valve actuation system which allowed high levels of exhaust gas to be retained in the cylinder through manipulation of the intake and exhaust valve events. All of these experiments were performed at stoichiometric fueling conditions and a range of speeds and loads.

The current phase of this activity is being performed using a multi-cylinder research engine developed by Delphi Automotive Systems and installed at the Delphi Technical Center in Rochester, New York. Specific tasks for the multi-cylinder effort include:

- Development and baseline of engine/management systems. The research platform under development is a 2.2-L four-cylinder engine equipped with direct-injection fuel delivery, production-realistic flexible valve train components, and an advanced high-speed controller.
- Mechanistic and physical modeling and control-algorithm development for improved understanding of physics governing mixed-mode operation and for real-time, multi-cylinder prediction and control.
- Conventional SI, mixed-mode, and HCCI steady-state experiments to explore the operational range and potential benefits of mixed-mode operation.
- HCCI and SI transient experiments which will include maneuvering within the HCCI envelope as well as mode switching between SI, mixed-mode, and HCCI operation.

Results

In our research, the transition between conventional SI and HCCI operation is achieved with high levels of exhaust gas retained in the cylinder through manipulation of the intake and exhaust valve events. Unfortunately, this results in a strong coupling between successive cycles with small variations in the thermal and chemical composition of the retained exhaust gas leading to large variations in the combustion process. Recent results from our research have shown that, due to this highly variable combustion, the SI-HCCI mode transition is very unstable with high torque variations, high unburned hydrocarbon emissions, and potential engine stall. Figure 1 illustrates the trend in engine stability and engine-out NOx emissions during the transition from SI to HCCI operation as well as four distinct modes of operation observed. This discussion will focus on observations from the transition region where combustion instability is highest but NOx emission levels are near HCCI levels. Appropriate application of control to limit variability in the transition region could not only smooth the SI-HCCI transition but also extend the window of steady-state operation with HCCI-like NOx emission levels.

We have developed a conceptual model to explain the dynamics of the SI-HCCI transition based on experimental observations. When dilution levels due to the trapped exhaust gas are low, combustion occurs as a conventional spark-ignited, propagating flame. As dilution level increases, flame speed and combustion efficiency decrease. At very high dilution levels, a propagating flame cannot be sustained; however, heat from compression and the residual gas is sufficient to auto-ignite the fuel, resulting in HCCI combustion. At

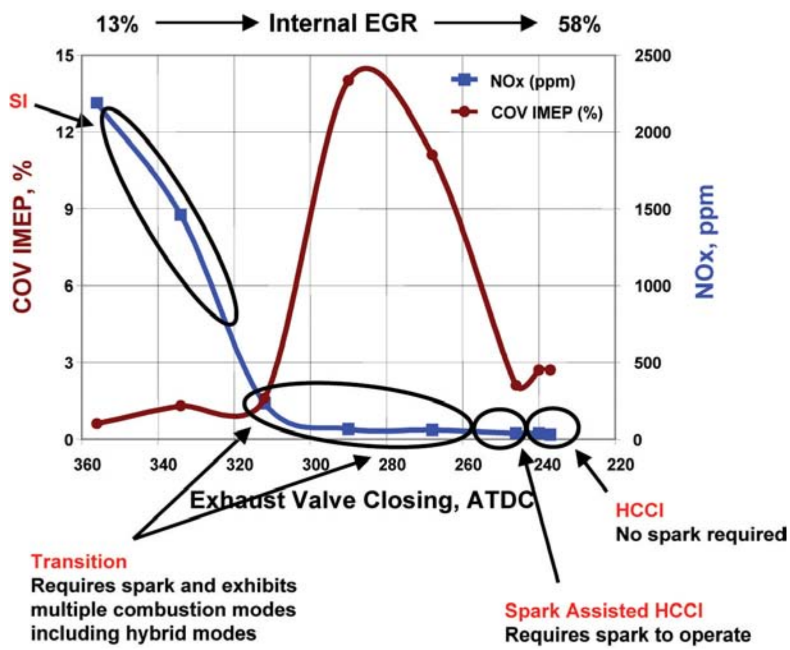

FIGURE 1. General combustion trends observed in the SI-HCCI transition experiments for 1,600 rpm, 3.4 bar BMEP. Internal EGR referenced in the figure was estimated using a full engine simulation code.

intermediate dilution levels, SI and HCCI combustion modes compete with one another and often occur together in the same cycle in what we refer to as spark-assisted HCCI. We hypothesize that competition between the two combustion modes is driven by the presence or absence of sufficient concentration of some intermediate fuel species that accumulates in the cylinder through exhaust recirculation and acts as an enabler for HCCI combustion (with charge temperature and stratification also playing important roles). The high levels of combustion variability observed at intermediate exhaust gas recirculation (EGR) levels results from changes in the relative strength of the two competing combustion modes as the in-cylinder conditions vary due to feedback from the previous cycle. SI-HCCI combustion becomes unstable when one of the two modes becomes dominant and is most stable when the strengths of the two modes are relatively balanced (suggesting that this would be an appropriate target for control).

Based on this conceptual understanding of the combustion dynamics, we have developed a low-order model to predict cycle-resolved combustion dynamics during the SI-HCCI transition. The model combines a diluent-limited laminar flame speed model for SI combustion and an HCCI model which accounts for temperature and residual-gas composition with a set of rules governing the competition between the two modes.

The propagating-flame model is based on empirical correlations for laminar flame speed limited by diluent concentrations (i.e., burned gases in the residual). In the literature, flame-speed correlations have been developed by fitting data to a form dependent on temperature, pressure, and diluent fraction:

$$S_L(x) = S_L(x=0)\left(\frac{T}{T_*}\right)^{\alpha}\left(\frac{p}{p_*}\right)^{\beta}\left[1-ax^b\right]$$

where S_L is flame speed, T is temperature, p is pressure, * represents a reference condition, x is diluent fraction, and α, β, a and b are fitting coeffients. In our model, combustion follows a Wiebe form, which governs combustion efficiency for the cycle:

$$C = 1-\exp\left[-k(S_{L,x}/S_{L,0})^m\right]$$

where k and m are coefficients which can be determined from experimental data. Unburned fuel mass that is fed forward to the next combustion cycle via the residual gas is:

$$z(i+1) = (1-C)\cdot(1+z(i))\cdot R$$

where R is the nominal residual fraction and z is unburned fuel mass. All masses are balanced on the basis of stoichiometric fueling in the first iteration of model development.

The HCCI model is governed by residual-gas composition and temperature. During the compression stroke, temperature rise from compression and from residual gases can achieve some combustion under conducive conditions. During the power stroke, combustion occurs following a Wiebe form using empirically derived ignition timings:

$$C_2 = 1-\exp\left[-\log(1-w)/\xi^{n+1}\right]$$

where w is a mass-depletion parameter, n is a fitting parameter and ξ is a normalized burn rate. As reported by us and others previously, for certain fuels and conditions, ignition delay exhibits a negative temperature coefficient effect, with a non-monotonic dependence on temperature, as seen in Figure 2.

The mixed-mode model is a combination of the two separate models. During the compression stroke, both modes are viable depending on conditions (residual-gas composition). At a defined critical point (e.g., at or near top-dead center beginning the power stroke), conditions are evaluated. If HCCI dominates, then the propagating flame is quelled by the rapid global combustion; if conditions are not conducive to HCCI, then the flame propagates as conditions permit.

Figure 3 shows a conceptual diagram of the additive nature of the combustion modes. The actual mechanisms for the way the combustion modes interact, especially regarding for the chemical and thermal feedback from the residual gases, are not fully understood but will be the subject of modeling and experimental analysis. The upcoming data from the multi-cylinder engine will be needed to refine and calibrate the model to match the actual variations seen in experimental operation.

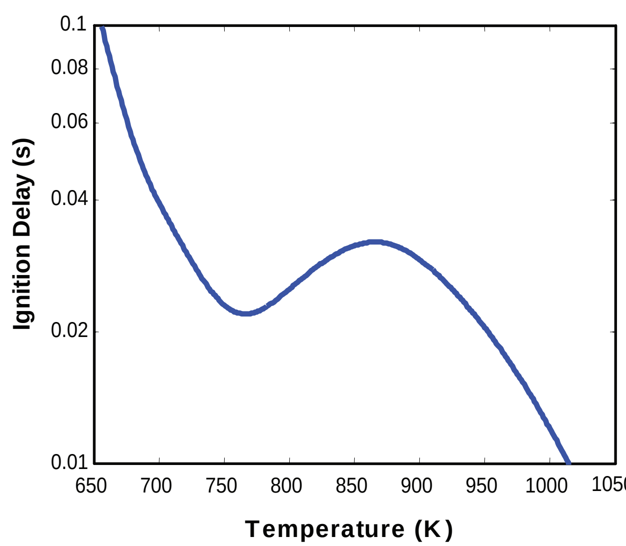

FIGURE 2. Variation of Ignition Delay with Temperature

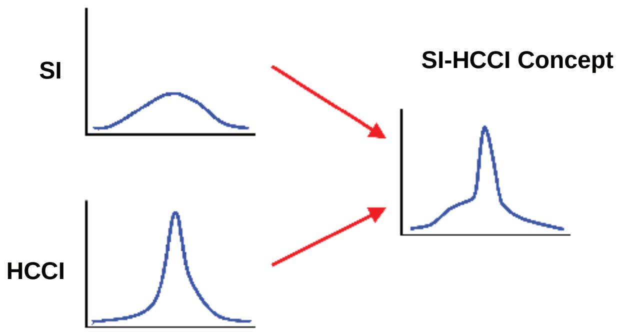

FIGURE 3. Conceptual diagram of the combining of two combustion rate profiles (SI, top left, and HCCI, bottom left) into a composite combustion mode (SI-HCCI, right).

Development of the multi-cylinder platform has begun at the Delphi Technical Center. One of the first tasks is designating the high-lift (for SI operation) and low-lift (for HCCI operation) cam profiles that will be used in 2-step valve-lift hardware. A study has been performed using the stock cams to determine the optimal cam phasing for SI operation over the speed/load range. A merit-function technique was used to compare (with appropriate weighting) several experimentally measured performance indicators (including brake specific fuel consumption [BSFC], coefficient of variation [COV] of brake mean effective pressure [BMEP], etc.) and determine optimal intake and exhaust cam phasings at each speed and load (see Figure 4). GT-Power simulations were used to identify a low-lift cam design which should allow HCCI operation. The stock cams have now been replaced

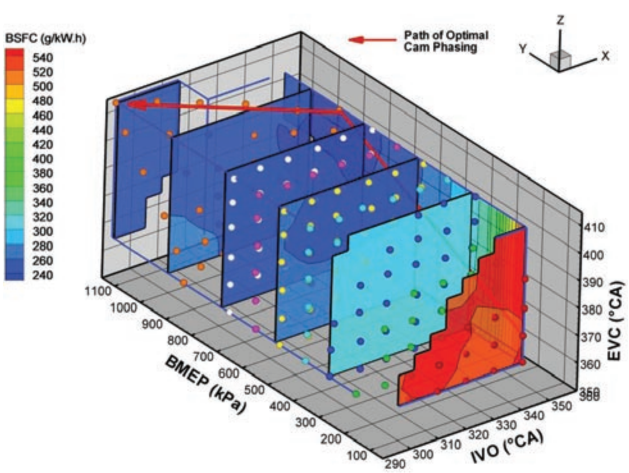

FIGURE 4. Sample results of the cam-phasing optimization study showing changes in BSFC with load and cam phasing at an engine speed of 2,000 rpm. The red trajectory indicates optimum phasing over a load transient. (IVO - intake valve opening; EVO - exhaust valve opening; CA - crank angle)

with these low-lift cams and experiments have begun to explore the HCCI operating regime.

Conclusions

The results of this study indicate that the combustion variability observed during SI- HCCI operation is driven by competition between SI and HCCI combustion modes. Stabilizing SI-HCCI operation relies on the ability to maintain a balance between these two modes. A low-order model has been developed which is capable of simulating the complex dynamics observed experimentally on a single-cylinder engine. The next phase of this activity involves adapting these concepts to a multi-cylinder engine for the development and implementation of adaptive control strategies.

FY 2008 Publications/Presentations

1. W.J. Glewen, R.M. Wagner, K.D. Edwards, C.S. Daw "Analysis of cyclic variability in spark-assisted HCCI combustion using a double Wiebe function". Proceedings of the 32nd International Symposium on Combustion (3–8 August 2008; Montreal, Canada).

2. C.S. Daw, K.D. Edwards, R.M. Wagner, J.B. Green Jr. (2008) "Modeling cyclic variability in spark-assisted HCCI". ASME Journal of Engineering for Gas Turbines and Power, 130(5), 052801.

3. W.J. Glewen, R.M. Wagner, K.D. Edwards, C.S. Daw (2008) "Analysis of cyclic variability in spark-assisted HCCI combustion using a double Wiebe function". 2008 Technical Meeting of the Central States Section of the Combustion Institute (20–22 April 2008; Tuscaloosa, AL, USA).

4. K.D. Edwards, R.M. Wagner, C.S. Daw, C.E.A. Finney, J.B. Green Jr., K. Confer (2008) "Ignition control for HCCI". US DOE Office of Vehicle Technologies 2008 Annual Merit Review (25–28 February 2008; Bethesda, MD, USA).

5. K.D. Edwards, C.S. Daw, R.M. Wagner, J.B. Green Jr., V.K. Chakravarthy, C.E.A. Finney (2008) "Modeling dynamical instability of homogeneous charge compression ignition (HCCI) in combustion engines". Dynamics Days 2008 (3–6 January 2008; Knoxville, TN, USA).

6. K.D. Edwards, C.S. Daw, R.M. Wagner, J.B. Green Jr., W.J. Glewen (2007) "Understanding the dynamics of spark-assisted HCCI combustion". 2007 American-Japanese Flame Research Committees' International Symposium (22–24 October 2007; Waikoloa, HI, USA).

7. C.S. Daw, K.D. Edwards, R.M. Wagner, J.B. Green Jr. (2007) "Modeling cyclic variability in spark-assisted HCCI". ASME ICEF2007-1685.

Special Recognitions & Awards/Patents Issued

1. US Patent 7,431,011. "A method for diagnosing and controlling combustion instabilities in internal combustion engines operating in or transitioning to homogeneous charge compression ignition modes".

2. Activity was recognized as 2008 DOE FreedomCAR and Fuel Partnership technical highlight “A Predictive Model has been Developed for the Practical Implementation of HCCI Combustion”.

II.A.11 KIVA-4 Development

David J. Torres (Primary Contact) and
David Carrington
Los Alamos National Laboratory (LANL)
Theoretical Division, Group T-3, MS B216
Los Alamos, NM 87545

DOE Technology Development Manager:
Gurpreet Singh

Subcontractor:
Iowa State University, Ames, IA

Objectives

- Implement and perform parallel LES (large eddy simulation) turbulence simulations in KIVA-4.
- Implement and perform parallel KIVA-4 multi-zone simulations.
- Test KIVA-4's implementation of the University of Wisconsin's Engine Research Center (UW-ERC) combustion and spray models in KIVA-4.
- Compare KIVA-4 simulations against experimental engine data.
- Perform calculations of soot distribution with KIVA-4 and compare data with the experimental data of Pickett and Siebers [1].
- Implement and perform parallel partitioning strategies in KIVA-4.

Accomplishments

- A parallel LES implementation of KIVA-4 was completed. Calculations were performed which compared the LES model against the k-epsilon model in a vertical valve engine.
- A parallel multi-zone model in KIVA-4 was implemented. Calculations were performed and results compared very well with Lawrence Livermore National Laboratory's (LLNL) multi-zone KIVA-3 model in a 3-dimensional (3-D) sector mesh.
- The UW-ERC chemistry and spray submodels were tested in a constant volume 3-D geometry. Results compared very well with UW-ERC's code.
- Pressure histories of KIVA-4, KIVA-3V and experimental data were compared in a Caterpillar 3401 engine running at different loads and injection timings.
- Soot calculations were performed with KIVA-4 in a constant volume chamber and compared against Pickett and Siebers' experimental data [1].
- Partitioning strategies were implemented and tested in four different engine geometries. A paper was submitted to Computers and Fluids.

Future Directions

- Enable KIVA-4 to run with a cut-cell grid which will improve the numerical accuracy in the interior of the mesh and resolve rezoning issues.
- Develop a software package to produce a cut-cell grid from a stereolithographic surface.
- Perform parallel 3-D calculations with the KIVA-4 multi-zone method.
- Perform calculations with the grid overset method in complex geometries.

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Introduction

KIVA-4 is a 3-D parallel code capable of simulating engine combustion, spray and turbulence in unstructured meshes. As engine meshes become more resolved and computational power increases, LES models become increasingly used to simulate engines. A LES turbulence model was implemented in KIVA-4 to allow the code to take advantage of the benefits an LES model has to offer. In contrast to RANS (Reynolds Averaged Navier-Stokes) turbulence models, LES models approximate only the smaller length scales of turbulence. RANS models such as the k-epsilon model approximate all turbulent length scales. While LES calculations require more resolved grids than RANS models, LES models tend to capture more of the smaller scales and are less diffusive compared to RANS models. We implemented the two-equation LES model of Sone and Menon [2] into KIVA-4 and performed parallel computations with the code comparing the fuel distribution with the k-epsilon model in a vertical valve engine.

LLNL has invested a great deal of time in developing their multi-zone chemistry model which can dramatically reduce computational time when performing engine calculations with combustion. Los Alamos collaborated with LLNL and implemented their multi-zone model in KIVA-4, thus enabling KIVA-4 to perform combustion calculations more efficiently. The multi-zone model does not solve the chemistry in every cell but rather divides up the cells into temperature and equivalence ratio zones. The chemistry is solved within each zone and the information is mapped back into the individual cells. Since the chemistry is the most expensive component of an engine calculation, solving the chemistry in a reduced set of zones reduces the computational time significantly. KIVA-4 multi-zone results were compared with LLNL's results in a 3-D sector mesh. The two codes results generated very similar results which were visually identical.

The UW-ERC submodels for combustion and spray have undergone extensive testing. UW-ERC combustion models include mixing controlled models and ignition models which versions of KIVA-3V had not incorporated. Previous KIVA-4 development activities integrated these existing models into KIVA-4. Recently efforts were devoted to testing these models in KIVA-4. Soot and NOx distribution was compared in KIVA-4 and KIVA-3 ERC in a constant volume chamber. Iowa State performed numerical simulations and experimental tests and compared KIVA-4 pressure traces in a Caterpillar 3401 engine for different loads and for single and double injections. Iowa State also performed simulations studying soot distribution in a combusting constant volume chamber and compared their results with the experimental results of Pickett and Siebers [1].

Parallel computations in a static grid are relatively straightforward. One divides up or partitions the grid among available processors once and computes with this initial partitioning for the entire simulation. Processors should be given approximately the same number of cells to ensure the computational load is balanced equally. In addition, the partitioning should minimize the amount of data that needs to be passed between processors.

Engine calculations pose a more difficult challenge if portions of the mesh become deactivated or activated during the course of the simulation. For example, when the piston ascends, layers of cells become deactivated and when the piston descends these layers of cells become reactivated. Similarly entire ports can become activated.

Considerable time was spent in developing partitioning strategies for engine meshes to accommodate an engine's moving surfaces. In the first strategy, the entire mesh was partitioned once using a vertical partitioning. In the second strategy, the bowl, squish and ports regions were partitioned separately. In the third strategy, the entire mesh was periodically repartitioned during the course of the simulation to effect load-balance. These strategies were tested on four different 3-D engine meshes.

Approach

We have focused our efforts on continued development of KIVA-4. Our approach is to develop KIVA-4 in areas that are most essential and will have the greatest impact. We believe that KIVA-4 will continue to be adopted more readily and have more applicability if it is complemented with an additional parallel turbulence LES model, a multi-zone combustion capability, the capability to run with tested UW-ERC models and an effective way to partition the mesh for parallel computations.

Results

The LES KIVA-4 model was compared with the RANS k-epsilon model. Figure 1 shows the fuel distribution using a k-epsilon RANS model and Figure 2 shows the fuel distribution using the implemented LES model. Both calculations were performed in parallel with four processors using an unstructured vertical valve engine mesh. The grid contains 128,000 cells at bottom dead center. Fuel is convected into the cylinder region

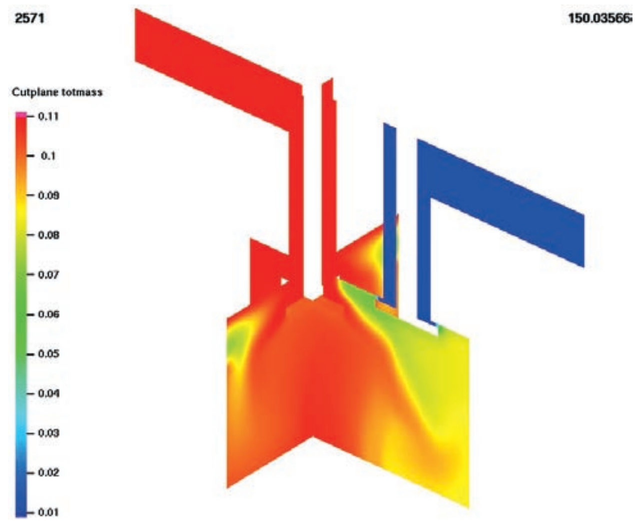

FIGURE 1. Fuel Concentration at 150 Crank Angle Degrees after Top-Dead Center using the K-Epsilon Model

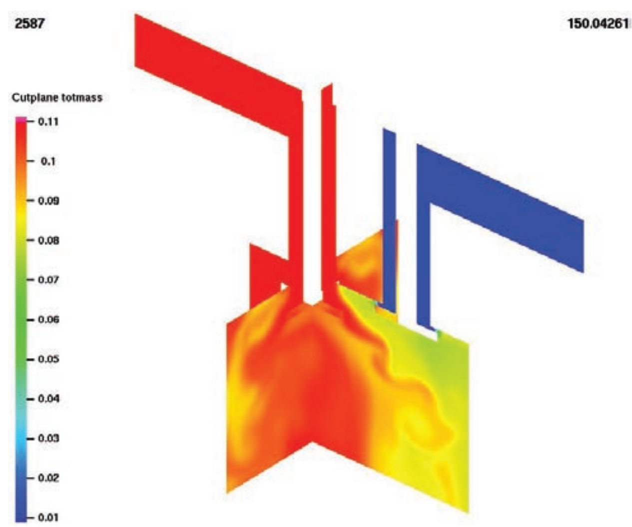

FIGURE 2. Fuel Concentration at 150 Crank Angle Degrees after Top-Dead Center using the LES model

using a pressure gradient. The LES simulation captures more of the finer length scales compared to k-epsilon at 150 crank angle degrees after top dead center.

Figure 3 shows a comparison of the multi-zone KIVA-4 model against Lawrence Livermore's multi-zone KIVA-3V model using a 3D sector mesh. The pressure and temperature history of both codes compare very well. Thus KIVA-4 is capable of performing parallel combustion calculations using the multi-zone model.

Figure 4 shows a comparison of KIVA-4 ERC implementation against the UW's KIVA-3V ERC model. In these simulations, n-tetradecane was injected into a constant volume chamber. Soot and NOx creation compare very well in both models. We are currently reconciling emissions from both codes in moving geometries.

Figure 5 shows a comparison of KIVA-4 (green K4ERC line), KIVA-3 (red K3r2 line) and experimental data (black Expt line) in a Caterpillar 3401 engine for a high-load single-injection case. Both codes match the experimental pressure trace reasonably well. Different load and injection cases were also performed experimentally and computationally and compared.

Table 1 shows a comparison of two different parallel partitioning strategies when running a four-valve diesel mesh (135,158 cells at bottom dead center) using 1,2,4,8 and 16 processors. The computational time as well as the speed-up (how much faster the parallel computation runs compared to the single-processor computation) are listed for both strategies. Table 1 shows that the second strategy improves the parallel performance for 8 and 16 processors. This trend was also seen in another relatively large vertical valve mesh (128,000 cells at bottom dead center). For smaller meshes, the first strategy proved to be an effective strategy. The first

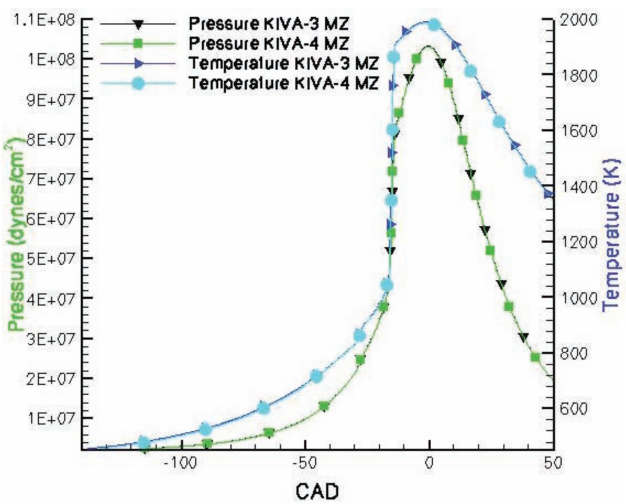

FIGURE 3. Comparison of KIVA-4 Multi-Zone Model with LLNL KIVA-3V Multi-Zone Model

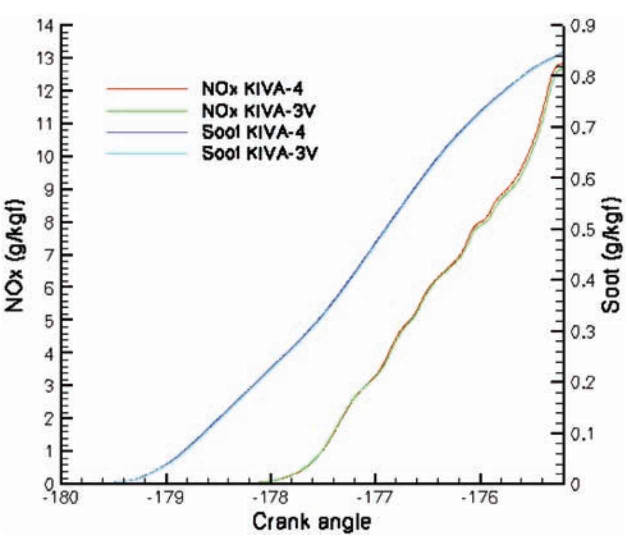

FIGURE 4. Soot and NOx Comparison using KIVA-4 ERC Model and UW-ERC KIVA-3V Model

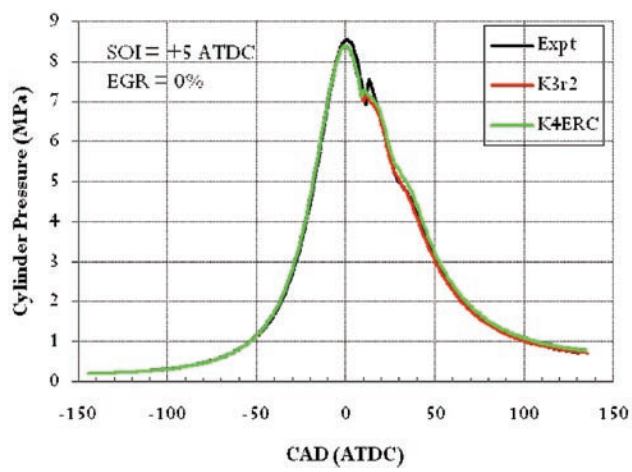

FIGURE 5. KIVA-4, KIVA-3V and Experimental Pressure History Comparison in a 3401 Caterpillar Engine

TABLE 1. Computational Time and Speed-Up for Two Different Partitioning Strategies in a Four-Valve Diesel Mesh

Number of processors	Time Strategy 1	Speed-up Strategy 1	Time Strategy 2	Speed-up Strategy 2
1	23.6 hours	1.0	23.6 hours	1.0
2	12.4 hours	1.9	12.7 hours	1.86
4	7.5 hours	3.1	7.5 hours	3.1
8	5.3 hours	4.5	4.85 hours	4.9
16	3.7 hours	6.4	3.5 hours	6.7

strategy partitions the entire mesh simultaneously. The second strategy partitions the bowl and port regions separately from the squish region of the engine. A third partitioning strategy which periodically repartitions the mesh using a shell script was also tested in a 3-valve geometry and demonstrated small improvements in parallel performance. Partitioning was done by developing codes which used METIS (a free partitioning software package).

Conclusions

Much progress was made this year in developing KIVA-4. An LES model was implemented in KIVA-4 and compared against the traditional k-epsilon model in a 3-D vertical valve geometry. A collaborative effort between Los Alamos National Laboratory and LLNL resulted in a multi-zone KIVA-4 model. This model was compared against LLNL's multi-zone model in a 3-D sector geometry. The UW-ERC models were tested in KIVA-4 in a constant volume cylindrical chamber. Results matched well with the UW-ERC KIVA-3V simulations. Iowa State made comparisons with KIVA-4 against experimental data in a Caterpillar 3401 engine and soot comparisons of KIVA-4 against experimental data in a constant volume combustion chamber. Three different partitioning strategies were implemented. These strategies were tested in four 3-D engine geometries. Specific results were documented in a paper submitted to Computers and Fluids.

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FY 2008 Publications

1. D.J. Torres, Y.H. Li and S.C. Kong, Partitioning Strategies for Parallel KIVA-4 Engine Simulations, submitted to Computers and Fluids.

2. Li, Y., S.C. Kong and D.J. Torres, Parallel KIVA-4 in Realistic Geometries, International Multidimensional Engine Modeling Group Meeting Proceedings, April 2008.

FY 2008 Presentations

1. D.J. Torres, "Partitioning Strategies for Parallel KIVA-4," Advanced Engine Combustion Working Group Meeting, Detroit, August 2008.

2. Y. Li, "Parallel KIVA-4 in Realistic Geometries," International Multidimensional Engine Modeling Group Meeting, Detroit, April 2008.

3. D.J. Torres, "KIVA-4 Development," Advanced Engine Combustion Working Group Meeting, Livermore, CA, March 2008.

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II.A.12 Chemical Kinetic Models for HCCI and Diesel Combustion

William J. Pitz (Primary Contact),
Charles K. Westbrook, Marco Mehl
Lawrence Livermore National Laboratory (LLNL)
P. O. Box 808, L-372
Livermore, CA 94551

DOE Technology Development Manager:
Gurpreet Singh

Objectives

- Develop detailed chemical kinetic models for fuel components used in surrogate fuels for diesel and homogeneous charge compression ignition (HCCI) engines.
- Develop surrogate fuel models to represent real fuels and model low-temperature combustion strategies in HCCI and diesel engines that lead to low emissions and high efficiency.
- Characterize the role of fuel composition on low-temperature combustion modes of advanced combustion engines.

Accomplishments

- Validated a low- and high-temperature mechanism for normal alkanes from C8 to C16, including n-hexadecane, a primary reference fuel for diesel engines.
- Further validated a detailed chemical kinetic mechanism for a large biodiesel surrogate.
- Developed a reduced mechanism for a large biodiesel surrogate for use in computational fluid dynamics (CFD) codes.

Future Directions

Develop and validate a detailed chemical kinetic mechanism for heptamethylnonane, a primary reference fuel for diesel engines.

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Introduction

Hydrocarbon fuels for advanced combustion engines consist of complex mixtures of hundreds or even thousands of different components. These components can be grouped into a number of chemically distinct classes, consisting of n-paraffins, branched paraffins, cyclic paraffins, olefins, oxygenates, and aromatics. Biodiesel contains its own unique chemical class called methyl esters. The fractional amounts of these chemical classes are quite different in gasoline, diesel fuel, oil-sand derived fuels and bio-derived fuels, which contributes to the very different combustion characteristics of each of these types of combustion systems.

Approach

To support large-scale computer simulations of each kind of engine, it is necessary to provide reliable chemical kinetic models for each of these chemical classes in fuels. However, few specific hydrocarbon components of some of these fuel classes have been modeled. For example, models for benzene and toluene have been developed, although models for few if any larger aromatic compounds such as naphthalene or styrene currently exist. Similarly, detailed models for small iso-paraffins such as iso-octane have been developed, but detailed models do not yet exist for the much larger versions such as heptamethylnonane, characteristic of diesel fuels. Biodiesel is composed of large methyl esters, but few detailed chemical kinetic models of these components have been developed. Current approaches to this problem are to construct a detailed model, containing one or more representatives of each class of components to serve as a surrogate mixture. In order for such a surrogate mixture model to be useful, each component must have a well-tested detailed kinetic model that can be included. This high-level approach can create realistic substitutes for gasoline or diesel fuel that reproduce experimental behavior of the practical real fuels. Detailed kinetic models for surrogate fuels can then be simplified as needed for inclusion in multidimensional CFD models or used in full detail for purely kinetic modeling.

Results

There is a need to extend chemical kinetic models to address large alkanes because they are recommended as surrogate components for diesel fuel and one particular recommended component is n-hexadecane [1]. Recently, the LLNL chemical kinetics team developed a chemical kinetic model for all n-alkanes from n-octane to n-hexadecane [2]. This model allows the simulation of both low- and high-temperature chemistry of these n-alkanes. The inclusion of low-temperature chemistry in the model is important for simulation of new modes of combustion in engines such as HCCI, premixed charge compression ignition, and smokeless rich combustion. This year, the LLNL kinetics team validated their new model for C8 to C16 n-alkanes and published it in one of the most recognized combustion journals, Combustion and Flame [2]. Figures 1 and 2 show some examples of the mechanism validation by comparison of computed results with experimentally measured results. Figure 1 compares predictions from the LLNL detailed chemical kinetic model and measurements [3] of intermediate species in a stirred reactor when n-hexadecane is the fuel. The agreement between the predicted and measured intermediate species concentrations is good. Figure 2 shows a comparison of predictions of the model with experiments when n-decane is the fuel component. The experiments were performed at engine-like conditions of 80 bar and at temperatures from 800 to 1,100 K, including the negative temperature coefficient region [4]. Predictions of n-decane ignition compared well with experimental measurements (Figure 2). The comparison covers the full low- to high-temperature chemistry regime which is important for low-temperature combustion strategies in diesel combustion. Finally to assess the ignition behavior for all n-alkanes, the ignition of C8 to C16 alkanes were computed over the low- to high-temperature range at 13 bar, a pressure relevant to an internal combustion engine (Figure 3). The calculations show that all the large n-alkanes exhibit nearly the same ignition behavior. Therefore, a small n-alkane like n-octane can be used to represent the ignition behavior of a much larger n-alkane like n-hexadecane. Using n-octane to represent the ignition of n-hexadecane has the advantage of allowing the use of a much smaller chemical kinetic model requiring less computer resources. Finally, the development of a chemical kinetic model for all n-alkanes up to n-hexadecane allows a broad choice of surrogate fuel components in the n-alkane chemical class for use in surrogate fuel models for diesel fuel. For example, a broad range of n-alkanes is needed to model the distillation characteristics of the diesel fuel and properly simulate the diesel spray volatility in the engine.

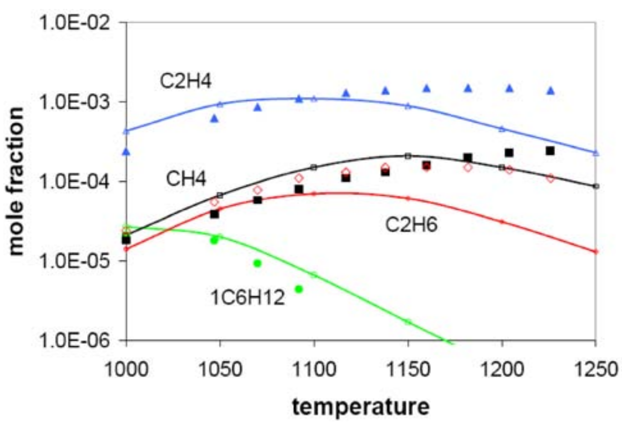

FIGURE 1. Comparison between computed and experimental [3] results for intermediate species in n-hexadecane oxidation in a jet stirred reactor. Conditions are equivalence ratio = 1.5, 1 atm pressure, and 0.07 s residence time.

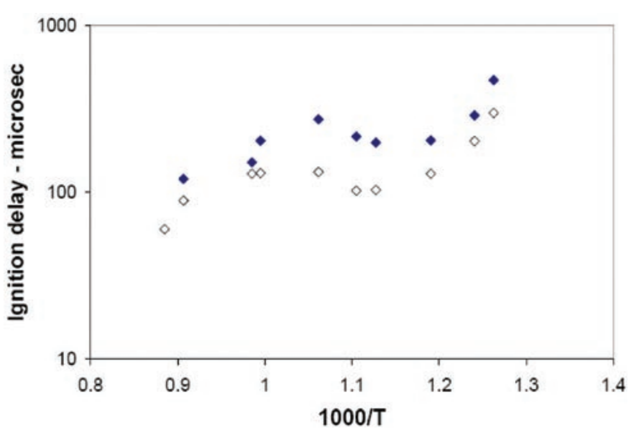

FIGURE 2. Computed and experimental ignition delay times for stoichiometric, n-decane/air at 80 atm pressure versus inverse temperature [K^{-1}]. Experiments (◊) from Zhukov et al.[4], present model (♦).

In Fiscal Year 2008, we further validated our detailed chemical kinetic model for a biodiesel surrogate. We use methyl decanoate, a large methyl ester, to represent biodiesel. Since there is not a lot of experimental data available on methyl decanoate, we compare the computed ignition behavior of methyl decanoate with experiments on n-decane [5], a similarly sized n-alkane (Figure 4). As can be seen, the ignition times of methyl decanoate nearly match those of n-decane. We found that the ignition behavior of methyl decanoate matches n-decane for a variety of shock tube experiments and for flame speed. This point is further illustrated in the Combustion and Flame paper that we composed and published on methyl decanoate during the last year [6].

It is important to reduce large chemical kinetic models so that they can be used effectively in multidimensional reacting flow simulations. During the last year, we reduced our large chemical kinetic mechanism for a biodiesel surrogate so that it could be used in a reacting flow code. The work allowed us

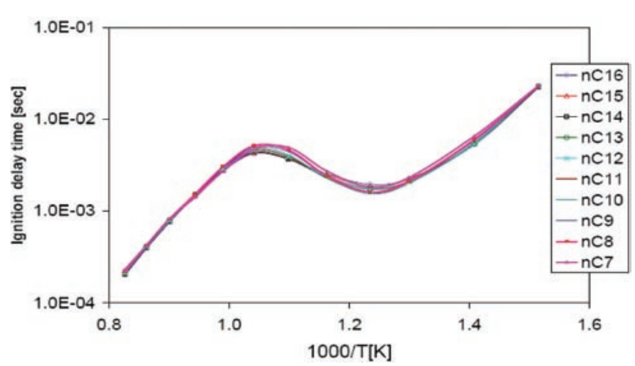

FIGURE 3. Computed ignition delay times for stoichiometric mixtures of n-alkanes in air at 13.5 bar [2].

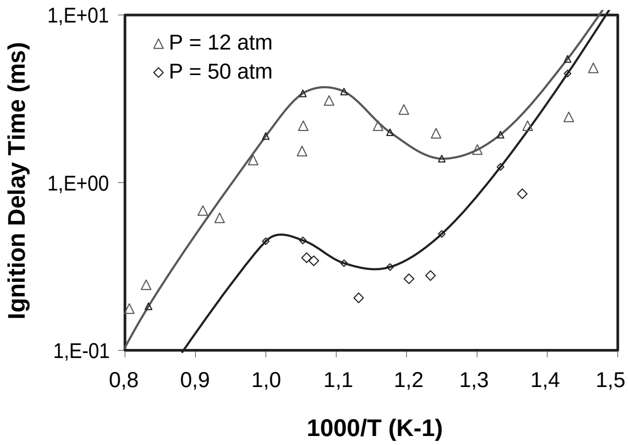

FIGURE 4. Comparison of fuel reactivity under shock tube conditions in stoichiometric fuel/air mixtures. Lines – methyl decanoate model predictions. Open symbols – n-decane experimental data [5].

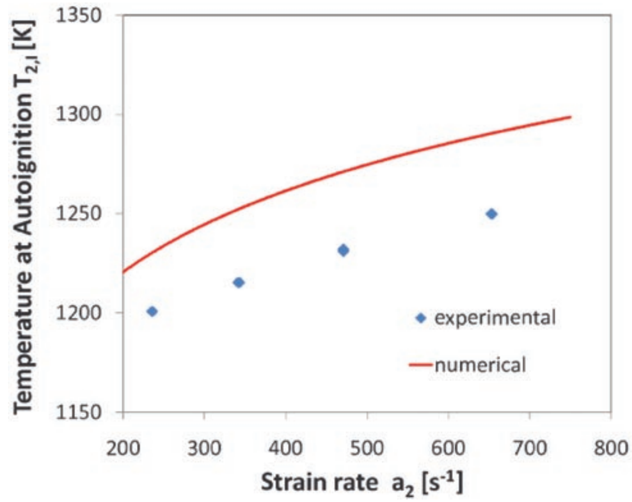

FIGURE 5. The measured and predicted temperature for autoignition in a counterflow flame [11]. The air flow is heated up slowly until ignition occurs. The strain rate increases with the velocity of the air flow.

to test a new method for mechanism reduction called the directed relational graph (DRG) method [7]. This method is a graphical technique that analyses the reaction paths in the mechanism and removes paths that do not affect the concentration of important species of interest. The DRG method reduced the detailed mechanism of methyl decanoate from 3,036 species and 8,555 reactions down to 125 species and 713 reactions. The number of species was reduced by a factor of 5, a dramatic reduction. Since a conservation equation must be solved for each species considered in a reacting flow code, reducing the number of species greatly shortens code execution times. To validate the reduced mechanism, we employed a counterflow flame configuration which consists of fuel and air flowing in opposite directions, towards each other. When ignition occurs, a flame develops near the stagnation plane formed by the two flows. The flame configuration has relevance to diesel engines because the fuel and air are initially separate in this flame just as it is the case in a conventional diesel engine. Also, the counter-flow flame includes the effect of fluid dynamic strain, an effect also found in diesel engine flows. To compute this flame, a 1-dimensional reacting flow code that computes fluid flow, transport of heat and species, and chemical reactions is required [8]. Figure 5 shows good agreement between experimentally measured and computed ignition temperatures in the counter flow flame. This work will be published in the Proceedings of the Combustion Institute [9].

Conclusions

- A chemical kinetic model for C8-C16 n-alkanes was validated for low- and high-temperature chemistry regimes. This model is available to represent n-alkanes in diesel fuel [10].
- The detailed chemical kinetic mechanism for methyl decanoate was further validated. The chemical kinetic model is available [10].
- A reduced chemical kinetic mechanism for biodiesel surrogate was developed and validated for use in a reacting flow code.

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Special Recognitions & Awards/Patents Issued

1. Charles K. Westbrook: 2008 Bernard Lewis Gold Medal awarded by the Combustion Institute.

2. Charles K. Westbrook: 2008 - 2012 President of the Combustion Institute.

3. William J. Pitz: Invited Plenary Lecture at the 2008 International Conference on Modeling and Diagnostics for Advance Engine Systems (2008 COMODIA), Sapporo, Japan.

II.A.13 Achieving and Demonstrating FreedomCAR Engine Efficiency Goals

Robert M. Wagner (Primary Contact),
K. Dean Edwards, Thomas E. Briggs, Jr.
Oak Ridge National Laboratory (ORNL)
2360 Cherahala Boulevard
Knoxville, TN 37932

DOE Technology Development Manager:
Gurpreet Singh

Objectives

- Demonstrate Fiscal Year 2008 DOE FreedomCAR milestones of 43% peak brake thermal efficiency (BTE) and 27% part-load BTE on a light-duty diesel engine.
- Perform component-by-component evaluation of thermodynamic availability on a light-duty diesel engine to characterize thermal energy recovery (TER) potential for meeting FY 2010 milestones.
- Develop and evaluate feasibility of an organic Rankine cycle for TER through analysis, modeling, and bench-scale experiments.
- Estimate potential benefits of and identify issues associated with TER for improving fuel economy over the Federal Test Procedure (FTP) drive cycle.

Accomplishments

- Demonstrated 2008 FreedomCAR milestones of 43% peak BTE and 27% part-load BTE on a light-duty diesel engine.
- Characterized the thermodynamic availability of engine systems (*e.g.*, exhaust system, exhaust gas recirculation [EGR], etc.) across the speed-load operational range of a light-duty diesel engine and estimated potential fuel economy improvements over FTP drive cycle.
- Developed TER model of an organic Rankine cycle and constructed bench-scale system which will be transitioned to engine in early FY 2009.
- Developed well-defined path to meeting FY 2010 efficiency and emissions milestones.

Future Directions

- Continue component development of TER system and evaluate on the exhaust system of a light-duty diesel engine.
- Evaluate prototype turbo-compounding system being developed and supplied to ORNL by Woodward Governor.
- Explore low-temperature combustion approaches in combination with appropriate aftertreatment systems for improving overall system efficiency while meeting FY 2010 emissions targets.
- Develop vehicle systems model with integrated transient capable TER model using GT-Drive and/or PSAT to estimate the potential benefits of and manage implementation issues associated with TER on light-duty vehicle applications.

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Introduction

Modern light-duty diesel engines have peak BTEs in the range 40-42% for high-load operation and lower efficiencies for part-load operation. The FreedomCAR roadmap has established efficiency and emissions goals for the next several years with a 45% peak efficiency being demonstrated in 2010, while meeting the Tier 2 Bin 5 emissions levels. The objective of this project is not to develop all the necessary technology to meet the efficiency and emissions goals but to serve as a focus for the integration of technologies into a multi-cylinder engine platform and to provide a means of identifying pathways for improved engine efficiency.

Approach

This activity makes use of knowledge discovery from internal ORNL activities, other national laboratories, universities, and industry. Internal activities include those focused on advanced combustion operation, aftertreatment, fuels, and unconventional approaches to improve combustion efficiency. This activity also makes use of technical contributions from external sources through regular interactions with the Advanced Engine Combustion working group administered by Sandia National Laboratories, the Cross-Cut Lean Exhaust Emissions Reduction Simulations working group administered by ORNL, and one-on-one interactions with industry teams such as Cummins Engines, Caterpillar, BorgWarner, Woodward Governor, etc.

Substantial improvements in engine efficiency will require a reduction in thermal energy losses to the environment and a better understanding of thermodynamic loss mechanisms associated with the combustion process. With less than ½ of fuel energy converted to useful work in a modern engine, opportunity exists for significant advancements in engine efficiency. A fundamental thermodynamics perspective in combination with simulations and laboratory experiments is being used toward this purpose to provide guidance on developing and evaluating a path for meeting 2010 and intermediate milestones as well as longer term insight into the potential of future high efficiency engine-systems.

The following methodology is and has been used in this activity:

1. Characterize current state-of-the-art light-duty engine technology. Note that this is a moving target as more advanced engines enter the market place.
2. Improve fundamental understanding of internal combustion engine efficiency losses and opportunities.
3. Identify and evaluate promising strategies to recover and/or reduce thermodynamic losses to the environment through engine-system simulations and experiments.
4. Perform proof-of-principle demonstrations of selected concepts.

Technologies for improving efficiency and emissions in light-duty engines are being evaluated at ORNL on a General Motors (GM) 1.9-L common rail four-cylinder diesel engine. Earlier experiments were performed on a Mercedes-Benz (MB) 1.7-L common rail four-cylinder diesel engine. The engine platform was upgraded to reflect a change in the state-of-the-art in the market place. The GM engine is equipped with a microprocessor-based dSpace control system which permits unconstrained access to engine hardware including the integration of custom control algorithms. This engine also has an electronic control unit donated by GM which allows for the monitoring and manipulation of the base engine calibration.

Results

A peak BTE of 43% and a part-load BTE of 27% has been demonstrated on a GM 1.9-L diesel engine. These accomplishments are interim milestones on the path to 2010 FreedomCAR goals of 45% peak BTE with Tier 2 Bin 5 emissions. Advanced engine technologies identified and investigated in FY 2008 include thermal energy recovery, electrification of auxiliary components, advanced lubricants, and fuel properties. In addition, a flexible microprocessor-based control system was used for re-optimization of engine parameters to make better use of these technologies. Thermal energy recovery was not used to meet the FY 2008 milestone but significant progress has been made in developing this technology for light-duty applications, including modeling and on-engine experiments under conditions consistent with a light-duty vehicle drive cycle. Peak BTE milestones and demonstration status are shown in Figure 1 for FY 2005 to FY 2010.

As noted earlier, substantial improvements in engine efficiency will require a reduction in thermal energy losses to the environment and a better understanding of thermodynamic loss mechanisms associated with the combustion process. A thermodynamic Second Law perspective has been adapted to aid in the identification, assessment, and implementation of TER technologies. Noteworthy progress in FY 2008 includes (1) a component-by-component evaluation of the thermodynamic availability (or potential to do work) of a light-duty diesel engine based on experimental data and simulations, (2) an improved understanding of issues associated with vehicle implementation based on simulations and chassis dynamometer data, and (3) advancements in the design and on-engine implementation of TER systems. The continued development of this perspective and maturation of TER technologies is expected to have a major impact on vehicle efficiency and fuel usage of the transportation sector.

A significant amount of fuel energy is discarded to the environment and potentially available for recovery in internal combustion engines. An example of thermodynamic availability for the EGR and exhaust systems across the speed/load range of a GM 1.9-L engine is shown in Figure 2. Thermodynamic availability is shown in Figure 2 as a fraction of the input fuel availability to the system. While the most significant available energy occurs in the exhaust for high load/speed operation, a useful amount of energy is also available under low load/speed conditions. As an example, a condition of 1,500 rpm 2.0 bar brake mean effective pressure (BMEP) is considered representative of part-load (or road-load) operation on a light-duty vehicle. This condition corresponds to approximately 1.5% fuel energy available in the EGR system and 3.0% fuel energy available in the exhaust system. The estimated improvement in BTE across the speed/load range is shown in Figure 3 for three assumed TER

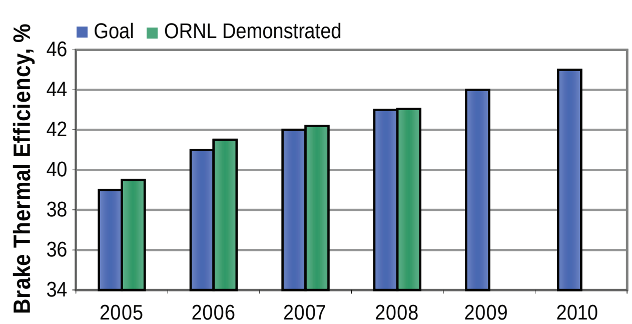

FIGURE 1. On path to demonstrating FY 2010 FreedomCAR engine and efficiency milestones including 45% peak BTE.

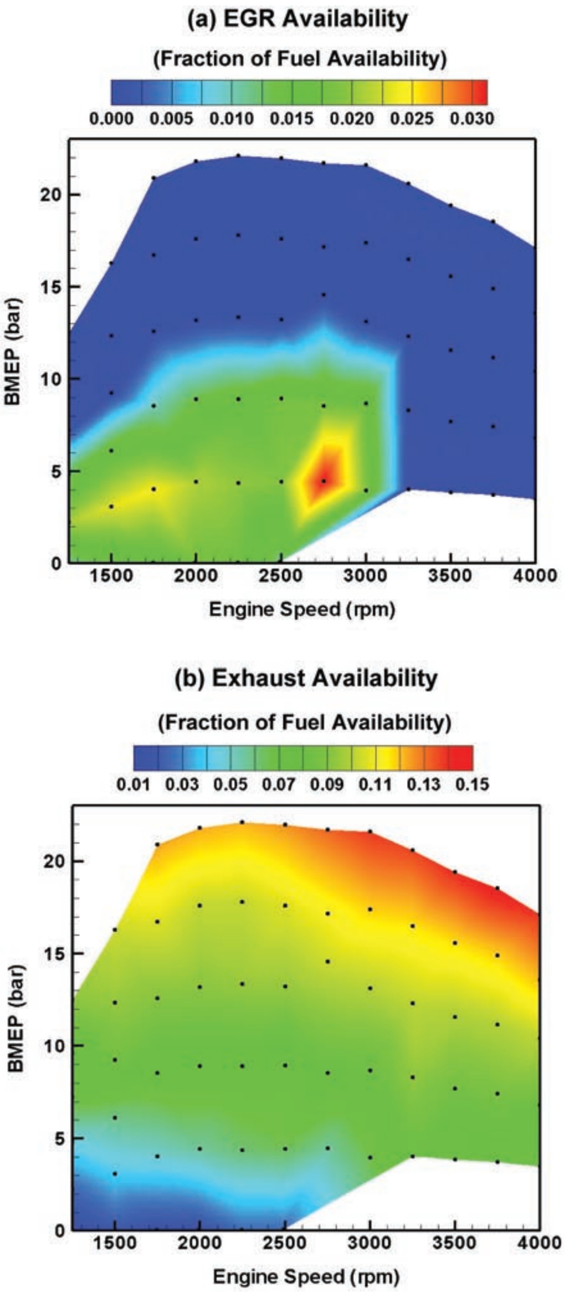

FIGURE 2. Thermodynamic availability of the (a) EGR and (b) exhaust systems on a GM 1.9-L engine shows a significant amount of fuel energy is discarded to the environment and potentially available for recovery.

recovery efficiencies. Note that for these examples the TER recovery efficiency is based on availability and assumed constant across the speed/load range with a Second Law TER efficiency of 30% considered realistic for on-engine recovery. The location of the engine-system peak BTE was observed to shift for higher TER efficiencies due to the increasing role of exhaust availability in the engine-system peak BTE estimation.

Potential fuel economy improvements over the FTP drive cycles were estimated using composite modal experiments and simulated TER of the EGR and exhaust systems. More information on the modal experiments may be found in the literature, SAE 2006-01-3311. While this approach makes use of many assumptions, the analysis was undertaken to have a better understanding of the potential of a TER system with light-duty applications. Specifically, the composite modal approach does not take into account cold-start, transient phenomena, or the added mass of the TER system. In addition, the TER system efficiency was assumed constant for all speed/load combinations. The TER system efficiency would be influenced by many factors in implementation including the temperature and mass flow rate of the thermal source. Estimates for drive cycle fuel savings with TER based on data from the GM 1.9-L engine are summarized in Table 1. The results of this analysis show a non-negligible potential for fuel savings with light-duty applications, even for 30% TER efficiency which is considered reasonable for this application. A vehicle systems model with an integrated transient capable TER model is under development with GT-Drive. This model will be used to further assess the potential of TER technologies, thermal management strategies, and thermal damper and/or capacitor technologies for damping thermal transients.

TABLE 1. Estimated fuel economy improvements for FTP drive cycle using composite efficiency estimates based on modal experiments and assumed TER efficiencies.

2nd Law TER System Efficiency	Estimated Fuel Savings
30%	8.6%
50%	11.4%
100%	17.0%

An organic Rankine system was developed in FY 2008 for on-engine recovery of EGR and exhaust system energy. A literature review and modeling showed the potential to recover sufficient energy to achieve a 45% peak BTE on the GM 1.9-L engine. A system was constructed and evaluated on-bench and on-engine with an initial focus on exhaust energy recovery. The system was designed around off-the-shelf components including a scroll expander from an automotive air conditioning system and made use of R123 for the working fluid. R123 was chosen for early experiments for comparison with the literature. R245 will be the long-term candidate and is currently used by Cummins Engines for TER system development due to favorable characteristics including high efficiency, low global warming potential, and non-flammability. The off-the-shelf expander was not able to meet expectations due to sealing issues and will be further addressed during FY 2009.

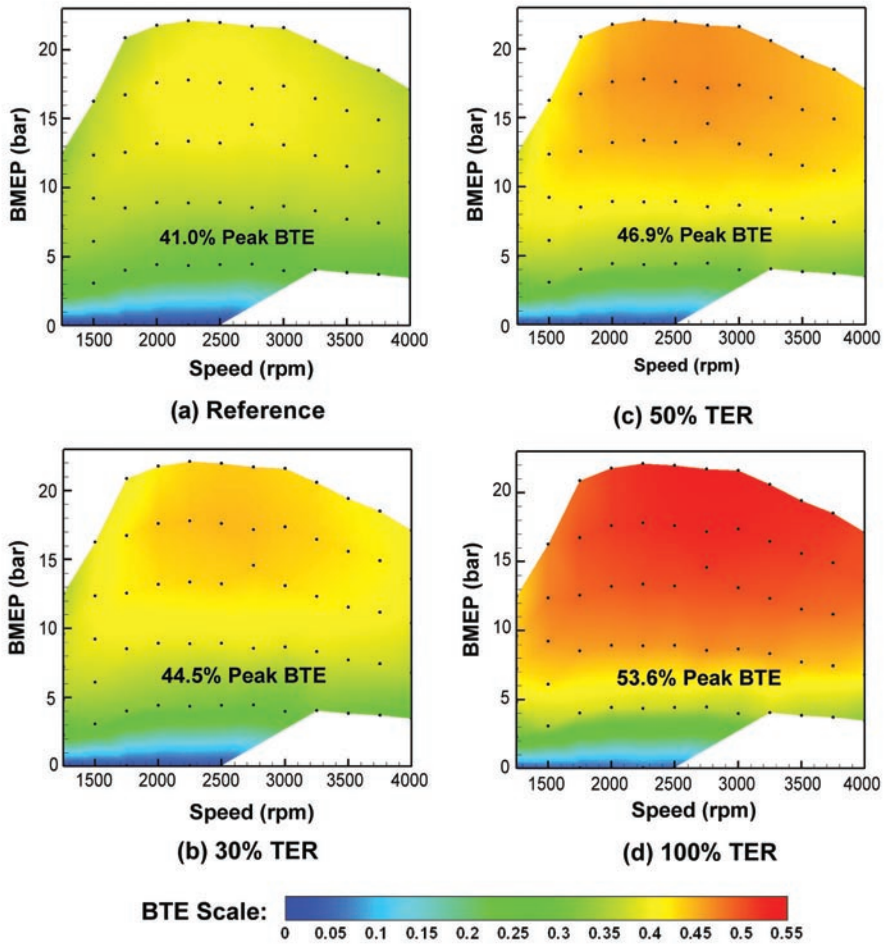

FIGURE 3. (a) BTE of the unmodified GM 1.9-L engine calibration and the estimated potential improvement in BTE with TER from EGR and exhaust systems for Second Law TER efficiencies of (b) 30%, (c) 50%, and (d) 100%.

The FY 2008 milestone of 43% peak BTE was met with low viscosity oil, high cetane number fuel, electrification of the engine coolant pump, and re-optimization of engine parameters including turbo-machinery and fuel parameters. The efficiency improvement potential of these technologies was sufficient to meet the 43% peak BTE and also serve to move the reference peak BTE for a future TER recovery system. Recall that in Figure 3 the reference was 41% peak BTE.

The path forward to the demonstration of FY 2010 efficiency and emissions milestones has been developed through extensive modeling, experiments, and interactions with the scientific community. The path will include a combination of the efficiency enabling technologies used this year as well as TER in combination with advanced combustion operation and the integration of appropriate aftertreatment systems. The advanced combustion and aftertreatment research is also being performed at ORNL and in close communication with this activity. Demonstration and verification of the milestones will be accomplished with on-engine experiments with a prototype TER system and vehicle system modeling with GT-Drive and/or PSAT.

Conclusions

This activity has shown progress toward the development, implementation, and demonstration of technologies for meeting and possibly exceeding FreedomCAR engine and efficiency milestones. Specific accomplishments are as follows:

- Demonstration of FY 2008 FreedomCAR milestones including 43% peak BTE and 27% part-load BTE on a light-duty diesel engine.
- New insight into the thermodynamic availability of engine systems (*e.g.*, exhaust system, EGR, etc.) across the speed/load operational range of a light-duty diesel engine and estimated potential fuel economy improvements over the FTP drive cycle.

- Development and evaluation of a first generation organic Rankine cycle through modeling and experiments on-bench and on-engine.
- Finalization of path forward to demonstration of FY 2010 efficiency and emissions milestones.

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1. R.M. Wagner, K.D. Edwards, Thomas E. Briggs, "Engine efficiency activities at ORNL", Meeting with Cummins (Columbus, IN; October 2008).

2. K.D. Edwards, R.M. Wagner, R.L. Graves, "Identification and evaluation of near- and long-term opportunities for efficiency improvement", AEC Working Group meeting (Auburn Hills, MI; September 2008).

3. K.D. Edwards, R.M. Wagner, R.L. Graves, "Identification and evaluation of near-term opportunities for efficiency improvement", Diesel Engine-Efficiency and Emissions Research conference (Dearborn, MI; August 2008).

4. K.D. Edwards, R.M. Wagner, R.L. Graves, "Identification of potential efficiency opportunities in internal combustion engines using a detailed thermodynamic analysis of engine simulation results", SAE Paper 2008-01-0293 (Detroit, MI USA; April 2008).

5. R.M. Wagner, K.D. Edwards, T.E. Briggs, "Achieving FreedomCAR fuel efficiency goals for light-duty diesel engines", Meeting with Caterpillar (Peoria, IL; March 2008).

6. R.M. Wagner, K. Cho, C.S. Sluder, "Achieving high-efficiency clean combustion in multi-cylinder light-duty engines (Agreement 15936)", 2008 DOE Office of Vehicle Technologies Annual Merit Review (Bethesda, MD; February 2008).

7. R.M. Wagner, K.D. Edwards, T.E. Briggs, "Achieving and demonstrating FreedomCAR engine fuel efficiency goals (Agreement 13704)", 2008 DOE Office of Vehicle Technologies Annual Merit Review (Bethesda, MD; February 2008).

8. R.M. Wagner, K.D. Edwards, "Update on ORNL efficiency and advanced combustion activities for LD diesel engines", 2007 AEC Working Group Meeting at USCAR (Southfield, MI; September 2007).

Special Recognitions & Awards/Patents Issued

Activity was recognized as a 2008 Advanced Combustion & Emissions Controls Technical Accomplishment in the reports to USCAR Board of Directors; "Demonstrated 2008 FreedomCAR engine efficiency milestones of 43% peak and 27% road-load BTE on light-duty engine" and "2nd Law thermodynamics perspective helps to define path to 45% peak BTE in light-duty internal combustion engines".

II.A.14 Hydrogen Free-Piston Engine

Peter Van Blarigan
Sandia National Laboratories
PO Box 969, MS 9661
Livermore, CA 94551-0969

DOE Technology Development Manager:
Gurpreet Singh

Objectives

- Design and begin fabrication of opposed-piston research experiment.
- In collaboration with General Motors (GM) and the University of Michigan, assess the performance of a free-piston generator as the auxiliary power unit (APU) in a series hybrid vehicle.
- Improve the efficiency of small output (30 kW) reciprocating generators by at least 20% along with reduced emissions.

Accomplishments

- Designed the opposed-piston research experiment utilizing SolidWorks/COSMOS and experience base available from Sandia National Laboratories Combustion Research Facility.
- Analyzed the research experiment for stability of piston coupling with Mathematica-based model.
- Designed a gas-powered dynamometer to maintain piston oscillation of generator at any fueling condition, including full motoring.
- Conducted engineering analysis of experimental hardware to show performance and safety margins.
- Produced the engineering drawings of all components and began fabrication.

Future Directions

- Continue fabrication and assembly of a two-stroke, opposed-piston research experiment utilizing optimized coupling of dual Magnequench linear alternators as a proof-of-concept tool.
- Operate the research experiment fueled by hydrogen to measure indicated efficiency in a continuous operation regime as well as the stability of the electrically-coupled opposed pistons.
- Demonstrate flexibility and multi-fuel capability by operating on alternative fuels at various operating conditions (compressions ratios, equivalence ratios).
- Optimize the battery charging application for higher power-to-weight ratio.

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Introduction

As fuel efficiency of the typical American automobile becomes more important due to hydrocarbon fuel cost and availability issues, powertrain improvements will require smaller output engines combined with hybrid technologies to improve efficiency. In particular, the plug-in hybrid concept will require an electrical generator of approximately 30 kW output. Unfortunately, current crankshaft spark ignition internal combustion engines with optimized power outputs of 30 kW have thermal efficiencies of less than 32%.

The free-piston generator of this project has a projected fuel-to-electricity conversion efficiency of 50% at 30 kW output. The project has progressed by conducting idealized combustion experiments, designing and procuring the linear alternators required for control and power conversion, and conducting computational fluid dynamics design of the inlet/exhaust processes. The design has evolved into a dynamically balanced configuration suitable for seamless incorporation into an automotive application. The ultimate goal is to combine the developed components into a research prototype for demonstration of performance. Figure 1 shows the improvement based on single cycle experiments.

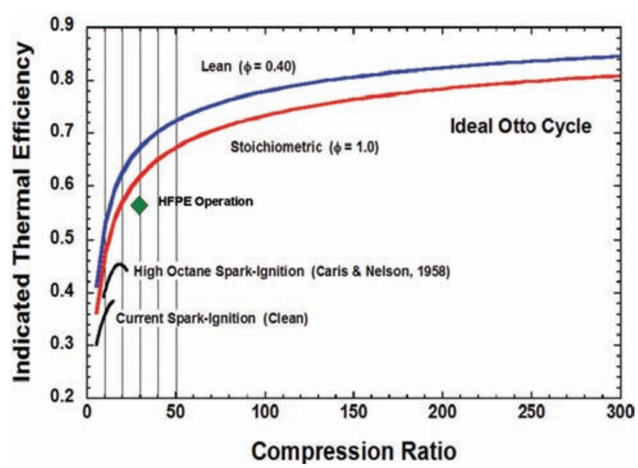

FIGURE 1. Indicated Efficiency as a Function of Compression Ratio (Expected hydrogen free-piston engine operation shown by diamond.)

Approach

By investigating the parameters unique to free-piston generators (linear alternator, opposed-piston coupling, uniflow port scavenging) as separate entities, each piece can be used at its optimum design point. More importantly, upon assembly of a research prototype for performance demonstration (the goal of this project), understanding of the pieces in the device will allow proper contribution of each component to the combined performance of the assembly.

This year, our activities concentrated on the design and fabrication of the opposed-piston research prototype experiment and preparation of the laboratory in building 979 that will house the experiment. We have also developed a gas dynamometer concept to maintain the oscillation of the pistons at the desired compression ratio independent of the fueling level. Our collaborators (GM and the University of Michigan) have concentrated on a ground-up hybrid vehicle model to optimize the size and configuration of the free-piston APU.

Results

The majority of our efforts this year have been concentrated on designing the opposed-piston experiment and preparing the laboratory in building 979 to house the research prototype. This laboratory still contained the single-cylinder lean-burn hydrogen engine experiment from several years ago. The lab has been updated with new combustible gas sensors and other environmental, safety, and health required equipment to meet current day requirements. Figure 2 shows the completed computer-aided design model of the opposed-piston research prototype. The majority of the parts have been procured and assembly is currently underway.

As part of the experimental design process it was realized that the capability to start the piston oscillation and bring the compression ratio to the desired value before fuel is introduced would be an important capability. We began investigating various concepts to introduce extra gas into the bounce chambers when the pistons are near their full outward travel position (maximum combustion chamber volume) and a method for venting the extra gas when the pistons are near the full inward travel position (minimum combustion chamber volume). In this way the energy to drive the pistons inward can be provided and controlled. We have investigated using both helium and air as the working fluid in the bounce chamber. The gas is introduced through a piston actuated valve in the bounce chamber cylinder head and vented into a plenum that surrounds the venting ports in the bounce chamber cylinder walls. Figure 3 shows the configuration.

Figure 4 shows the pressure-volume (PV) diagrams for bounce chamber operation under three modes. Full motoring mode occurs when no fuel is injected on the combustion side and all power comes from injected gas into the bounce chamber. Full combustion power mode means all power comes from engine combustion; no gas is injected into the bounce chamber, which acts like a sealed gas spring. Half motoring mode is a 50/50 power combination of fuel combustion and bounce chamber gas injection. The various compression lines represent different starting pressures for the gas in the bounce chamber at the start of the bounce chamber compression stroke (denoted by 1, 2, and 3). This pressure can be determined by controlling the vent plenum pressure. Gas injection is by means of a piston-actuated valve that opens and closes at the same point. This valve controls the supply of a constant pressure gas supply. This ensures the same amount of gas is present in the bounce chamber during expansion across all modes

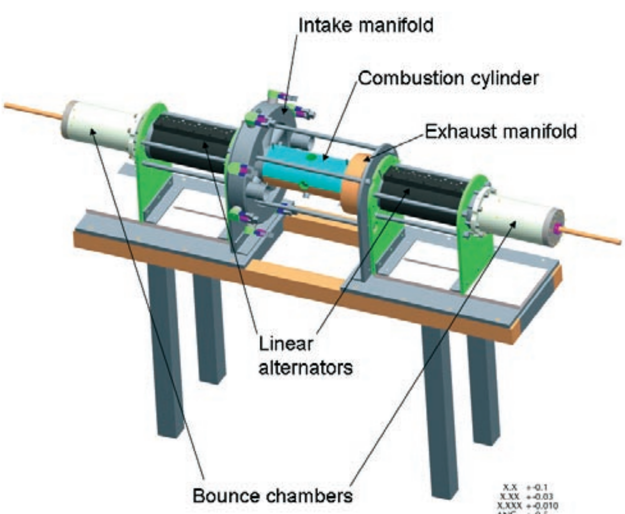

FIGURE 2. The Opposed-Piston Research Prototype Overview

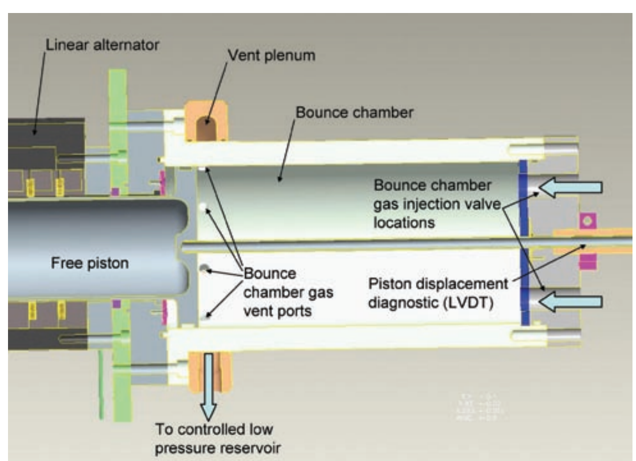

FIGURE 3. Bounce Chamber Gas Dynamometer Operation (Block arrows show gas flow direction.)

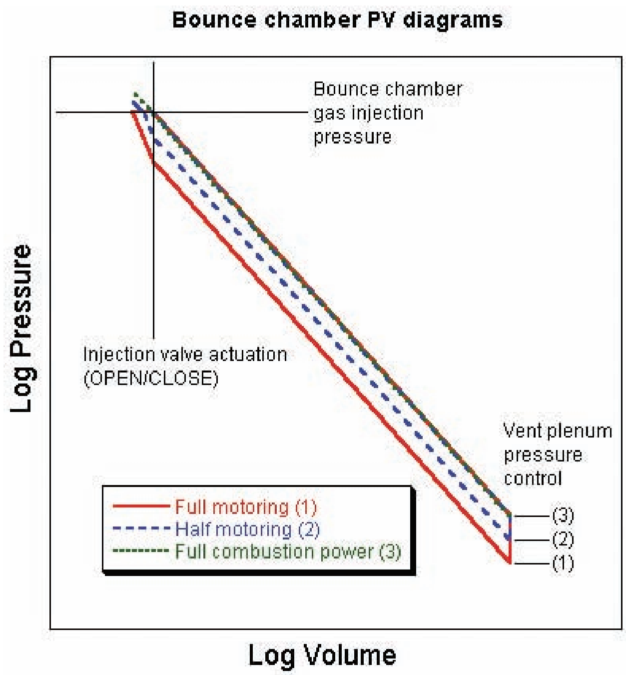

FIGURE 4. Bounce Chamber PV Diagrams for Various Operating Modes

of operation. Thus the quantity of gas added to the bounce chamber is controlled by the pressure in the bounce chamber exhaust plenum. By raising the plenum pressure sufficiently, no extra gas will be admitted to the bounce chamber, requiring all of the alternator power output and losses to be provided by combustion. A feedback control system can therefore utilize the piston displacement diagnostic to control the plenum pressure as the fuel rate is changed, resulting in a constant compression ratio under all fueling conditions.

Conclusions

- Laboratory preparation and research prototype design/fabrication are on track for operation in Fiscal Year 2009.
- A gas dynamometer concept is being incorporated into the experiment for starting and maintaining piston oscillation under all fueling conditions.

II.A.15 Optimization of Direct Injection Hydrogen Combustion Engine Performance Using an Endoscopic Technique

Thomas Wallner
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439

DOE Technology Development Manager:
Gurpreet Singh

Objectives

- Apply advanced mixture formation and combustion techniques to close in on the efficiency and emissions goals set for hydrogen combustion engines.
- Optimize the hydrogen combustion engine through improved injection strategies, injector location and injector nozzle designs.
- Utilize advanced diagnostic tools such as endoscopic imaging to gain further insight into hydrogen mixture formation and combustion.

Accomplishments

- Determined that the injector location has significant influence on the engine efficiency and emissions behavior.
- Found that the injection strategy and nozzle design are closely related and highly dependent on injector location.
- Evaluated the potential of water injection for NOx emissions reduction and found that an emissions reduction of up to 50% with no significant loss in engine efficiency is feasible.
- Gained further understanding of mixture formation mechanisms by running case studies with single-hole injector.
- Intensified collaboration with Ford and Sandia National Laboratories (SNL) by closely coordinating experimental conditions.

Future Directions

- Characterize the efficiency improvement of fast acting injectors (piezo-actuated).
- Develop improved injector nozzle designs for specific operation conditions (injector location, injection strategy) supported by optical engine results (SNL) and 3-dimensional (3-D) computational fluid dynamics (CFD) simulation.
- Evaluate the effects of external exhaust gas recirculation on engine efficiency and emissions.
- Evaluate hydrogen direct injection in a multi-cylinder engine (separate project proposal for Fiscal Year 2009).

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Introduction

The favorable physical properties of hydrogen make it an excellent alternative fuel for internal combustion engines and hence it is widely regarded as the energy carrier of the future. The U.S. Department of Energy has set challenging targets for the performance and emissions behavior of hydrogen combustion engine vehicles. These targets include a peak brake thermal efficiency of 45%, NOx emissions as low as 0.07 g/mile and a power density comparable to gasoline engines [1]. Hydrogen direct-injection is a promising approach to close in on above-mentioned goals as it offers additional degrees of freedom by influencing mixture stratification which in turn affects the combustion process and the exhaust emissions.

Approach

The research project at Argonne National Laboratory has been funded to evaluate hydrogen combustion strategies in a research engine and apply advanced diagnostics to identify areas for further improvement.

This report summarizes research results on the effect of injector location and nozzle design on engine efficiency and emissions. A special cylinder head that allows central (adjacent to the spark plug) as well as side (between intake valves) injector location is used for these studies. An endoscopic imaging technique is also applied to gain further insight into the combustion intensities and allows correlating local air/fuel ratios and NOx emissions. In addition, water injection is employed as an additional measure to reduce engine-out NOx emissions by lower in-cylinder combustion temperatures.

Results

Influence of Injector Location on Mixture Formation and Combustion

Two custom-built injector nozzles were used to determine the influence of injector nozzle design as well as injector location on the mixture formation and consequently combustion and emissions behavior. A symmetric 6-hole nozzle was specifically designed for operation with central injection to allow the injection cone to penetrate the combustion chamber. An asymmetric nozzle was designed for operation in the side location. With the holes pointing towards the spark plug, it is expected that a locally rich zone in proximity of the spark plug can be created. Multiple configurations were possible with respect to injector location and position. The following four configurations were used for this study.

- 6-hole symmetric injector in central location (6-hole central).
- 6-hole symmetric injector in side location (6-hole side).
- 5-hole asymmetric injector in the side location with holes pointed towards the spark plug (5-hole side-up).
- 5-hole asymmetric injector in the side location with hole pointed towards the piston (5-hole side-down)

The indicated thermal efficiency as a function of start-of-injection (SOI) timing for low engine load of 2 bar indicated mean effective pressure (IMEP) is shown in Figure 1. The SOI timing for the 6-hole injector in the central location was not retarded beyond 100° crank angle (CA) before top-dead center (BTDC) because stable combustion was not possible for the low load. For the injectors in the side location with the holes pointing up, SOI was retarded until injection was completed just before spark timing (20° CA BTDC). It is observed that higher efficiency is achieved when the injectors are in the side location with retarded SOI. An approximately 1% increase in peak efficiency is observed for the 5-hole injector in the side location with the jets towards the spark as compared to the 6-hole injector in the side location whereas an approximate 4% increase is observed when compared with the 6-hole injector in the central location. The 6-hole and the 5-hole side-down configurations allowed SOI as late 40° CA BTDC before unstable combustion occurred. It is expected that SOI later than 40° CA BTDC does not allow enough time for an ignitable mixture to form around the spark plug.

Figure 2 shows the indicated thermal efficiency as a function of SOI timing for the high engine load of 8 bar IMEP. It is observed that for the high load the efficiency is increased as the SOI timing is retarded. However the efficiency drops after an optimum SOI timing. The unburnt hydrogen emissions in the exhaust increased by approximately six times and a noticeable decrease in combustion stability was observed after the optimum SOI timing because of disadvantageous mixture stratification which resulted in formation of non-combustible mixture around the spark plug.

The NOx emissions relative to SOI timing for the different injector configurations for the high load of 8 bar IMEP are shown in Figure 3. For the retarded SOI timing of 80° CA BTDC it is seen that the NOx emissions are reduced by approximately 50% for the 6-hole injector in the side location as compared to the injector in the central location. It can also be observed that there is almost a constant decrease in NOx emissions by approximately 33% when the fuel jets are pointed towards the spark plug as against being pointed towards the piston. This trend is seen from retarded SOI of 80° CA BTDC to early SOI of 120° CA BTDC.

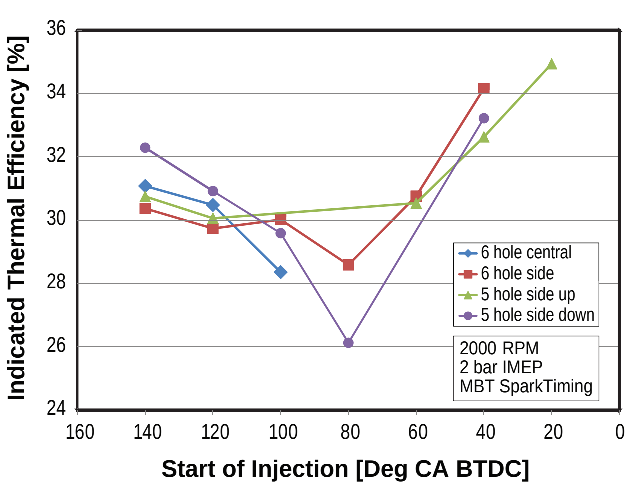

FIGURE 1. Indicated thermal efficiency as a function of start of injection at low engine load (2 bar IMEP).

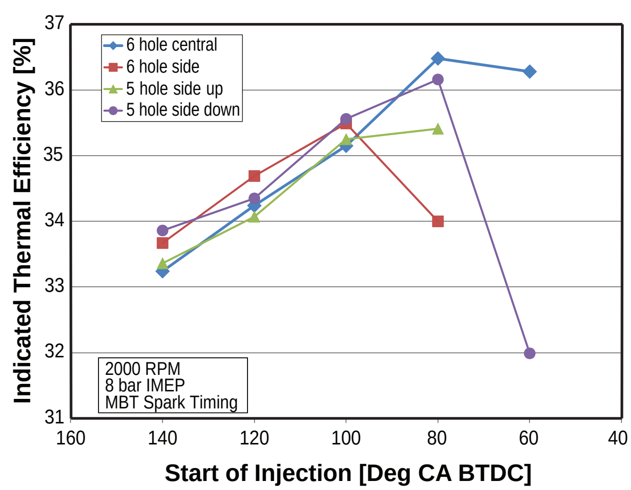

FIGURE 2. Indicated thermal efficiency as a function of start of injection at high engine load (8 bar IMEP).

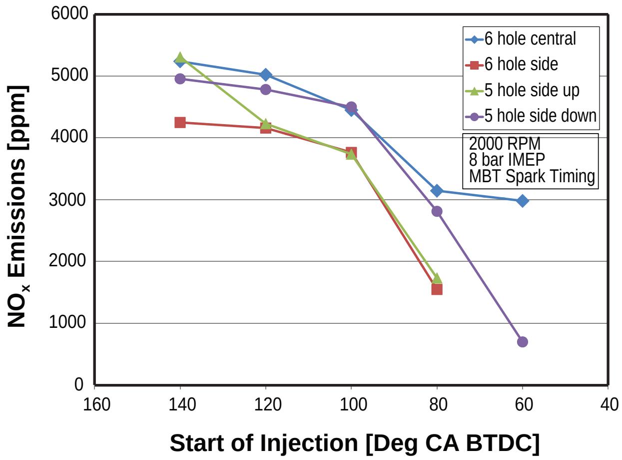

FIGURE 3. Influence of start of injection on NOx emissions at high engine load (8 bar IMEP).

This can be attributed to the formation of localized rich mixture zones near the spark plug as the jets are towards the spark. When the jets are pointed towards the piston, the jets reflect of the piston area towards the walls of the cylinder and a partial homogenous mixture is formed leading to higher NOx emissions.

A visualization of the combustion event for all the injector configurations with a SOI timing of 80° CA BTDC for a high engine load of 8 bar IMEP is shown in Figure 4. Each image represents an average of ten combustion events at a certain crank angle. The range of the crank angle was from 10° CA after top dead center (ATDC) to 30° CA ATDC in steps of 2° CA. The average fuel/air equivalence ratio (Φ) for these tests was ~0.8. From Figure 3 maximum NOx emissions are observed for the 6-hole injector in central location. Combustion images for this particular injector configuration show maximum peak OH* intensity. High OH* intensities are also seen for the 5-hole injector in the side location with the jets towards the spark. However, from Figure 3 a decrease in NOx emissions can be observed for this configuration. This is because of the contrasting trends followed by the NOx emissions and the OH* intensities at air/fuel ratios close to stoichiometric.

The correlation between average peak OH* intensity numbers calculated from the images and the NOx emissions for a high engine load of 8 bar IMEP are shown as function of SOI timing in Figure 5. The average of the peak OH* intensity is calculated by averaging the peak OH* intensity of each frame over the total number of frames. It is difficult to generalize a trend but a very good correlation between the NOx emissions and the OH* intensities can be observed.

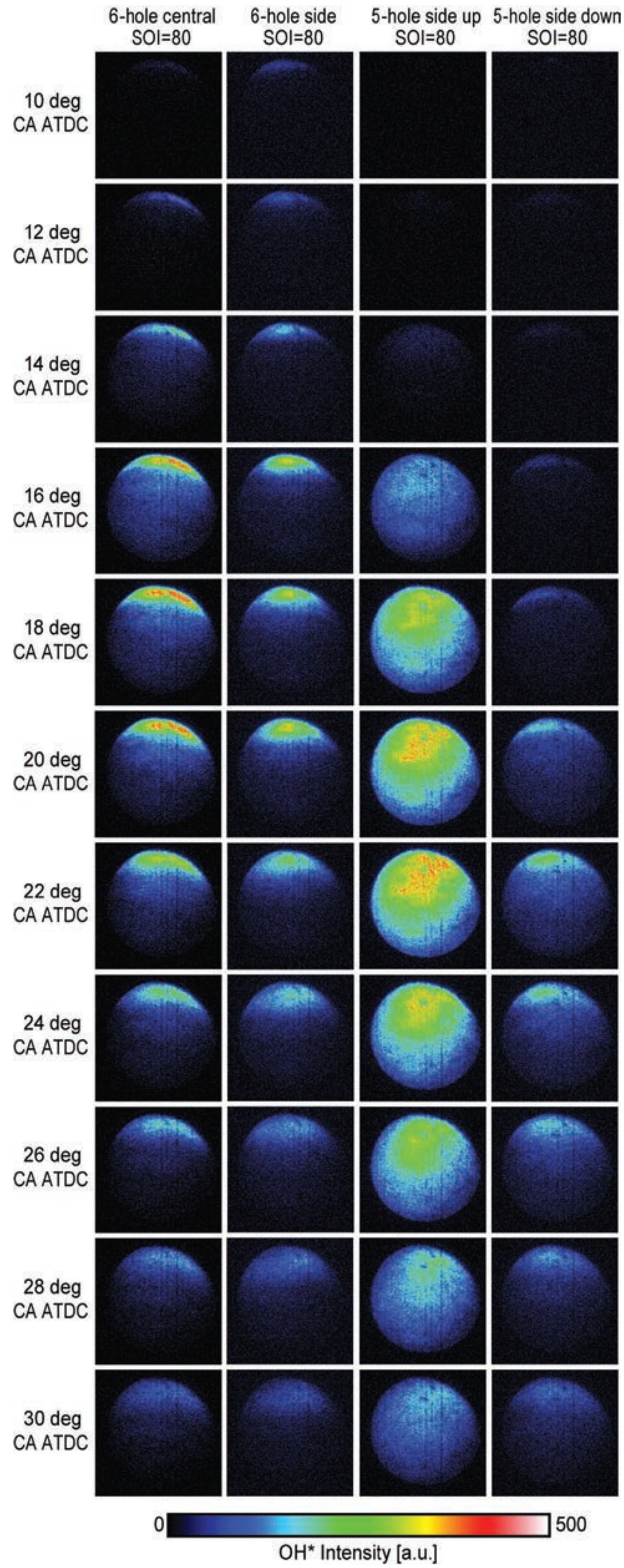

FIGURE 4. Sample OH* intensity plots for different nozzle configurations at high engine load (8 bar IMEP; SOI=80 deg CA BTDC).

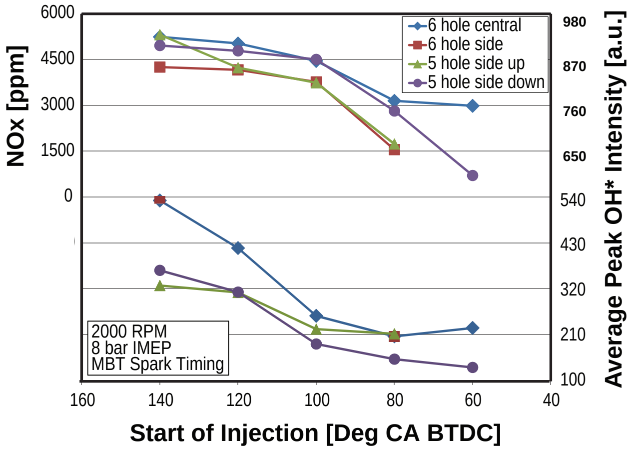

FIGURE 5. Correlation of NOx emissions and average peak OH* intensity as a function of start of injection at high engine load (8 bar IMEP).

Influence of Water Injection on Engine Efficiency and Emissions

The effect of water injection on the NOx emissions and engine efficiency for the maximum efficiency point is shown in Figure 6. The location of 50% mass fraction burned was monitored to maintain maximum brake torque (MBT) conditions for this set of tests. As the water level was increased beyond 0.8 kg/hr, the location of 50% mass fraction burn was retarded and hence the ignition timing had to be advanced to maintain MBT conditions. The results from this case are plotted as Case 1 in Figure 6. For the Case 2 condition in Figure 6, the ignition timing for all the tests was maintained at 2° ATDC which was the MBT timing for the maximum efficiency point when no water was injected into the combustion chamber. Under both the cases the overall trend which can be observed is that the NOx emissions are decreased by approximately 55% as the water flow rate is increased to 1.4 kg/hr. Correspondingly, the efficiency drops by only 1.1 percentage points, which is a relative efficiency loss of less than 2.5%. It is also observed that for the maximum water flow rate of 1.4 kg/hr, the relative efficiency loss for Case 1 is less than that for Case 2 by nearly 0.8% whereas the NOx emissions are higher by only about 100 ppm. The NOx emissions for the two cases shown are still significantly higher than the Tier II Bin 5 emissions targets; however, the corresponding operating point of 8 bar net IMEP at 2,000 RPM is not representative of an operating point on the Federal Test Procedure 75 drive cycle.

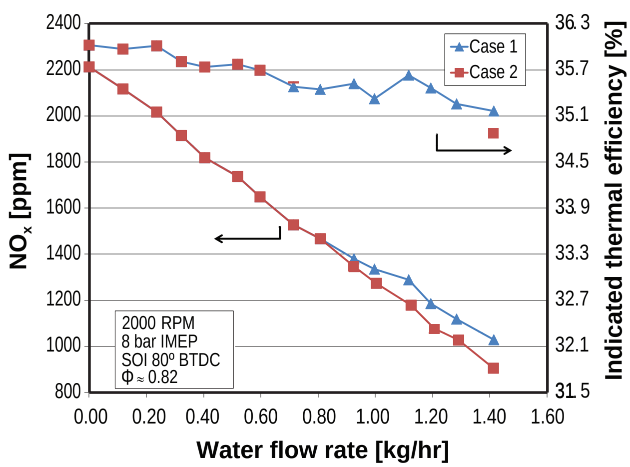

FIGURE 6. Indicated thermal efficiency and NOx emissions vs water flow rate for maximum efficiency SOI for high engine load (8 bar IMEP).

Conclusions

- Injection parameters, such as injection timing and injector nozzle design, in combination with the respective injector location have a significant influence on engine efficiency and emissions behavior.
- Endoscopic imaging allows local determination of combustion intensities and ultimately NOx emissions and shows good correlation with NOx emissions measurement.
- Water injection is an effective tool to reduce engine-out NOx emissions by up to 50% without compromising engine efficiency.
- Optimized nozzles for specific injector locations need to be developed supported by optical results as well as 3-D CFD simulation.

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II.A.16 Advanced Hydrogen-Fueled ICE Research

Sebastian A. Kaiser
Sandia National Laboratories
P.O. Box 969, MS 9053
Livermore, CA 94551

DOE Technology Development Manager:
Gurpreet Singh

Objectives

The hydrogen internal combustion engine (ICE) project aims to provide the science base for the development of high-efficiency hydrogen-fueled vehicle engines. The technical focus is on direct-injection strategies, using laser-based in-cylinder measurements closely tied to advanced numerical simulations (performed by J. Oefelein at Sandia, see "Large Eddy Simulation Applied to Low-Temperature and Hydrogen Engine Combustion Research"). Specifically, at this point the goals of the project are to:

- Quantify the influence of injection strategies on pre-combustion in-cylinder mixing of fuel and air.
- Complement metal-engine research and development (R&D) at Ford and partially-optical engine research at Argonne National Laboratories (ANL).
- Provide data for and collaborate in large-eddy simulation (LES) validation.
- Investigate influence of charge stratification on the combustion event and NOx formation.

Accomplishments

- Two-dimensional measurement technique to quantify in-cylinder fuel distribution was improved substantially to be able to make measurements under more realistic operating conditions.
- Evaluation of injection strategies, coordinated with metal-engine experiments at ANL, is in progress.
- Detailed velocity measurements in two orthogonal planes help understand interaction of intake-induced and injection-induced flow.
- Velocity and fuel distribution measurements are initial building blocks of a database for the validation of companion LESs by J. Oefelein at Sandia.

Future Directions

- Install new engine head, supplied by Ford R&D, featuring central or side injection and central ignition. Engine geometry will then be identical to that of collaborating labs at Ford and ANL.
- Compile extensive database of fuel distributions and velocity maps as a function of varying injector geometry and location, injection timing, speed, and load. Data will be used to complement metal engine data and for simulation validation.
- Supplement quantitative laser-based techniques (see above) with qualitative high-speed Schlieren "movies" to understand temporal development mixture formation.
- Use hydroxyl ion planar laser-induced fluorescence (OH-PLIF) to investigate the influence of mixture formation on combustion, in particular with multiple injections per cycle.

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Introduction

Hydrogen internal combustion engine (H_2ICE) development efforts are focused to achieve an advanced hydrogen engine with peak brake thermal efficiency greater than 45%, near-zero emissions, and a power density that exceeds gasoline engines. Such advanced engines can be part of a powertrain with efficiency similar to systems based on fuel cells [1]. With respect to these efforts, the direct-injection (DI) H_2ICE is one of the most attractive options [2]. With DI, the power density can be approximately 115% that of the identical engine operated on gasoline. In addition, the problems of preignition associated with port fuel injection can be mitigated. Lastly, in-cylinder injection offers multiple degrees of freedom available for controlling emissions and optimizing engine performance and efficiency.

The challenge with DI-H_2ICE operation is that in-cylinder injection affords only a short time for hydrogen-air mixing, especially when start-of-injection (SOI) is retarded with respect to intake valve closure to reduce the compression work of the engine and to mitigate preignition. Since mixture distribution at the onset of combustion is critical to engine performance, efficiency, and emissions, a fundamental understanding of the in-cylinder mixture formation processes is necessary to optimize DI-H_2ICE operation. Correct prediction of mixture formation before the onset of combustion is also of great importance for any engine simulation. The experimental results will therefore provide a benchmark test for advanced computations also being developed at Sandia.

Approach

In the optically accessible DI-H_2ICE, separate two-dimensional, quantitative measurements of in-cylinder fuel distribution and charge motion were made. Particle-image velocimetry (PIV) enabled two-dimensional velocity measurements in both horizontal and vertical planes. The velocity measurements were continuing the characterization of an operating point chosen for studies in Fiscal Year 2007. That work indicated that jet-wall interaction had a major influence on the mixture preparation. Since all the previous measurements had been made in a horizontal plane (parallel to the piston top), imaging in an orthogonal (vertical) plane through central axis of the cylinder was performed to obtain complementary information. In addition to measurements after the injection event, data were collected for the intake stroke, which are being used for simulation validation.

Previous measurements of fuel distribution and velocity had been made at an operating point with relative low injection pressures. The technique for velocity measurements is not influenced by the injection pressure, but the fuel-distribution (equivalence ratio) measurement is. As in previous studies, equivalence ratio was measured using PLIF of acetone seeded in small amounts into the hydrogen fuel. Higher gas pressures mean lower concentration of acetone if condensation of the tracer is to be avoided, hence lower fluorescence signal. Consequently, the system for fuel-distribution imaging was significantly improved in order to be able to make quantitative measurements with the higher injection pressures used in second-generation hydrogen injectors. A detailed assessment of measurement accuracy and precision was performed. The current system is briefly described in the Results section.

Upon completing improvements to the experimental technique, we are now collaborating with ANL (principal investigator Thomas Wallner) to study the influence of the injector location and geometry on the mixture formation [3]. At ANL, thermal efficiency, emissions, and combustion duration were studied for four different combinations of injector tip geometry and location. Several different load points (= global equivalence ratios) were examined. Two different injectors were used: a symmetric 6-hole nozzle with 90° included angle between two opposite jets, and an asymmetric 5-hole injector. The hole patterns are shown in Figure 1a. Four different combinations of injector geometry and location were investigated: the 6-hole injector in the central position and in the side position, as well as the 5-hole injector mounted from the side with the holes either pointing upwards along the pent-roof, or downwards toward the piston top (Figure 1b). With our experiment, we can directly and quantitatively measure the in-cylinder equivalence ratio before combustion starts. Coupled with ANL's thermodynamic and emissions data from the metal engine this will improve our understanding of how the injection system can be used to distribute the hydrogen fuel in an optimal way. Data acquisition and analysis are still in progress.

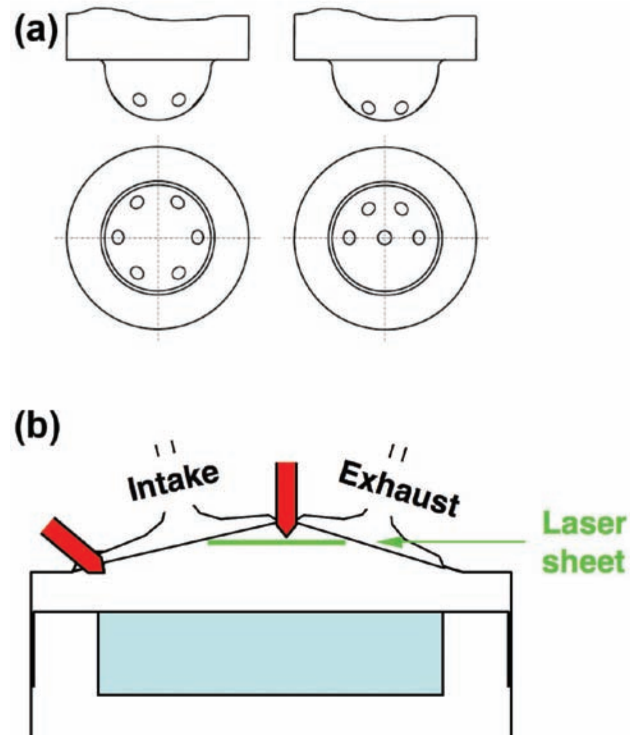

FIGURE 1. (a) 6-hole and 5-hole injector tip geometries. (b) Schematic of the side and central injector mounting position. The approximate location of the laser sheet used for the images in Figure 4 is also shown.

Results

In previous work (FY 2008 Publications/Presentation 2) we had conjectured that with the 6-hole injector in side position late injection (past about 100° crank angle [CA] before top-dead center [BTDC]) is unfavorable because the redirection of the hydrogen jets by the walls of the combustion chamber pushes the fuel towards the injector. In fired engine operation, this would lead to high heat losses to the walls. As more complete velocity data-sets from compression with and without injection have been assembled, a detailed picture of the influence of injection on the charge motion for this geometry has emerged.

Figure 2 summarizes our current understanding. The injection event has a strong influence on the in-cylinder flow, increasing charge velocities by more than a factor of two. However, the injection-induced flow creates a stable counter-flow pattern (Figure 2, top), which inhibits mixing and keeps the fuel close to the injector, i.e., close to the cylinder wall and away from the spark plug (Figure 2, middle – mean velocity vectors overlaid onto the mean fuel distribution). This can be expected to lead to high thermal losses and misfires. Velocity measurements in the vertical r-z plane (Figure 2, bottom two image sets) indicate why the flow is so stable: the flow induced by the injection has some similarity to the flow already present from the intake stroke. It can be seen that in the field of view the flow with as well as without injection consists of an upward-sweeping counter flow. This similarity is not because the injection event is too weak to change the flow, as evidenced by the large increase in mean velocity and turbulence, but rather is due to the fact that intake valves and injector issue fluid into the cylinder from similar locations and in a similar direction. As an overall result, for retarded injection, the current 6-hole injector is not suitable when side-mounted.

The PIV flow-field studies with the 6-hole injector in the side location were concluded in the 2nd quarter of FY 2008. An optimized experimental set-up and engine operating procedures for PIV have been established. More flow-field studies are planned after the current fuel-distribution measurements (see below) have been completed. It is evident that fuel-distribution and velocity measurements together are a powerful tool for understanding mixture preparation in the DI-H_2ICE.

To be able to obtain quantitatively precise images of the fuel distribution at the operating conditions used by our collaborators at ANL [3] and Ford [4], several improvements were made over earlier fuel-concentration measurements. They are summarized in Figure 3. As an improved method for seeding the fuel tracer acetone into the hydrogen, a high-pressure bubbler was used. This moves the point of seeding from the highest pressure in the system (gas storage bottle) to the lowest (just upstream of the injector), allowing for higher acetone concentrations. The detection system (camera and lens) was optimized. In particular, the use of an unintensified charge-coupled device (CCD) yields gains in both signal and resolution. When compared at the same resolution, the signal/noise ratio of the unintensified CCD is 3–4 times higher than that of the intensified CCD (ICCD). The excitation system (laser and sheet optics) was improved. This includes adding a passive-cavity pulse stretcher, allowing for higher laser energy (= more signal) without window damage.

These improvements may seem incremental, but together they are critical enablers for performing quantitative measurements on the fuel-air mixing process over a wide range of practical engine and injector operating conditions. Equally important for any quantitative measurement is knowledge of the measurement's accuracy and precision. For the current experiment, the results of this characterization, which would be too lengthy for this report, are described in FY 2008 Publications/Presentation [1].

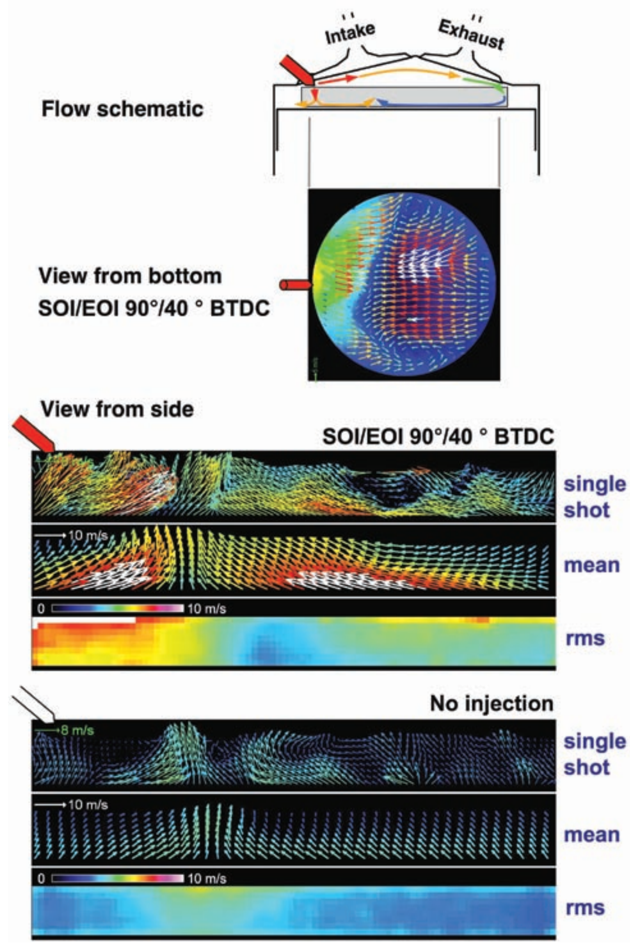

FIGURE 2. Top: Schematic of injection-induced flow for injection late in the compression stroke. Middle: corresponding mean flow (vectors) and fuel distribution (background) as seen from the piston bottom (r-θ plane). Bottom: Flow as seen from the side (r-z plane), with and without hydrogen direct injection. Images are taken at 32°CA BTDC, injection pressure 25 bar, global equivalence ratio (ϕ) = 0.55, 1,200 rpm, 0.5 bar intake pressure (EOI - end of injection).

The current study on the influence of the injector location and geometry on mixture formation, which makes use of the enhanced capabilities in imaging the fuel distribution, is in progress. Initial results on mixture ignitability near the spark plug are shown in Figure 4. The images show the equivalence ratio in a horizontal plane just below the spark plug. We can see that stably firing operation in the metal engine (frames) is possible for either homogeneous mixtures (early injection), or for mixtures where the spark plug is on the mean boundary of fuel-rich and fuel-lean regions. Unstable operation (no frames) often corresponds to a "hole" in the equivalence-ratio field around the spark plug, i.e., the fuel is away from the spark plug for most cycles. Arrows indicate this lean region for two injection timings for the case of the 5-hole injector with upwards hole pattern. Across all conditions, the correspondence is not perfect.

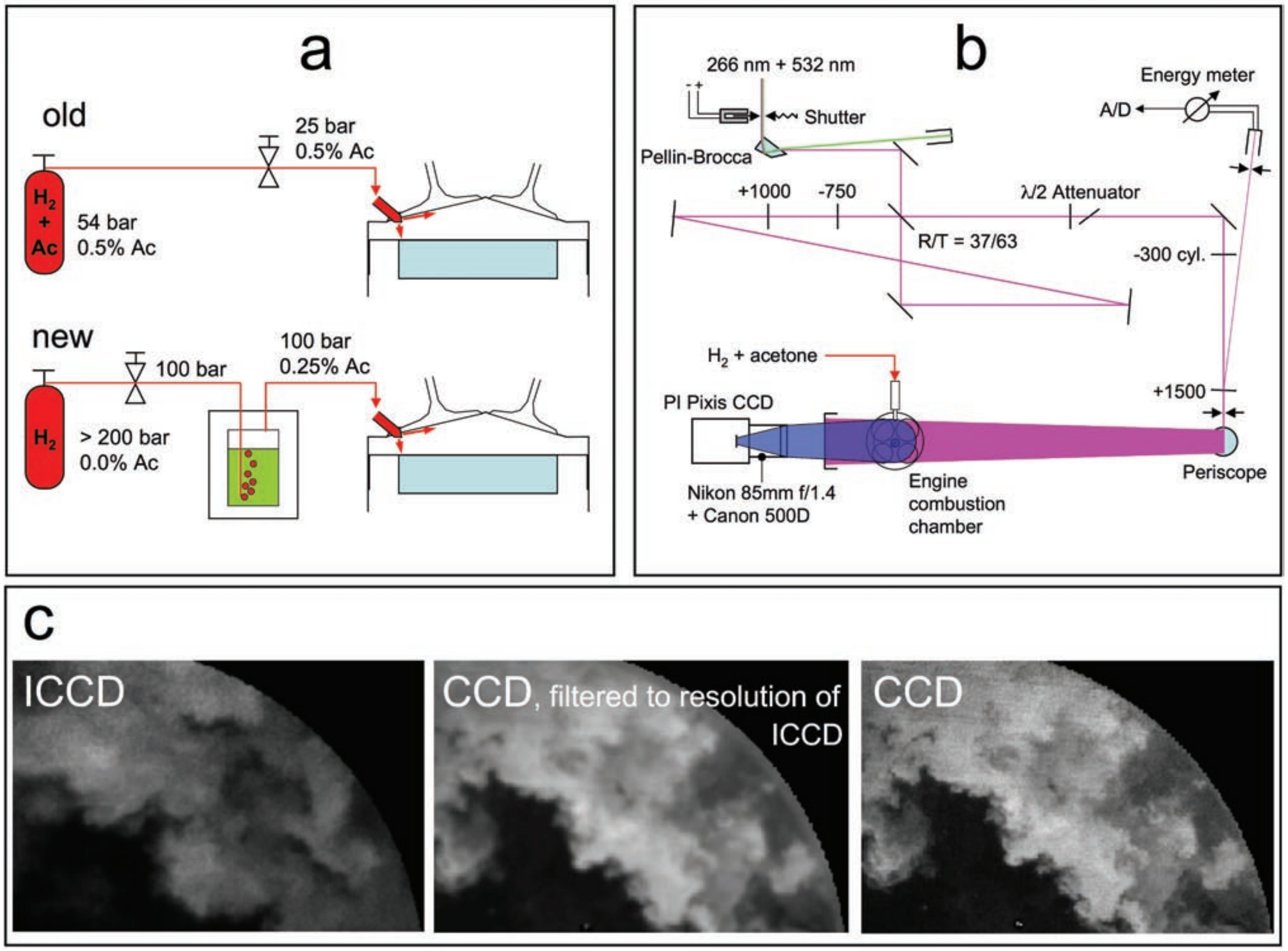

FIGURE 3. Overview of significant improvements in the experiment. (a) old and new method for seeding acetone into the hydrogen fuel, (b) experimental arrangement with passive-cavity pulse stretcher, (c) comparison between sample shots from intensified vs. unintensified camera.

This is to be expected, since the mean field contains no information about cycle-to-cycle variability, which is important for the stability of a particular operating point. Indeed, investigating mixture ignitability is not the focus of our current work, rather it was the intention of this paragraph to use some preliminary results to show what kind of information can be gained by complementing a parameter study in the metal engine with laser-based imaging. Current work focuses the physics underlying the relationship between mixture formation, efficiency, and NOx emissions.

Conclusions

- Laser-based measurements of in-cylinder velocity and fuel distribution are able to provide a detailed picture of the mixture formation process in the DI-H_2ICE.
- For the 6-hole injector in the side location and with retarded injection, the injection-induced flow couples into the intake flow and induces an unfavorable mixture distribution at the time of spark.
- After significant experimental upgrades, the fuel distribution can be measured with good precision and accuracy for practically any relevant injection pressure.
- Current work is complementing a study at ANL on injector geometry and location with data from Sandia's optical DI-H_2ICE to understand the relationship between mixture formation, efficiency, and NOx emissions.

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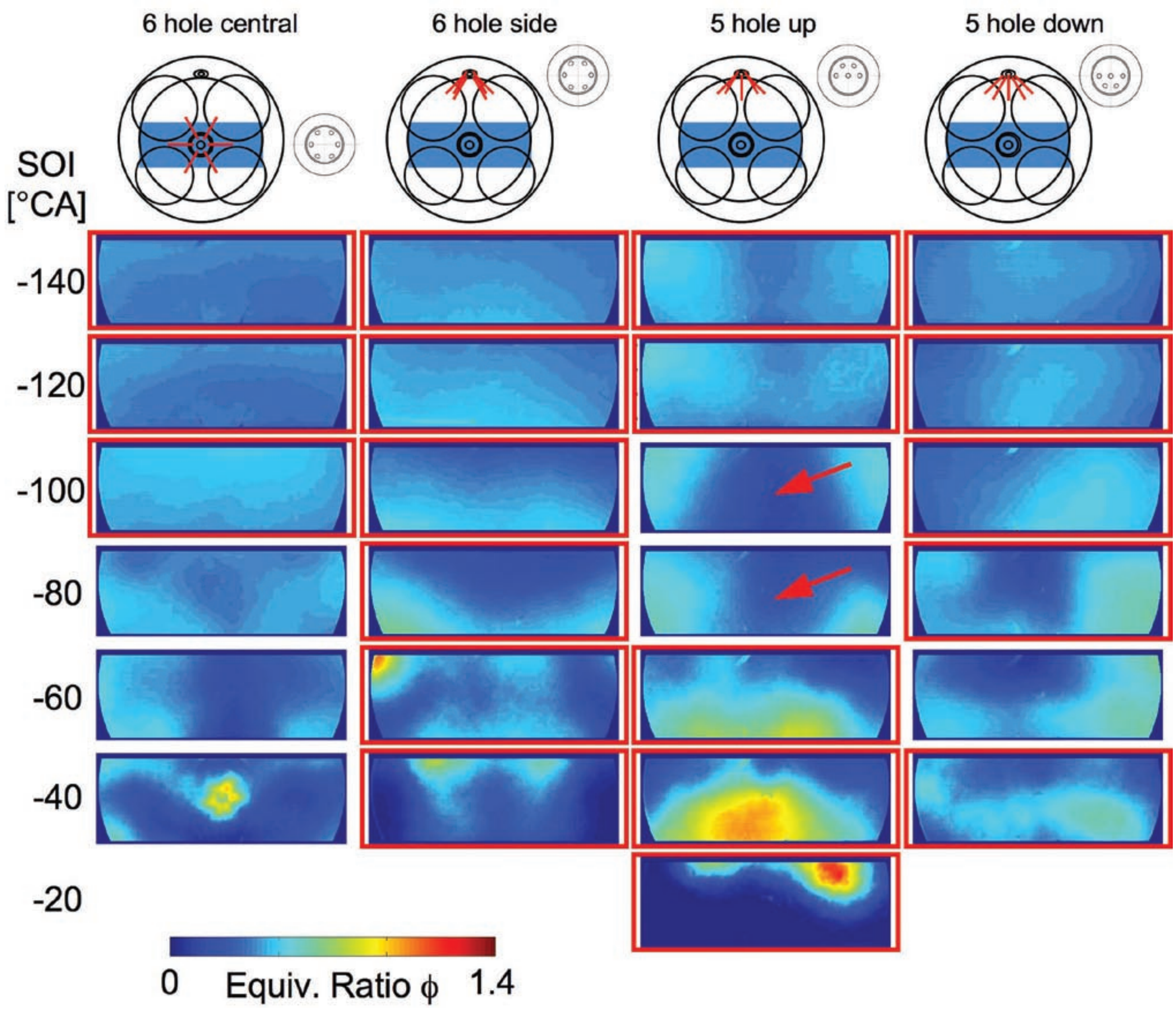

FIGURE 4. Mean equivalence-ratio fields for different injection timings and injectors in a horizontal plane close to the typical spark-plug location. The equivalent homogeneous, global equivalence ratio is 0.25. Framed images correspond to conditions for which stable, fired operation could be obtained at ANL. Arrows point to “fuel hole”; see text. Images are taken at the maximum-brake-torque spark timing from the ANL metal engine (different for each image, but generally, between 30°CA BTDC and TDC). 1,200 rpm, intake pressure 1 bar, injection pressure 80 bar.

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II.A.17 Advanced Diesel Engine Technology Development for High Efficiency, Clean Combustion

Donald Stanton
Cummins Inc.
1900 McKinley Ave.
Columbus, IN 47201

DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Carl Maronde

Subcontractors:
- Oak Ridge National Laboratory, Oak Ridge, TN
- BP Global Fuels Technology, Warrenville, IL

Objectives

- To design and develop advanced engine architectures capable of achieving U.S. Environmental Protection Agency (EPA) 2010 emission regulations while improving brake thermal efficiency by 10% compared to current production engines.
- To design and develop components and subsystems (fuel systems, air handling, controls, etc.) to enable construction and development of multi-cylinder engines.
- To perform an assessment of the commercial viability of the newly developed engine technology.
- To specify fuel properties conducive to improvements in emissions, reliability, and fuel efficiency for engines using high-efficiency clean combustion (HECC) technologies. To demonstrate a viable approach to reduce petroleum imports by at least 5% via renewable fuel sources. To demonstrate the technology is compatible with B20 (biodiesel).
- To further improve the brake thermal efficiency of the engine as integrated into the vehicle. To demonstrate robustness and commercial viability of the HECC engine technology as integrated into the vehicles.

Accomplishments

- Achieved a 13% to 15% improvement in efficiency compared to the project target of 10% using the HECC-developed technology with selective catalytic reduction (SCR) oxides of nitrogen (NOx) aftertreatment while meeting U.S. EPA 2010 emissions for Class 6, 7, and 8 commercial vehicles.
- Achieved an 8% improvement in efficiency compared to the project target of 10% using the HECC-developed technology with no NOx aftertreatment while meeting U.S. EPA 2010 emissions.
- Achieved a 13% to 15% increase in efficiency compared to the baseline engine results in a 5% fuel consumption avoidance while achieving an 8% to 10% net increase in efficiency compared to the 2007 current engine technology. The 5% fuel consumption avoidance is associated with the requirement to reduce system-out NOx from 1.2 g/bhp-hr to 0.2 g/bhp-hr.
- Fuel savings of 680 million gallons of oil per year for Class 8 trucks and fuel savings of 210 million gallons of oil per year for Class 6 and 7 trucks can be achieved based on the efficiency improvements demonstrated.
- Additional fuel consumption improvements of 3%-4% can be achieved through better integration of the engine with the transmission and vehicle systems.
- Supplier assessments for all the engine technologies have been completed. All key engine components will be supplied by Cummins Component Business units.
- U.S. EPA 2010 steady-state and transient NOx emissions compliance has been achieved without NOx aftertreatment for the 6.7L ISB engine used in the light-duty truck market while exceeding the 10% improvement in brake thermal efficiency project target. Drive cycle efficiency improvements range from 13% to 18%.
- Analysis and design of additional subsystem technology for the 6.7L ISB has been completed to enable an additional 5% improvement in brake thermal efficiency.
- The design and commercialization assessment of a new generation of Cummins XPI high-pressure common rail fuel system has been completed.
- Advanced turbomachinery has been designed and procured to provide fast transient response that is expected to allow engine-out transient NOx emissions compliance with acceptable particulate matter for the 15L ISX engine.
- A new exhaust gas recirculation (EGR) cooling system has been designed and tested that provides 1% to 2% fuel economy improvement on the 15L ISX and 6.7L ISB engine programs.
- New model-based air handling and combustion control algorithms have been created and validated for the 15L and 6.7L engine applications.

- HECC engine technology developed as part of this project has been shown to be robust for fuel economy and emissions with variations in diesel fuel properties representative of commercially-available fuels in the marketplace.
- The development of virtual and real fuel sensing technology is required to maximize the fuel economy benefit associated with the HECC technology when using renewable fuel sources such as biodiesel.
- The fuel economy benefits associated with the HECC engine technology developed can not be maintained when using biofuels at constant NOx emissions. However, a reduction of 20% to 40% in particulate matter can be achieved with the use of biofuels.

Future Directions

- Complete vehicle packaging studies for the engine and aftertreatment components.
- Development of aftertreatment thermal management techniques and hardware to optimize the engine and aftertreatment system to minimize the impact on engine efficiency.
- Development of an urea decomposition reactor to improve the SCR NOx conversion efficiency of the SCR catalyst. The urea decomposition reactor is used to convert aqueous urea to gaseous ammonia.
- Finalize the development of the SCR dosing system controls strategy.
- Improve the urea dosing system accuracy.
- Cost-thrift the ammonia slip catalyst.
- Reduce the aftertreatment pressure drop.
- Finalize the diesel particulate filter substrate material.
- Optimize the diesel oxidation catalyst formulation that thrifts the precious metal content.
- The impact of biofuels on diesel particulate filters will be explored.
- Development of on-board diagnostics associated with the implementation of the new HECC subsystem technology to achieve proper functioning during in-use operation.

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Introduction

Cummins Inc. is engaged in developing and demonstrating advanced diesel engine technologies to significantly improve engine thermal efficiency while meeting U.S. EPA 2010 emissions. The essence of this effort is focused on HECC in the form of low-temperature, highly premixed combustion in combination with lifted flame diffusion controlled combustion. Reduced equivalence ratio, premix charge in combination with high EGR dilution has resulted in low engine-out emission levels while maintaining high expansion ratios for excellent thermal efficiency. The various embodiments of this technology require developments in component technologies such as fuel injection equipment, air handling, EGR cooling, combustion, and controls. Cummins is committed to demonstrating commercially-viable solutions which meet these goals. Recent efforts have focused on integration of the engine technology with aftertreatment systems to maximize fuel efficiency improvements.

In addition to the engine technologies, Cummins is evaluating the impact of diesel fuel variation on the thermal efficiency, emissions, and combustion robustness of the HECC technology. Biofuels are also being evaluated as part of the fuels study to determine if the thermal efficiency improvements and emissions compliance can be maintained.

Approach

Cummins' approach to these project objectives continues to emphasize an analysis-led design process in nearly all aspects of the research. An emphasis is placed on modeling and simulation results to lead the way to feasible solutions.

Three areas of emphasis that lead to substantial improvements in engine thermal efficiency are the maximization of the engine closed cycle efficiency, the reduction of the open cycle losses and engine parasitics, and the integration of the HECC engine technology with aftertreatment. Engine system solutions to address the three areas of emphasis include air handling schemes, control system approaches, EGR cooling strategies, fuel system equipment, and aftertreatment design. Based on analysis and engine testing, subsystem component technologies are identified for further development. Cummins is uniquely positioned to develop the required component technologies via the Cummins Component Business unit. A variety of laboratory tests are conducted to verify performance and to tune system functions. Model predictions are verified and refined as necessary. Often, different portions of the system are pre-tested independently to quantify their behavior, and the data are analyzed in a model-based simulation before combined hardware testing is conducted. Concurrent to laboratory testing and tuning, vehicle system performance is planned and obtained. Once satisfactory test cell system performance is verified, the vehicle demonstration is conducted.

Data, experience, and information gained throughout the research exercise will be applied wherever possible to the final commercial products. Cummins intends to continue to hone its technical skill and ability through this research while providing satisfactory results for our customers. Cummins continues to follow this cost-effective, analysis-led approach both in research agreements with the Department of Energy as well as in its commercial product development. Cummins feels this common approach to research effectively shares risks and results.

Results

The U.S. EPA 2010 emissions standards pose a significant challenge for developing clean diesel powertrains that are affordable. Along with exhaust emissions, an emphasis on heavy-duty vehicle fuel efficiency is being driven by increased energy costs as well as the potential regulation of greenhouse gases. An important element of the success of meeting emissions while significantly improving efficiency is leveraging Cummins component technologies such as fuel injection equipment, aftertreatment, turbomahcinery, electronic controls, and combustion systems. Innovation in component technology coupled with system integration is enabling Cummins to move forward with the development of high-efficiency clean diesel products with a long-term goal of reaching a 57% peak brake thermal efficiency for the engine plus aftertreatment system. The first step in developing high-efficiency clean products has been supported by the DOE through the HECC project.

The Cummins global product strategy for diesel powertrain systems is to create engine architectures that allow system calibration to achieve a wide range of system-out NOx compliance to meet the diversity of future worldwide exhaust emissions standards. A variety of engine architectures is being explored by Cummins to meet U.S. EPA 2010 NOx emissions based on two primary strategies to control NOx: cooled EGR and SCR. An in-cylinder solution for NOx control based on cooled EGR can be achieved with advancements in component technology thus eliminating the need for NOx aftertreatment. The current in-cylinder architecture can achieve compliance with the 2010 NOx regulation along with particulate matter compliance with the use of a diesel particulate filter. The fuel economy of the system is comparable with the 2007 current product.

Much of the enabling technology for in-cylinder NOx control can also be used to provide significant fuel economy improvements for the variety of SCR-related architectures. However, there still remains a greater than 7% fuel economy benefit associated with the SCR architectures compared to the in-cylinder NOx control architecture using the same component technology. Additional engine performance capability can be achieved in the form of increased power density for an SCR engine architecture assuming the vehicle application can accommodate a larger catalyst size. The larger catalyst poses challenges for vehicle packaging, thermal management of the catalyst bed temperature, and cost. Therefore, there exists a complex system integration and optimization task to select the right SCR catalyst size for a given power density that can involve also the choice of engine displacement for a given application. Analysis and engine testing at Cummins indicate that the SCR engine architecture is better suited for engine downsizing compared to an in-cylinder solution. The power density of the in-cylinder NOx control architecture is limited by peak cylinder pressure (PCP) due to the high rate of charge flow. If the PCP capability of the engine is increased, higher power density levels can be achieved.

For the engine architectures that contain cooled EGR, there exists an opportunity to recover some of the waste heat from the EGR system and the exhaust stream. Analysis indicates that a 10% fuel economy improvement is possible with an organic Rankine cycle waste heat recovery (WHR) system. The fuel efficiency improvement can be obtained via 6% from EGR-derived WHR, 2% from exhaust-derived WHR, and 2% from the use of electrical accessories. Engine experiments have shown that a 5% improvement is possible from the EGR-derived WHR system which is in good agreement with the analysis. Additional engine testing is planned to validate the benefits of exhaust derived WHR and electrical accessories.

Conclusions

During the Fiscal Year 2008, all Phase 3 milestone and deliverables have been met for the Cummins HECC project with the successful close-out of the Phase 3 work. Accomplishments include:

- Achieving a 13% to 15% improvement in efficiency compared to the project target of 10% using HECC-developed technology with SCR NOx aftertreatment while meeting U.S. EPA 2010 emissions for Class 6, 7, and 8 commercial vehicles.
- Achieving an 8% improvement in efficiency compared to the project target of 10% using HECC-developed technology with no NOx aftertreatment while meeting U.S. EPA 2010 emissions.
- Achieving a 13% to 15% increase in efficiency compared to the baseline engine results in a 5% fuel consumption avoidance while achieving an 8% to 10% net increase in efficiency compared to the 2007 current engine technology. The 5% fuel consumption avoidance is associated with the requirement to reduce system-out NOx from 1.2 g/bhp-hr to 0.2 g/bhp-hr.
- Fuel savings of 680 million gallons of oil per year for Class 8 trucks and fuel savings of 210 million gallons of oil per year for Class 6 and 7 trucks can be achieved based on the efficiency improvements demonstrated.

- Additional fuel consumption improvements of 3%-4% can be achieved through better integration of the engine with the transmission and vehicle systems.
- Supplier assessments for all the engine technologies have been completed. All key engine components will be supplied by Cummins Component Business units.
- U.S. EPA 2010 steady-state and transient NOx emissions compliance has been achieved without NOx aftertreatment for the 6.7L ISB engine used in the light-duty truck market while exceeding the 10% improvement in brake thermal efficiency project target. Drive cycle efficiency improvements range from 13% to 18%.
- Analysis and design of additional subsystem technology for the 6.7L ISB has been completed to enable an additional 5% improvement in brake thermal efficiency.
- The design and commercialization assessment of a new generation of Cummins XPI high-pressure common rail fuel system has been completed.
- Advanced turbomachinery has been designed and procured to provide fast transient response that is expected to allow engine-out transient NOx emissions compliance with acceptable particulate matter for the 15L ISX engine.
- A new EGR cooling system has been designed and tested that provides 1% to 2% fuel economy improvement on the 15L ISX and 6.7L ISB engine program.
- New model-based air handling and combustion control algorithms have been created and validated for the 15L and 6.7L engine applications.
- HECC engine technology developed as part of this project has been shown to be robust for fuel economy and emissions with variations in diesel fuel properties representative of commercially available fuels in the marketplace.
- The development of virtual and real fuel sensing technology is required to maximize the fuel economy benefit associated with the HECC technology when using renewable fuel sources such as biodiesel.
- The fuel economy benefits associated with the HECC engine technology developed can not be maintained when using biofuels at constant NOx emissions. However, a reduction of 20% to 40% in particulate matter can be achieved with the use of biofuels.

II.A.18 High Efficiency Clean Combustion (HECC) Advanced Combustion Report

Chris Gehrke
Caterpillar, Inc.
PO Box 1875
Peoria, IL 61656-1875

DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Carl Maronde

Subcontractors:
- ExxonMobil, Paulsboro, NJ
- Sandia National Laboratories, Livermore, CA
- IAV Automotive, Detroit, MI
- eServ, Peoria, IL
- ENSYS, Madison, WI

Objectives

- Identify and develop technologies to enable low-temperature, high-efficiency combustion.
- Define technologies necessary to achieve a 10% reduction in fuel consumption while meeting Environmental Protection Agency 2010 on-highway and Tier 4 non-road emissions requirements.

Accomplishments

- Identified relationship between liquid fuel impingement, efficiency and emissions.
- Completed single-cylinder engine testing of gasoline/diesel fuel blends.
- Demonstrated emissions and fuel consumption benefit under laboratory conditions of premixed-charge, compression ignition (PCCI) combustion with a Caterpillar C15 engine.
- Developed and validated jacket water boiling model to allow accurate prediction of heat transfer to engine coolant.
- Identified cause of variable compression ratio (VCR) engine bearing failure and proposed design changes to eliminate failure mode.

Future Directions

- Single-cylinder engine testing of gasoline/diesel fuel blends with optimized engine hardware.
- Study evaporating and combusting sprays of gasoline/diesel fuel blends.
- Validate precision cooling design methodology and demonstrate reduced heat transfer to jacket water.
- Evaluate multi-hole spray impact on lifted flame diffusion combustion.
- Complete development and validation of wall film model to improve simulation accuracy of combustion using early injection timing, such as PCCI.
- Optimization of PCCI combustion system hardware to extend operating range.
- Complete bearing analysis of redesigned VCR and finalize design changes.

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Introduction

Improving fuel efficiency while meeting future emissions levels in the diesel on-road and off-road environments is an extremely difficult challenge but is necessary to maintain the level of customer value demanded by the end-users of compression ignition engines. Caterpillar® is currently engaged with several partners to address this challenge using advanced low-temperature combustion regimes enabled by advanced fuel system technologies and advanced engine design concepts. Advanced combustion regimes can provide a direct improvement in thermodynamic efficiency, as well as an indirect benefit in the form of lower particulate emissions, which in turn, require less fuel consumption for diesel particulate filter regeneration.

Approach

This project provides a fundamental understanding of the in-cylinder fuel/air mixing and combustion process, including the impact of fuel properties, through the use of single-cylinder engine testing, advanced optical diagnostics and computational fluid dynamics. We are actively developing high-efficiency, clean combustion (HECC) enabling technologies such as fuel injection technologies, controls strategies, heat rejection reduction technologies and advanced engine concepts. The integration of enabling technologies and advanced combustion recipes is performed using engine system simulation tools and validated through multi-cylinder engine testing. Successful completion of this project will provide Caterpillar® and DOE with a clear understanding of the technology hurdles that must be overcome to increase the thermal efficiency and reduce emissions on future compression ignition engines.

Results

Sandia Optical Engine Experiments: Activities at Sandia National Laboratories during Fiscal Year 2008 centered on studying a principal barrier to achieving HECC using early direct injection of diesel fuel: the creation of liquid fuel films on in-cylinder surfaces. The resultant understanding of the relationships between fuel films, efficiency, and emissions gained in FY 2008 can be summarized as follows. Liquid fuel films on in-cylinder surfaces should be avoided. For the conditions studied (which are representative of those proposed for future engine operating modes), the formation of fuel films can occur, leading to incomplete combustion, which in turn can cause increased fuel consumption and dilution of the lubricating oil. In addition, if the fuel vapor above a film ignites to produce an intensely luminous pool fire, the fuel-rich gas mixture produces soot well into the expansion stroke when bulk-gas temperatures and mixing rates are insufficient to oxidize it, leading to elevated smoke emissions. Meanwhile, near-stoichiometric regions around the rich mixture can produce nitrogen oxide (NOx) emissions. Radiative heat transfer from the pool fire to the fuel film enhances vaporization and combustion of the film, yielding lower unburned hydrocarbon (HC) and carbon monoxide (CO) emissions than if an intensely luminous pool fire is not produced; nevertheless, HC and CO emissions are still high enough to require the use of an oxidation catalyst to meet emissions regulations. On the other hand, if an intensely luminous pool fire is not produced above a fuel film, hot soot is not formed in the vapor region above the film. The lack of heat transfer to the film from radiating soot in a pool fire inhibits film vaporization and subsequent combustion, leading to even higher HC and CO emissions. NOx emissions may be high or low in this latter case, since they are controlled primarily by the bulk-gas mixture preparation (particularly in the absence of a pool fire).

The observations above are the result of experiments in the single-cylinder optical research engine engine using a conventional ultra-low-sulfur #2 diesel fuel (HV0), a high-volatility mixture of 20 vol% toluene with balance *n*-heptane (HV100), and blends of 28, 56, and 78 vol% of HV100 in HV0 (denoted HV28, HV56, and HV78, respectively). It is noted that HV100 was formulated to have approximately the same ignition quality as HV0 so that the results represent inasmuch as possible the effect of changing fuel volatility only (given the compositional differences between HV0 and HV100). Figure 1 shows selected frames from spray-visualization and natural-luminosity movies acquired with HV0 and HV100, and Figure 2 shows the efficiency and emissions data for all of the fuels. The figures show that the absence of liquid-fuel impingement on in-cylinder surfaces is accompanied by substantial improvements in efficiency, smoke, HC, and CO, while NOx compliance with 2010 on-highway regulations is maintained for intermediate injection timings. The new insights gained through these experiments are consistent with and help unify trends reported in the literature into a simple conceptual understanding. Such an enhanced understanding can assist engine designers and fuel producers in identifying improved operating strategies and fuel specifications.

Multi-Cylinder Combustion Development: A series of tests were conducted to assess the performance of part-load PCCI combustion on a production-like C15 engine at 2010 emissions levels. The premixing associated with PCCI enabled lower soot emissions by producing a leaner air-fuel mixture prior to ignition. The premixed mixture also burns more quickly. The shorter burn duration, if phased properly can lead to lower specific fuel consumption as shown in Figure 3. The results showed a 4% improvement in fuel economy at part-load versus conventional diffusion combustion. As load was increased the combustion phasing advanced due to increased boost levels and charge temperatures. This phasing shift caused the fuel consumption benefit to diminish.

Using an engine model simulation, based on the C15 PCCI test results, the potential thermal efficiency benefit was determined assuming optimal combustion phasing could be maintained. The results in Figure 4 show that a fuel consumption reduction of 3-7% can be achieved if the expansion ratio can be maintained, and if an acceptable equivalence ratio can be achieved with adequate premixing. Thus the challenge is to achieve sufficient ignition delay without sacrificing too much expansion ratio or trapped air mass in the cylinder.

Fuel Property Effects Investigation: One possible avenue to extend the load range of PCCI combustion is through the use of a fuel with more desirable ignition and volatility characteristics. Previous testing has shown that decreasing the indicated cetane number allows higher load to be achieved. Increased fuel volatility would allow fuel vaporization to occur earlier in the compressions stroke, increasing the allowable fuel injection window and thus increase premixing. Since no commercial fuel is available that meets those requirements, gasoline/diesel fuel blends were investigated. In collaboration with ExxonMobil, single-cylinder engine tests were conducted using a series of gasoline/diesel fuel blends. The results were encouraging and future testing is planned to study the fuel effects further.

VCR Engine Development: Another option for extending the PCCI load range is to reduce compression ratio as load increases. A potential mechanism for changing compression ratio is the VCR engine that was previously developed under this project. The engine functioned properly, and an initial round of engine testing was completed in FY 2007. However, an inspection of the engine revealed two significant bearing failures. An analysis of the failures was completed, and

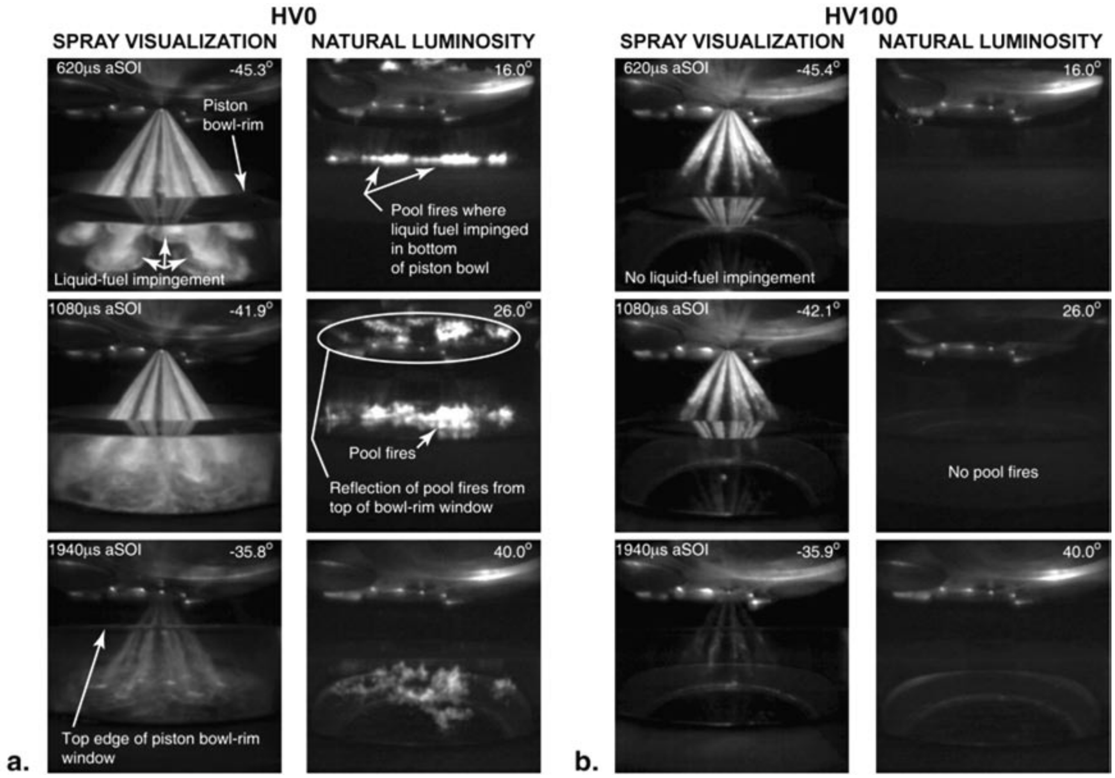

FIGURE 1. Images from spray-visualization and natural-luminosity movies acquired for: (**a**) a conventional ultra-low-sulfur #2 diesel fuel (HV0), and (**b**) a higher-volatility mixture of 20 vol% toluene with balance *n*-heptane (HV100). All images were acquired by viewing through a window in the cylinder wall. The spray-visualization images in (**a**) show that the lower-volatility HV0 leads to impingement of liquid fuel on the top of the piston, and the natural-luminosity images show that pool fires are observed later in the cycle at the impingement locations. In contrast, the images in (**b**) show that the higher-volatility HV100 does not exhibit liquid-fuel impingement or pool fires. The crank angle after top dead center (ATDC) at which each image was acquired is shown in the upper-right corner of the image frame. The engine operating parameters for all images are: 1,200 rpm speed, 4.82 bar gross indicated mean effective pressure load, actual start of injection -50° ATDC, 42°C intake temperature, 1.42 bar intake manifold pressure (abs.), 50% exhaust gas recirculation (simulated), 142 MPa injection pressure, and a dual-row injector tip with 15 orifices of 103-μm diameter (5 orifices at 35° included angle and 10 orifices at 70° included angle).

the root causes were identified. Design changes to the bearings have been proposed, and analysis of the new designs will be complete in early FY 2009.

Precision Cooling Development: To help mitigate the increased jacket water heat rejection associated with advanced low-temperature combustion regimes, efforts have been made to minimize heat transfer through the cylinder head and cylinder liner. An analytical tool has been developed to accurately predict the heat transfer from the combustion chamber to the block/head material, the jacket water and to ambient. The key challenge of the tool was accurately predicting the location and magnitude of coolant boiling. In FY 2008, a boiling model was successfully implemented that allowed the physics of heat transfer, fluid dynamics and boiling to concurrently predict heat transfer and metal temperatures. This tool will be used to optimize cylinder head and block designs that minimize heat transfer to jacket water.

Conclusions

- Liquid fuel impingement on in-cylinder surfaces results in lower combustion efficiency and increased NOx, soot and HC emissions. Liquid impingement should be avoided.
- Demonstrated 4% fuel efficiency improvement using PCCI combustion under laboratory conditions at part-load on a production-like C15 engine. If optimal phasing can be maintained, a fuel efficiency benefit of 4-7% over a larger load range would be possible under laboratory conditions.
- Identified root cause of VCR engine bearing failure, and proposed design changes. Analysis of the design changes will be completed in FY 2009.
- A boiling model was successfully implemented into the conjugate heat transfer analysis tool that allows accurate prediction of heat transfer and metal temperatures.

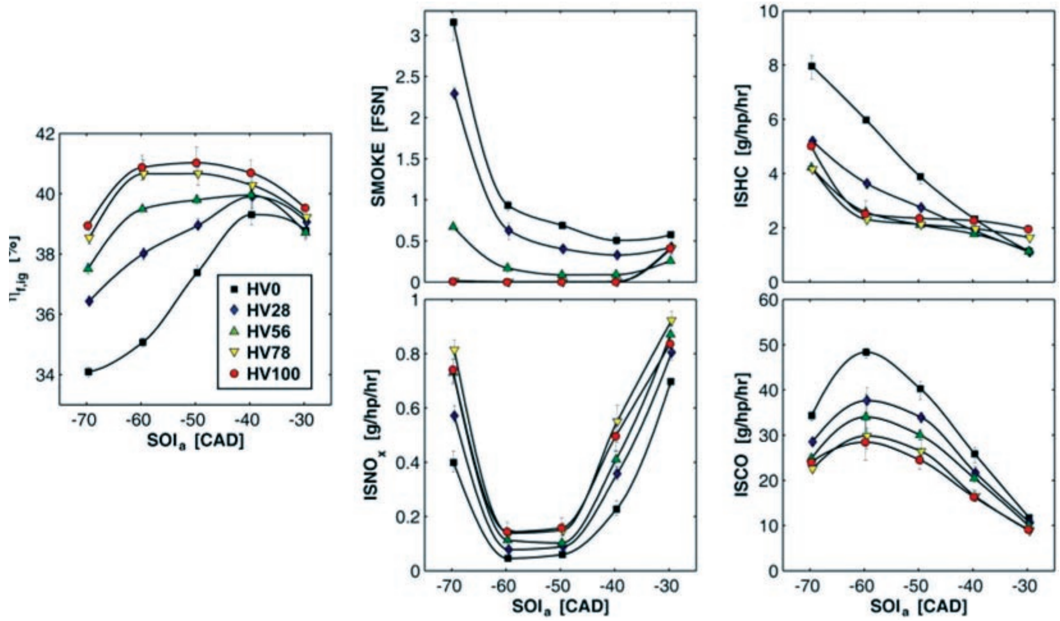

FIGURE 2. Gross indicated fuel-conversion efficiency ($\eta_{f,ig}$), smoke, and indicated-specific nitrogen oxides (ISNOx), unburned hydrocarbons (ISHC), and carbon monoxide (ISCO) emissions for HV0, HV28, HV56, HV78, and HV100 over a range of actual start-of-injection (SOI_a) timings. All other operating conditions are the same as those listed in the caption of Figure 1. In general, efficiency increases and smoke, HC, and CO emissions decrease as fuel volatility is increased, while NOx emissions are still compliant with 2010 on-highway truck engine limits for intermediate SOI_a timings.

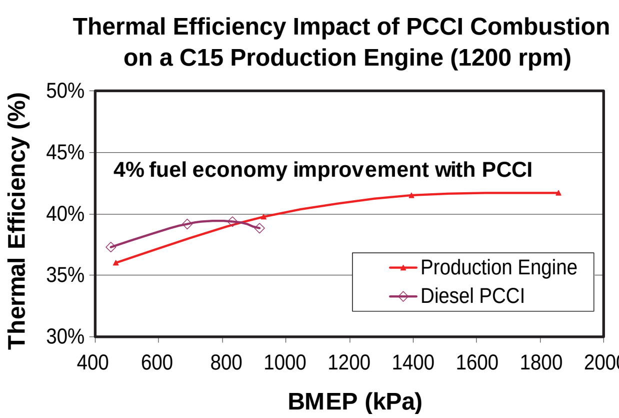

FIGURE 3. Impact of PCCI combustion on a production-like C15 engine at EPA 2010 on-highway emissions levels.

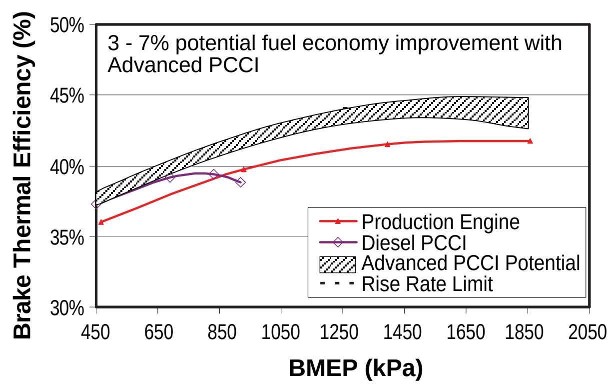

FIGURE 4. Simulated impact of advanced PCCI combustion with optimally phased combustion on the brake thermal efficiency of a C15 engine.

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2. David Milam, "Development of Enabling Technologies for High Efficiency, Low Emissions Homogeneous Charge Compression Ignition Engines", US DOE Program Merit Review, Feb. 26, 2008.

3. Chris Gehrke, Hari Sivadas, Tim Bazyn and David Milam, "The Role of Advanced Combustion in improving Thermal Efficiency", 2008 DEER Conference, August 4, 2008.

4. Charles J. Mueller, Glen C. Martin, David M. Milam, Michael S. Radovanovic and Christopher R. Gehrke, "Optical Engine Study of a Low Temperature Combustion Strategy Employing a Dual Row Narrow-Included-Angle Nozzle and Early, Direct Injection of Diesel Fuel", 2008 DEER Conference, August 6, 2008.

5. Glen C. Martin, Charles J. Mueller, David M Milam, Michael S. Radovanovic and Christopher R. Gehrke, "Early Direct-Injection, Low Temperature Combustion of Diesel Fuel in an Optical Engine Utilizing a 15-Hole, Dual Row, Narrow-Included-angle Nozzle," SAE 2008-01-2400.

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2. Kevin Duffy, et al., "Exhaust Gas Recirculation in a Homogeneous Charge Compression Ignition Engine", US Patent No. 7,377,270, May 27, 2008.

3. Kevin Duffy, et al. "Dynamic Control of a Homogeneous Charge Compression Ignition Engine", US Patent No. 7,380,540, June 3, 2008.

II.A.19 Low-Temperature Combustion Demonstrator for High Efficiency Clean Combustion

William de Ojeda, PhD, PE
Navistar, Inc.
10400 W. North Avenue
Melrose Park, IL 60160

DOE Technology Development Manager:
Kenneth Howden

NETL Project Manager: Samuel Taylor

Subcontractors:
- Lawrence Livermore National Laboratory
- Continental
- BorgWarner
- Mahle
- ConocoPhillips
- University of California, Berkeley
- Ricardo

Objectives

- Demonstrate low-temperature combustion (LTC) in a multi-cylinder engine with a power density of 12.6 bar brake mean effective pressure (bmep).
- Demonstrate engine operation over transient emission cycles.
- Achieve oxides of nitrogen (NOx) U.S. 2010 engine-out emissions without aftertreatment.
- Achieve 10% fuel efficiency improvement over conventional combustion.

Accomplishments

Present project applies LTC to the Navistar 6.4L V8 engine. Highlights over the course of this year include:

- Half way through 2008 Navistar achieved the **DOE load target of 12 bar bmep**. The work was later extended to **higher loads, attaining 16.5 bar bmep** by managing charge temperatures, dilution ratios, and fuel injection strategies. Testing was closely coordinated with computational fluid dynamics (CFD)-KIVA studies which correlated well with experiments, and provided a fundamental understanding of the combustion process.
- The impact of LTC on **fuel economy was 5 to 15% better** than the conventional engine.
- NOx levels were limited to below 0.2 g/bhp-hr with soot levels adequate for a diesel particulate filter.

Future Directions

- **Explore the impact of valve timing on LTC**. The engine demonstrator was reassembled with an electro-hydraulic variable valve actuation (VVA) system developed during the course of this project. The engine will be ready for testing on 1 November 2008. The VVA system will be used to explore the impact of valve timing on effective compression ratio and improved engine thermal efficiency.
- KIVA simulations have captured key elements of the combustion process, matching temperature and heat release traces. The simulations gave good correlations with experimental data in single- and multiple-injection conditions. This tool should be used to further **optimize combustion hardware and new boundary conditions** to extend the operation of LTC.
- The engine will run through the federal **transient heavy-duty cycle**. For this purpose, the project scope includes the development of a prototype electronic control unit to handle in-cylinder combustion diagnostics and feedback.

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Introduction

LTC has the potential to reduce engine-out NOx emissions to 2010 federal limits without the use of aftertreatment devices [1]. The benefits of LTC have been documented [2] as capable to lower NOx emissions due to low combustion temperatures. Improved fuel economy and lower soot emissions can likewise be attained with lean mixtures.

The attaining of low NOx has been attempted by various mechanisms, ranging from homogeneous charge compression ignition (HCCI) to LTC. HCCI is established by a lean, well-premixed mixture that autoignites at multiple points in the combustion chamber. HCCI is particularly difficult with diesel fuel due to its low volatility and high cetane number. The fuel needs to be injected late in the compression cycle to allow for sufficient temperatures to vaporize the fuel. The high cetane number or the high propensity to autoignite can cause large rates of pressure rise. LTC, conditioned by dilute mixtures with heavy exhaust gas recirculation (EGR), on the other hand can yield increased unburned hydrocarbon (UHC) emissions from long mixing times due to local equivalence ratios (ϕ) below the lean combustion limit [3].

In an attempt to harness the advantages of both HCCI and LTC the work at hand uses a partially premix charge compression ignition combustion [4] strategy. Work demonstrated NOx~0.2 g/hp-hr and an aftertreatment-tolerant soot level can be obtained with this concept up to a load of 16.5 bar bmep.

Approach

Implementation of LTC was integrated into the production engine using the following approach:

- Phase I (completed) consisted of applied research, determining engine boundary conditions, and combustion system design.
- Phase II (completed) consisted of exploratory development, engine hardware and control system procurement, and controls software development.
- Phase III (completed) consisted of steady-state engine testing, optimization of combustion hardware and fueling strategy, and further controls system development.
- Phase IV (in progress) consists of transient testing. This phase will also demonstrate the capabilities of the VVA version of the engine.

Results

Extending the LTC load range. The target lug line of the engine where LTC was to be applied is shown in Figure 1. This DOE target line is compared with the 2007 model year base engine lug line, and the area where LTC extended beyond the DOE target. The figure highlights three areas where the NOx target of 0.2 g/bhp-hr was attained: (**A**) attained either with high EGR and advanced timing or by very advanced timing and leaner conditions (less EGR) characteristic of HCCI; (**B**) by means of EGR and advanced timing, with one or multiple pilot injections; (**C**) with pilot and post injection.

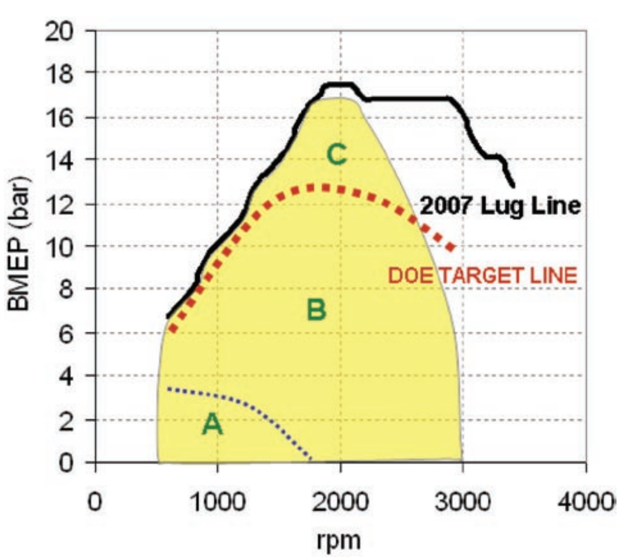

FIGURE 1. Operation Range of LTC

Combustion with pilot and main injection events. Pilot-main injection strategies enhanced homogeneity and were effective in reducing soot. Both quantity and timing contributed to homogenization. Figure 2 shows the effect of pilot quantity at 10 bar bmep and 1,750 rpm, a point representative of region (**B**). For a constant NOx, the increase of pilot reduced soot. The pilot injection timing was 50° before top-dead center and the combustion phasing was kept constant. The pilot quantity had negligible effect on efficiency and increased UHC minimally, below 1 g/bhp-hr.

CFD analysis. Pilot injection strategy helped reduce soot by 1 filter smoke number (FSN), the result of better fuel-air mixing during the long ignition delay provided by the pilot injection. KIVA-3V was used to understand this phenomenon. Figure 3 shows the NOx

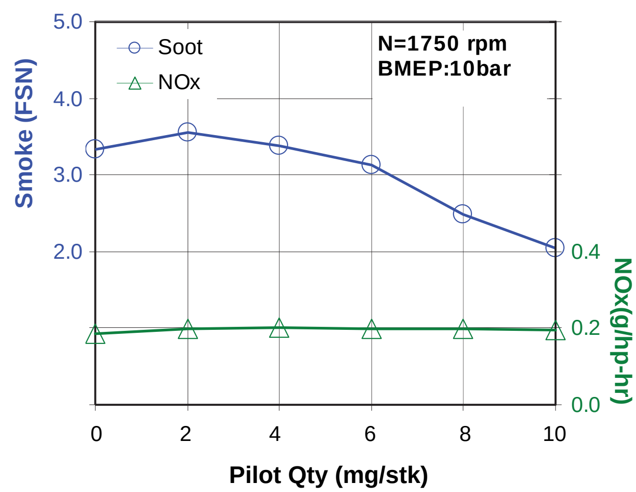

FIGURE 2. Effect of Pilot Injection Quantity

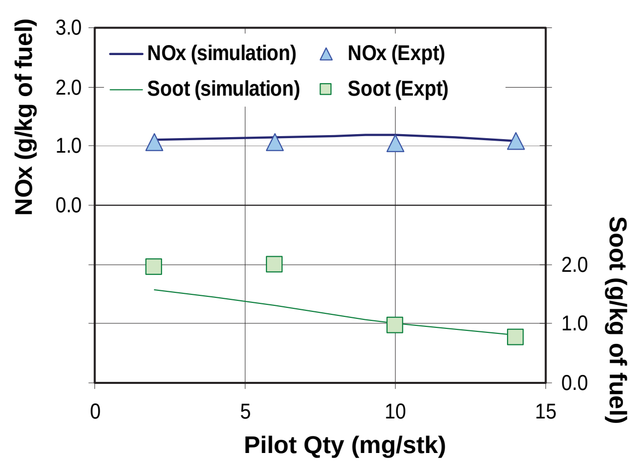

FIGURE 3. Predictive Capability of Emissions

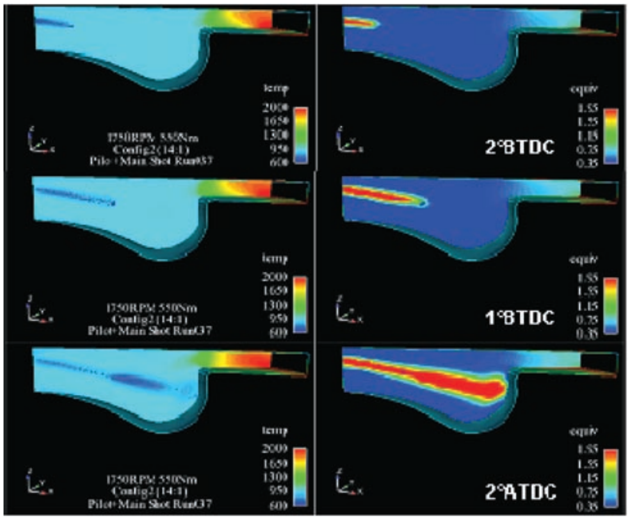

FIGURE 4. Simulation of a Main Following a Pilot Injection

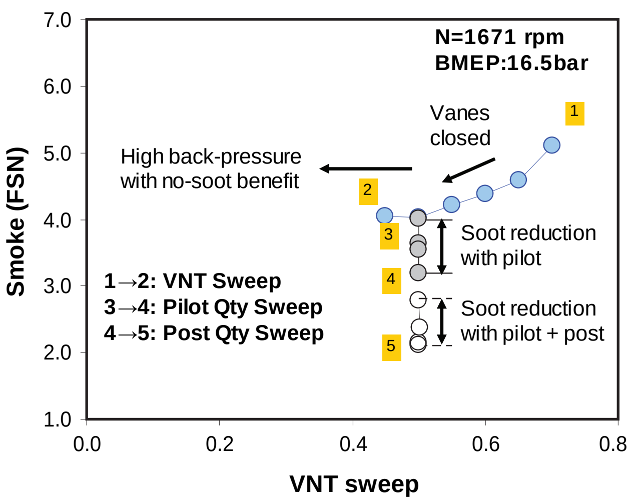

FIGURE 5. Effect of Injection Strategy (NOx = 0.2 g/bhp-hr constant; VNT = variable nozzle turbine)

predictions were accurate for pilot injection ranging from 2 to 14 mg. The soot trend was correct, though it was under-predicted at low pilot quantities. A detail of the simulation is shown in Figure 4. Here temperatures and ϕ contours are shown as the main injection takes place. The pilot combustion is visible at the edge of the cylinder wall in the squish region.

Combustion with post injection. At loads above 12 bar bmep the use of post injection was added to limit the soot emissions. Figure 5 shows a case at 16 bar, where the soot was treated by a combination of air system management (points 1-2), pilot injection (3-4) and post injection (5).

Fuel economy. LTC impact on emissions was accompanied by improvements to engine break thermal

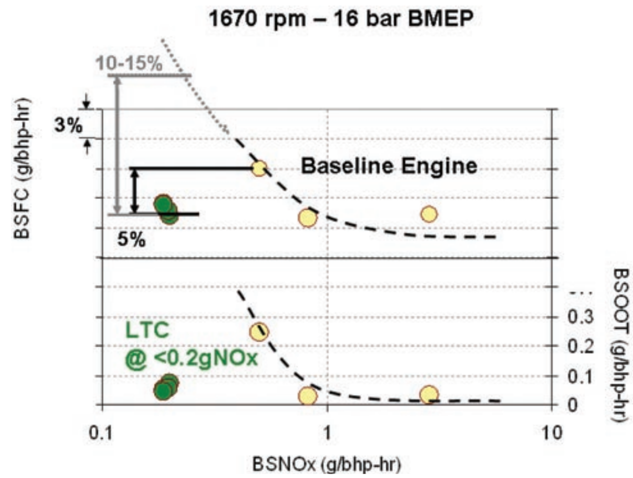

FIGURE 6. LTC Impact on Efficiency

efficiency. Figure 6 shows a load case of 16 bar running LTC compared with three base engine calibrations. LTC yielded 15% more efficiency at same emissions levels.

Conclusions

- Demonstrated 0.2 g NOx/bhp-hr with aftertreatment-tolerant soot level up to 16.5 bar bmep.
- Fuel efficiency improvements ranged from 5-15% over the conventional engine.
- EGR, intake temperature and injection strategy management were key enablers for LTC.
- A pilot-main injection strategy up to 12 bar was used to reduce soot largely in part due to lean homogenous cylinder charge mixtures prepared by the pilot injection.
- At high loads pilot injection strategy alone was insufficient for soot reduction and the soot reduction was enhanced by late cycle soot-oxidation of post injection.

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2. de Ojeda, W., Zoldak, P., Espinosa, R., Kumar, R., "Development of a Fuel Injection Strategy for Diesel LTC", SAE 2008-01-0057, SAE World Congress, Detroit.

3. de Ojeda, W., Zoldak, P., Espinosa, R., Kumar, R., Cornelius, D., "Multicylinder Diesel Engine Design for LTC operation", Diesel Engine Development, DEER 2008, August 4-8, Dearborn, Michigan.

II.A.20 Stretch Efficiency – Exploiting New Combustion Regimes

C. Stuart Daw (Primary Contact), Josh A. Pihl, V. Kalyana Chakravarthy, Jae-Soon Choi, Jim Conklin, A. Lou Qualls, Ronald L. Graves
Oak Ridge National Laboratory (ORNL)
National Transportation Research Center
2360 Cherahala Blvd.
Knoxville, TN 37932

DOE Technology Development Manager:
Gurpreet Singh

Objectives

- Analyze and define specific pathways to improve the energy conversion efficiency of internal combustion engines from nominally 40% to as high as 60%, with emphasis on opportunities afforded by new approaches to combustion.
- Establish proof-of-principle of pathways to stretch efficiency.

Accomplishments

- Developed conceptual design for bench-top cyclic constant volume combustor for demonstrating low-irreversibility combustion based on regenerative preheating with thermochemical recuperation.
- Confirmed with second law analysis that the fuel exergy losses associated with combustion irreversibility can be reduced by as much as 50% with thermochemical recuperation, thereby increasing overall engine efficiency by as much as 15% for fuels such as iso-octane.
- Characterized performance of reforming catalyst provided by an industrial partner in a flow reactor.

Future Directions

- Construct regenerative air preheating with thermochemical recuperation (RAPTR) bench-top constant-volume combustor.
- Experimentally demonstrate low-irreversibility combustion in the RAPTR bench-top apparatus.
- Analyze data from RAPTR experiments to determine efficiency implications and appropriate ways to model exergy losses under different operating modes.
- Continue exploring better ways for recuperating exhaust heat and utilizing compound cycles for extracting work.
- Continue exercising engine and combustion models to identify combustion modifications that would mitigate exergy losses.

Introduction

In conventional internal combustion engines, the largest efficiency losses (approximately 20-25% of the available fuel energy) occur in the combustion process itself. These losses are due to the generation of thermodynamic entropy by unrestrained chemical reactions. Processes that generate entropy are referred to as thermodynamically irreversible. Detailed analyses of the irreversibility of unrestrained combustion have shown that it comes mostly from 'internal heat transfer' between the products (exhaust gases) and reactants (fuel and air). Such heat transfer is inevitable in both pre-mixed and diffusion flames, where highly energetic product molecules are free to exchange energy with unreacted fuel and air [1]. Since these molecules have large energy (i.e., temperature) differences, considerable entropy is generated when they interact. The net effect is to divert some of the fuel energy into molecular motion and heat. According to the Second Law of Thermodynamics, this diverted energy becomes unavailable to produce useful work. However, it is theoretically possible to carry out combustion reactions in a more restrained way (closer to equilibrium) that produces less entropy and preserves more of the original fuel energy for work. The goal of this project is to identify and demonstrate strategies that enable combustion under conditions closer to chemical equilibrium and thereby increase the overall efficiency of the combustion process.

Approach

Our approach to improving internal combustion engine efficiency is to understand the losses in current engines and then develop ways to mitigate them. To this end, we previously conducted analytical studies of the exergy losses in current engines in collaboration with Professors Jerald Caton (Texas A&M University) and David Foster (University of Wisconsin). Exergy is a measure of the amount of energy available to do useful work. Based on these studies, we have quantified and reinforced that the irreversibility of the combustion step is the largest single contributor to fuel exergy loss. Our current efforts are focused on development, analysis, and experimental evaluation of novel approaches to combustion that can reduce this inherent irreversibility. A common theme of all the novel approaches being considered is that they attempt to create conditions under which the combustion reactions occur closer to a state of chemical equilibrium.

The first novel combustion approach being investigated combines two fundamental concepts to achieve reaction conditions closer to equilibrium:

- counterflow preheating of the inlet fuel and air with exhaust, and;
- catalytic steam reforming of the fuel as it is preheated.

Counterflow preheating brings the air and fuel feeds closer to the temperature of the combustion process in as reversible a manner as possible, minimizing the entropy generation due to internal heat transfer. Catalytic steam reforming converts the thermal energy recuperated from the exhaust into chemical energy in the fuel reformate. In essence, exhaust heat is used to upgrade the fuel to species with a higher heating value (hydrogen and carbon monoxide). These two concepts are specific implementations of more general concepts emerging from our previous analytical and literature investigations referred to as counterflow preheating with near-equilibrium reaction (CPER) [2] and thermochemical recuperation (TCR) [3].

Our efforts for Fiscal Year 2007 and early FY 2008 were focused primarily on constructing a bench-top experimental apparatus for studying the effects of CPER and TCR on constant-pressure combustion. However, reviewers at the FY 2008 Department of Energy Office of Vehicle Technologies Merit Review strongly suggested focusing the project on constant-volume combustion. In response to these comments, we changed course in the middle of FY 2008 and began studying recuperative preheating and reforming in the context of cyclic, unsteady, constant-volume combustion.

Results

Changing the focus of the project from steady-flow, constant-pressure combustion to cyclic constant-volume combustion required a shift in our approach to both the experimental demonstration and accompanying themodynamic analyses. In particular, where the constant pressure combustor relied on relatively simple counterflow heat exchangers, achieving reversible preheating in the context of cyclic constant volume combustion requires the use of a solid heat transfer material to store the residual heat in the combustor exhaust and transfer it to the feed streams. Placement of the reforming catalyst and its proximity to the combustion chamber is also complicated by the cyclical unsteady operation. Further, the combustion chamber itself must withstand higher pressures under constant-volume operation. These differences required us to create a completely new experimental apparatus.

Figure 1 shows our conceptual design for our revised experiment incorporating RAPTR. It incorporates three separate chambers and valves to control the transfer of gases between the chambers. The first chamber is used for precompression of the air. Once compressed, the air passes through the second chamber, which contains the thermal regenerator, and into the highly insulated combustion chamber. After fuel injection and ignition, the exhaust gases are passed back through the thermal regenerator and out through the exhaust valve. We will use measurements of temperature and pressure inside the combustion chamber to quantify the irreversibility of the combustion process while changing the degree of preheating and fuel reforming in the RAPTR system.

Shifting to a constant-volume approach also required modifications to our thermodynamic analysis tools. The key to achieving high efficiency in the RAPTR process lies in conducting the gas/solid heat transfer in the thermal recuperator as reversibly as possible. Accomplishing reversible heat transfer will require minimizing the temperature difference between the solid and the gas stream, which will necessitate careful management of the temperature profile inside the recuperator material. To this end, we are developing modeling tools that will enable First and Second Law thermodynamic analysis of thermal recuperator configurations to identify the most promising approaches for use in our experiments.

In parallel with development of the experiment apparatus and associated analysis tools, we have also evaluated a reforming catalyst for use in the RAPTR experiment. A commercial-intent reforming catalyst was obtained from an industrial partner. This catalyst was designed for partial oxidation reforming, so it was necessary to evaluate its performance in the steam reforming reactions used for thermochemical recuperation. This was accomplished using a bench-scale flow reactor. Experiments were conducted with methane or ethanol under various temperatures, space velocities, fuel concentrations, and fuel/steam ratios.

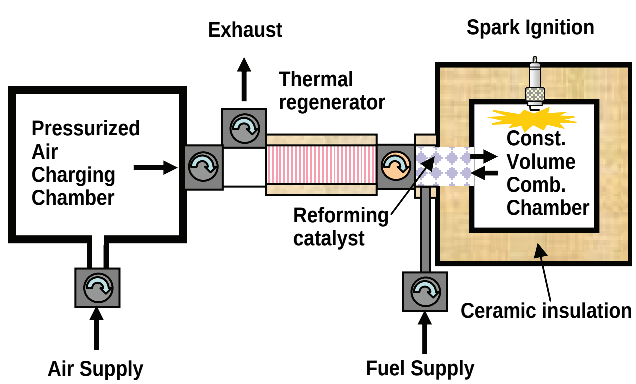

FIGURE 1. Conceptual Design of the RAPTR Experiment

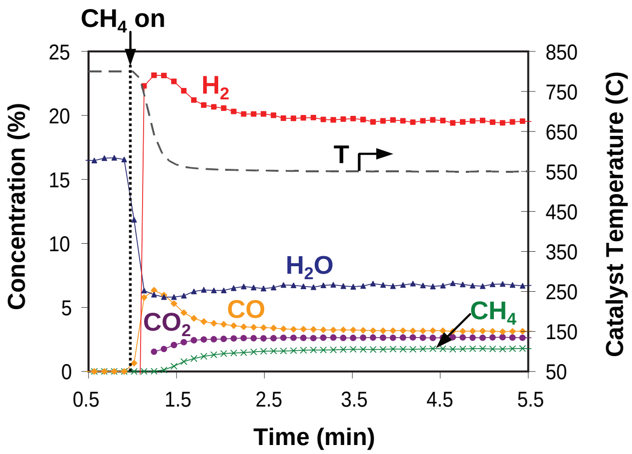

FIGURE 2. Typical reformer catalyst evaluation experiment. Catalyst heated to 800°C under 16.7% H_2O in N_2 at a space velocity of 60,000 h^{-1}. 8.3% CH_4 feed initiated at 1.0 min. Temperature measured with a thermocouple inserted into center of catalyst monolith core sample. CH_4, H_2O, CO, and CO_2 measured via Fourier transform infrared spectroscopy; H_2 calculated from H-atom balance.

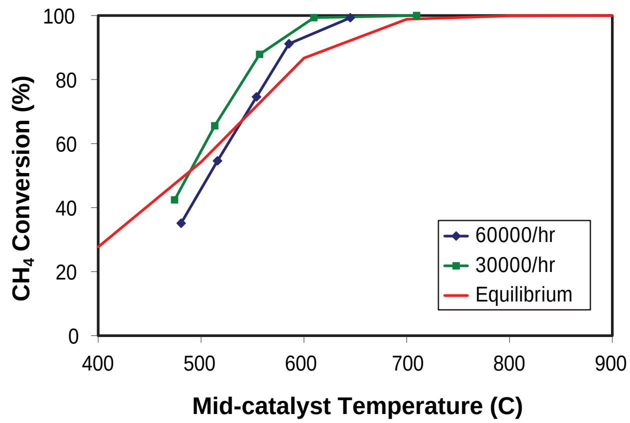

FIGURE 3. CH_4 reforming conversion as a function of catalyst temperature (measured in center of catalyst monolith core sample) and space velocity. Equilibrium values calculated assuming isothermal operation at measured catalyst temperatures and inlet feed concentrations.

Figure 2 shows the results of a typical methane reforming experiment. The catalyst monolith core sample was placed in a furnace and heated to 800°C under a flow of water vapor in nitrogen. After thermal equilibration, the methane feed was turned on. The endothermic nature of the reforming reactions caused a rapid decrease in the catalyst temperature by about 250°C. The RAPTR experiment will be designed such that the thermal recuperator will provide the necessary heat to drive the endothermic reforming reactions.

Figure 3 summarizes methane conversion as a function of temperature (measured in the center of the catalyst core sample) for all of our methane reforming experiments. For all operating conditions studied, we are achieving close to equilibrium conversion, showing the high effectiveness of the catalyst for steam reforming of methane. The drop-off in conversion with decreasing temperature also highlights the importance of thermal management in the regenerative preheater and reforming catalyst in the RAPTR experiment.

We also ran experiments with ethanol instead of methane. The reforming process was even more efficient with ethanol – we achieved conversions comparable to those obtained with methane at much lower temperatures. However, a continual degradation in catalyst performance was observed with ethanol feeds (see Figure 4). The cause of this degradation was identified as coking of the catalyst surface after a post-reforming oxidation step generated substantial carbon dioxide and a large exotherm (shown in Figure 5). We will continue to investigate operating conditions and/or different catalyst formulations that may minimize coking under ethanol reforming. We will also consider the efficiency impacts of coking in the RAPTR experiment.

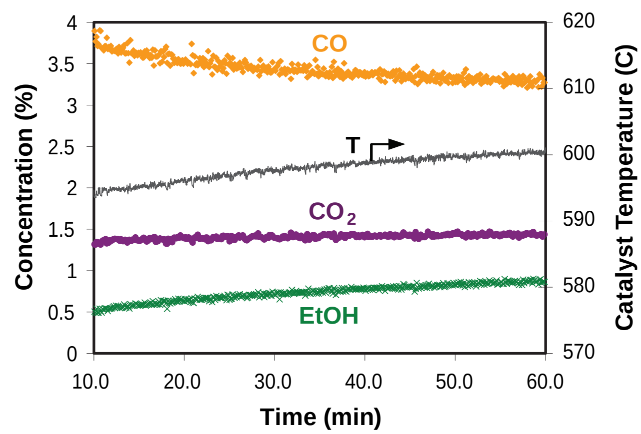

FIGURE 4. Typical ethanol reforming experiment. Feed composition: 4.2% EtOH, 12.5% H_2O, balance N_2, 60,000 h^{-1} space velocity. Furnace temperature: 700°C. Steadily decreasing CO and increasing EtOH and temperature illustrate slow degradation in catalyst performance.

Conclusions

Based on feedback from the 2008 DOE Vehicle Technologies Program Merit Review, we have shifted the focus of the project from a demonstration of preheating and thermochemical recuperation in an atmospheric pressure burner to one utilizing a constant-volume, cyclically operated combustor.

- A conceptual design for the new experiment (deemed RAPTR) has been created.
- Modeling tools needed to analyze the exergy balances in the system are under development.
- The performance of a reforming catalyst that will be used in the RAPTR experiment has been evaluated using a bench-scale flow reactor.

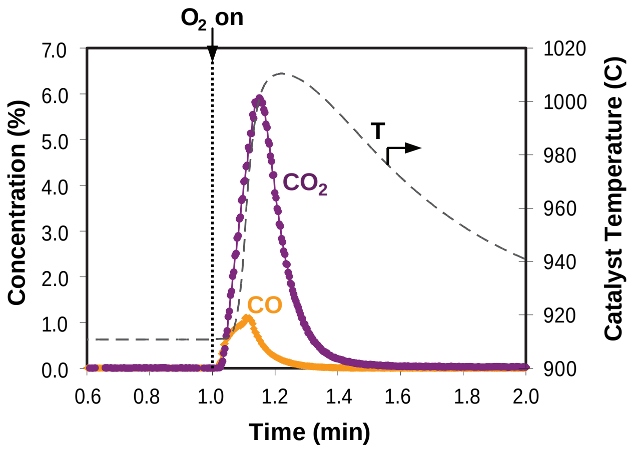

FIGURE 5. Post ethanol reforming oxidation experiment. Catalyst was heated to 900°C under N_2 at a space velocity of 30,000 h^{-1}. 10% O_2 flow initiated at 1.0 min. Large increase in temperature and CO_2 concentration is indicative of carbon oxidation, illustrating that performance degradation under ethanol steam reforming is due to coking of catalyst surface.

- Design and construction of the combustor will begin shortly.

Once completed, this combustor should provide the opportunity for the first experimental demonstration of a thermal combustion process that can retain a significant fraction of the exergy now destroyed in conventional combustors and combustion engines.

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II.A.21 Advancements in Engine Combustion Systems to Enable High-Efficiency Clean Combustion for Heavy-Duty Engines

Houshun Zhang (Primary Contact), Yury Kalish
Detroit Diesel Corporation
13400 Outer Drive, West
Detroit, MI 48239-4001

DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Carl Maronde

Objectives

Explore advancements in engine combustion systems to enable high-efficiency clean combustion (HECC) techniques to improve thermal efficiency and minimize cylinder-out emissions.

Accomplishments

- Experimentally demonstrated 5% thermal efficiency improvement on a multi-cylinder engine using advanced premixed charge compression ignition (PCCI) combustion concept at one engine operating point while maintaining the same emissions level
- Experimentally demonstrated over 4% fuel economy benefits on a multi-cylinder engine through transient Federal Test Procedure (FTP) cycle while simultaneously reducing particulate matter (PM) by 25% and oxides of nitrogen (NOx) by 15%, using validated next generation model-based control.
- Successfully completed project annual review with DOE in August 2008, passing the second "Go/No-Go" decision point by achieving 5% thermal efficiency improvement experimentally.
- Procured and flow bench tested variable injection nozzle hardware and evaluated its feasibility for injection mode switching.
- Evaluated advanced combustion concepts with advanced and flexible fuel injection system experimentally and analytically.
- Developed and validated model-based control modules for the simultaneous control of injection timing, injection pressure, pilot injection timing and exhaust gas recirculation (EGR) in an off-line computational environment.
- Explored potential of Detroit Diesel patented piston for optimal emissions and combustion through detailed combustion optimization and analysis. It is demonstrated that substantial benefits on soot reduction can be obtained with compromise on fuel economy.

Future Directions

- Consolidate fuel injection strategy and multiple combustion modes to maximize thermal efficiency while maintaining the same or lower engine-out emissions as baseline.
- Continue evaluation of different advanced combustion concepts with advanced fuel injection system.
- Continue steady-state advanced combustion development with implementation of genetic optimization recommendations for hardware procurement.
- Continue transient combustion and control development using next-generation model based control technology.
- Continue development and implementation of closed-loop real-time combustion control using novel in-cylinder sensors.

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Introduction

Detroit Diesel is conducting a multi-year cooperative agreement project with DOE on heavy truck engine development focusing on HECC. This project consists of three major tasks – (1) advanced concept development, (2) subsystem development, and (3) system integration. The primary objective of this project is to explore advancements in engine combustion systems using HECC techniques to improve thermal efficiency while minimizing cylinder-out emissions. Throughout the project, the integrated analytical tool box has been developed to define various promising conceptual engine system technologies and component enhancements, and then validate them with hardware experiments. The key enabling technologies have been aggressively pursued, making significant progress. This annual report will summarize the progress and key findings achieved during this annual report period.

Approach

Detroit Diesel has developed a proven concept and methodology of combining experimental and analytical tools to facilitate integrated engine, aftertreatment and vehicle development. Using the modes selected from typical vehicle operations, an advanced and integrated analytical tool box is used to carry our systematic simulation and design not only on individual components, but also on an integrated engine system. Those optimized individual component designs as well as the whole system will be validated experimentally through both steady-state and transient engine tests. With careful calibration optimization in a transient engine testing cell, the engine system will be then installed in a vehicle, performing comprehensive validations. The results from vehicle tests will again provide feedback to simulations, and then engine dyno tests. Thus iterations continue until an optimal system is obtained. During this iteration process, model-based control employing multiple input and output techniques plays a key role in enabling efficient integration of the various subsystems, ensuring optimal performance of each system within the total engine package. This system approach results in a shortened development cycle, and substantial NOx-PM trade-off and fuel economy improvement in both engines and vehicles.

In this specific combustion focused project, the technical approach is tailored to key combustion enabling technologies. One of them is a fully flexible fuel injection system, which can facilitate different advanced combustion modes. Working with fuel injection suppliers, a highly flexible fuel injection system was selected, which results in an unprecedented technical road map as shown in Figure 1. As can be seen in Figure 1, a highly flexible fuel injection system can greatly simplify the combustion strategy into three combustion zones, which feature emerging multi-mode combustion. Introduction of a genetic combustion optimization technique to the project in conjunction with advanced control technology can considerably enhance the project outcomes.

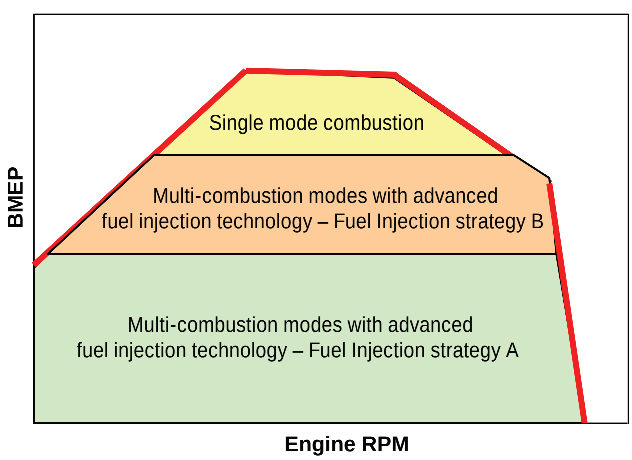

FIGURE 1. Strategy for Combustion Concepts Integration (BMEP - brake mean effective pressure)

Results

Advanced fuel injection system and advanced next generation model-based control were identified in the early stage of the project as key enabling technologies in achieving the project goals. This flexible fuel injection system is essentially a hybrid fuel injection system that consists of accumulator rail and unit injectors, allowing flexible multiple injection events and high injection pressure, which are key to facilitate different advanced combustion concepts. Use of advanced three-dimensional combustion and spray models with the help of a genetic optimization algorithm was made to down-select promising combustion concepts that have the potential to achieve the project goals. One of the specific combustion concepts under investigation is PCCI combustion. Table 1 shows parametric studies with injection timing, spray angle, and injection pressure in order to achieve optimal combustion, targeting 10% thermal efficiency benefits while maintaining the same emissions as baseline. As can be seen from Table 1, the case 12 demonstrated 10.8% improvement in fuel economy while maintaining about the same soot and NOx emissions as the baseline. With a proper selection of combustion timing and phasing guided by analytical results, use of this specific PCCI combustion realized 5.03% fuel economy improvement experimentally during preliminary testing stage, thanks to advanced flexible fuel injection system used in this project. It is likely that more thorough investigation will result in more favorable outcomes moving forward.

TABLE 1. PCCI Combustion Optimization

run	Soot	NOx	ISFC	Fuel economy improvement
	g/kgf	g/kgf	g/kW-hr	%
base	0.23	3.24	233.3	-
1	0.12	5.27	201.1	13.8
2	0.41	7.76	223.0	4.4
-----	-----	-----	-----	-----
11	0.33	1.98	212.9	8.7
12	0.19	3.72	208.1	10.8

ISFC - indicated specific fuel consumption

A multi-mode combustion concept was also thoroughly investigated. Early analytical simulations demonstrated that a unique dual-combustion mode with assistance of variable nozzle technology can provide substantial benefits in both engine fuel economy and emissions [1]. At the present, variable injection nozzle hardware was procured and flow bench tested and its feasibility for injection mode switching is currently under evaluation. Figures 2a and 2b display the flow bench test results, showing the two distinct spray patterns within one cycle. Figure 2a is of a narrow spray angle

FIGURE 2A. First Phase Injection with Conical Spray and Narrow Spray Angle

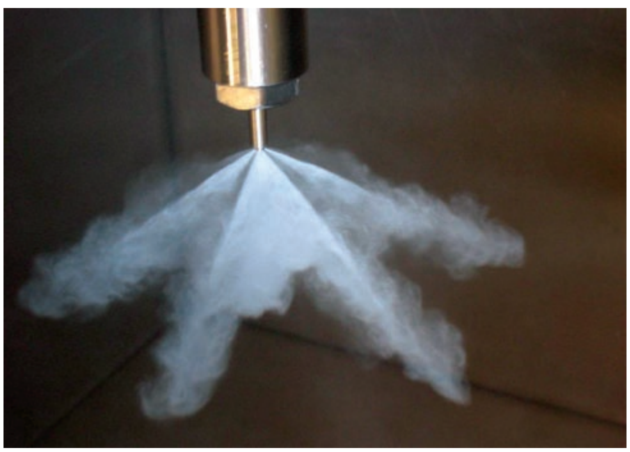

FIGURE 2B. Second Phase Injection with Multi-Jet Spray and Wide Spray Angle

injection with conical spray, specifically used in the early injection, while Figure 2b is of a wide spray angle injection with noticeable multi-jet pattern that would be typically used in convectional injection around top-dead center. More flow bench tests are being arranged in the hope that one of the promising variable nozzle hardware designs will be implemented in a multi-cylinder engine, and then tested.

In parallel with exploration of a fuel injection system with variable nozzle and advanced combustion concepts, development of next generation control is moving forward. Currently, model-based control (MBC) modules for the simultaneous control of injection timing, injection pressure, pilot injection timing and EGR have been developed and implemented in an off-line computational environment. These MBC modules employ engine operating parameters (engine speed and fueling) in real-time with a set of control inputs from the previous time step to predict engine operating and emissions outputs. These outputs are calculated using a set of forward computational models to predict real-time torque and emissions of NOx, carbon monoxide (CO), smoke and carbon dioxide. These predicted engine outputs are then used by a real-time optimizer as the inputs to a set of inverse models to calculate the desired control outputs that meet the optimization objectives. The ability of the optimization scheme to guide or steer the engine control in real-time has been demonstrated, resulting in a series of engine control schemes for low NOx, low PM or optimized fuel efficiency. Displayed in Figures 3 and 4 is the direct outcome of the implementation of this MBC into an engine control unit. Figure 3 shows the trade-off between NOx emissions and brake thermal efficiency. As can be seen, 4% fuel economy improvement is

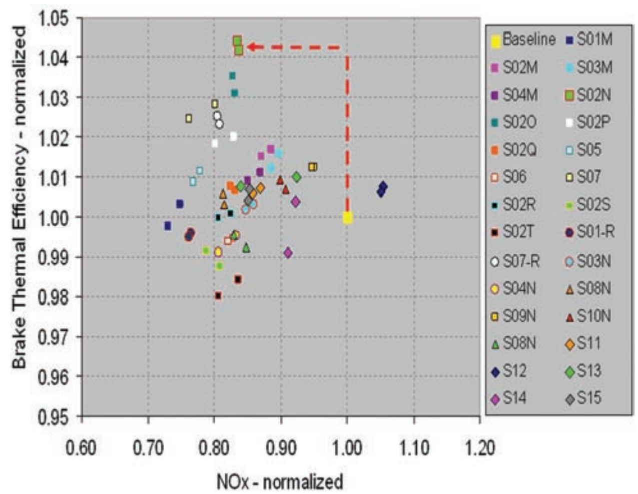

FIGURE 3. Trade-Off of Brake Thermal Efficiency and NOx with Advanced Control and Calibration Optimization (Each point marker designates one calibration FTP set point.)

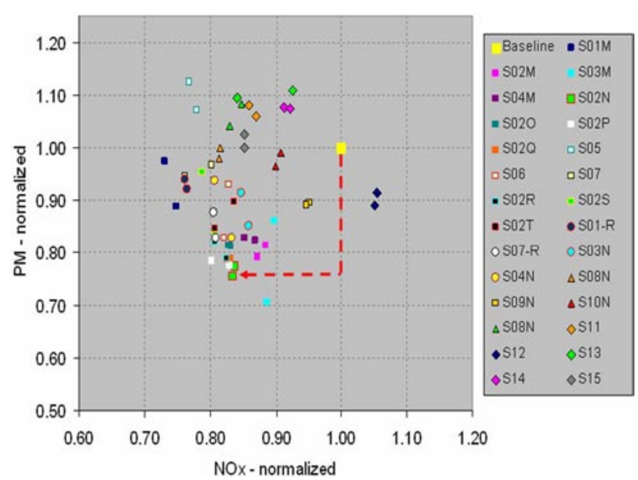

FIGURE 4. Trade-Off of NOx and PM with Advanced Control and Calibration Optimization (Each point marker designates one calibration FTP set point.)

obtained with substantial NOx reduction. Figure 4 shows the trade-off between NOx and PM emissions with simultaneous reduction of PM by 25% and NOx by 15%.

Conclusions

The DOE-Detroit Diesel Corporation heavy truck engine development project is progressing well. A project annual review with DOE in August 2008 was completed successfully, and passed the critical milestones with a "Go" decision point by achieving 5% thermal efficiency improvement experimentally on a multi-cylinder engine. Other key accomplishments are summarized as follows.

- Experimentally demonstrated over 4% fuel economy benefits on a multi-cylinder engine over the transient FTP cycle while simultaneously reducing PM and NOx by 25% and 15% respectively, using a validated next generation model-based control.
- Developed and validated MBC modules for the simultaneous control of injection timing, injection pressure, pilot injection timing and EGR and the control logic has been implemented in an off-line computational environment.
- Procured and flow bench tested variable injection nozzle hardware and evaluated its feasibility for injection mode switching. More flow bench tests are being conducted.

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II.A.22 Development of High Efficiency Clean Combustion Engine Designs for Spark-Ignition and Compression-Ignition Internal Combustion Engines

1. Spark-Ignition Portion: Development of High Efficiency Clean Combustion Engine Designs for Spark-Ignition Internal Combustion Engines

Kenneth J. Patton
GM Powertrain Advanced Engineering (GM)
895 Joslyn Ave.
Pontiac, MI 48340

DOE Technology Development Manager:
Ken Howden

DOE Project Manager: Carl Maronde

Objectives

- Develop and demonstrate engine designs which enable homogeneous charge compression ignition (HCCI) combustion systems.
- Use analysis, design, prototype builds, and testing of prototype builds to confirm capability and performance of individual components, subsystems, and complete engine systems.
- Develop and demonstrate an "enabling" engine which uses a lower-risk variable valvetrain system to enable HCCI operation in an effort to express a production-feasible hardware solution.
- Develop and demonstrate a fully-flexible engine which uses a higher-risk, but more capable, variable valvetrain system to explore the benefits of HCCI operation.
- Reduce technical risk and cost of all components and systems by defining component and subsystem requirements, evaluating alternative technologies, working with the supply base, identifying areas for improvement and simplification, and executing hardware solutions.

Accomplishments

- Enabling engines have been demonstrated on dynamometer and in vehicle. Functionality of engines and vehicle was as expected. While some specific challenges remain, the demonstration properties have been highly successful in meeting the stated objectives.
- One remaining specific challenge is the durability and robustness of production-feasible and cost-effective in-cylinder pressure sensing subsystems. This project continues to evaluate alternative technologies and supplier solutions in efforts to identify acceptable solutions. Major progress has been made in developing good requirements for cylinder pressure sensing subsystems.
- One remaining specific challenge for the enabling engine is the robustness of mode-switching from spark ignition (SI)-to-HCCI and HCCI-to-SI regimes. Demonstration of hardware which enables good switching has been completed, and execution of capable/robust/responsive engine controls is an ongoing development project which will extend beyond the scope of this project.
- One remaining specific challenge is the noise and vibration performance of the engine in HCCI mode and during mode-switching. This is important in terms of customer acceptance of HCCI. Demonstration hardware has been shown to be sufficiently capable, and the tradeoff between fuel economy improvement and noise/vibration performance has been explored. Ongoing development which will extend beyond the scope of this project will continue to focus on maximizing the fuel economy benefit while meeting noise performance requirements.
- Fuel efficiency improvements demonstrated by the enabling engine have been as expected. In the zone of operation for HCCI mode, fuel efficiency improvements in the range of 8% to 20% have been measured, depending on the specific engine operating condition. Overall vehicle fuel economy benefits are highly dependent on the engine speed/load and on the amount of time spent in HCCI mode, so many challenges remain in extracting HCCI fuel economy benefits in the real world and on fuel economy driving cycles.
- The majority of the fully-flexible multicylinder engine design has been completed, procurement is well underway, and engine builds are expected to proceed in early 2009.
- Heavy use of analytical tools has enabled execution of a valve actuator design which stays true to the prototype actuator concepts which were executed earlier in the project. This is a significant advance in electrohydraulic valve actuation technology.
- Although many specific challenges remain for the fully-flexible valve actuation system, the demonstrated prototype actuator functionality appears to be likely to deliver the expected capabilities in the multicylinder engine.
- One specific challenge for the fully-flexible actuation system is its performance under the wide variety of ambient temperature and pressure conditions

expected in normal vehicles. The demonstration hardware will be capable of quantifying this performance, and will be an important source of data to be used for developing more complete subsystem requirements for production fully-flexible engines.

- One specific challenge for the fully-flexible actuation system is its noise and vibration performance. Both the prototype hardware already demonstrated, and the upcoming multicylinder hardware, will be important contributors to the identification of specific noise source in the fully-flexible actuation system.

Future Directions

- Close out the remaining tasks (primarily generation of performance data) on the already-demonstrated enabling engine hardware.
- Continue to use the enabling engine as the testbed for production-style cylinder pressure sensing subsystems.
- Build and demonstrate the fully-flexible engine.

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Approach

- Using analysis, design tools, prototype subsystem builds, multicylinder engine builds, and vehicle builds, demonstrate enabling and fully-flexible engine systems which run HCCI combustion systems.
- Focus on the engine design and base engine hardware portions of the HCCI solution for this project, but use other necessary GM efforts outside this project to contribute combustion system operating strategy and powertrain control system development and execution.

Results

In the zone of HCCI operation, fuel efficiency benefits of as low as 8% and as high as 20% have been measured. Outside the zone of HCCI operation, of course, the measured benefits are essentially zero since they are normal SI mode. Real-world and on-cycle fuel economy benefits will be highly dependent on the speed/load operation of the engine and the amount of time the vehicle can spend in HCCI mode.

Base engine hardware capability for the enabling engine is sufficient to enable HCCI operation.

Conclusions

This project is continuing to be a successful demonstration of gasoline engine designs which enable HCCI combustion systems. The gasoline engine hardware designed and demonstrated so far have been key contributors to GM's overall efforts to understand, develop, and demonstrate HCCI vehicle solutions. Next steps in the project are being pursued as planned.

2. Compression-Ignition Portion: Diesel Single-Cylinder Engine Fully Flexible Variable Valve Actuation and Multi-Cylinder Simple Mechanism Variable Valve Actuation

Manuel Gonzalez, Russ Durrett, Xin He, Jonathan Burton
GM Diesel
895 Joslyn Ave.
Pontiac, MI 48340

DOE Technology Development Manager:
Ken Howden

DOE Project Manager: Carl Maronde

Objectives

- Quantify the benefits and limitations of using variable valve actuation (VVA) to reduce engine-out pollutant emissions and improve fuel economy at the Tier 2 Bin 5 engine-out NOx emission level using a single-cylinder engine with a fully flexible valve actuation (FFVA) system.
- Explore the operating conditions where the strategies can be applied, and identify any potential simple VVA mechanisms to be used in a multi-cylinder diesel engine.
- Design and implement simple VVA mechanism solutions including advanced charging components into multi-cylinder engine targeted to below Tier 2 Bin 5 engine-out NOx emission levels.
- Explore the trade-offs and synergies of VVA with an advanced charging system and calibration on the multi-cylinder engine.

Accomplishments

- Assessed the brake thermal efficiency and emission benefits of three simple VVA mechanisms for enabling late intake valve closing (LIVC).
- Quantified the benefits of a simple VVA mechanism for reducing hydrocarbon (HC) and carbon monoxide (CO) emissions at low/idle loads using internal exhaust gas recirculation (EGR).
- Assessed the benefits and limitations of early exhaust valve opening (EEVO) for controlling the exhaust temperature.

- Assessed the potential application of combining recompression and fuel reforming for NOx reduction.
- Preliminary package of VVA hardware for intake and exhaust valvetrains installed into a prototype multi-cylinder engine.

Future Directions

- Update and re-commission the FFVA system using production-intent hardware on the single-cylinder engine.
- Develop system requirements for the multi-cylinder engine using the updated FFVA system and support the multi-cylinder VVA system development.
- Validate emissions and fuel efficiency benefits found on the single-cylinder engine with the multi-cylinder engine.

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Approach

An FFVA system was developed for a prototype single-cylinder diesel engine. Comprehensive studies of the benefits of VVA on diesel fuel economy and emissions have been conducted at the Tier 2 Bin 5 engine-out NOx emission levels. The fully flexible system was also used to assess the benefits of several specific simple VVA designs. The design and implementation of these simple VVA systems in the multi-cylinder engine are under current development.

Results

- By adopting LIVC in the appropriate operating range, fuel economy is slightly improved by about 1% over the Federal Test Procedure (FTP) cycle and 0.5% over the US06 cycle. Smoke emissions are reduced by approximately 40% over the US06 cycle and ~50% over the FTP cycle (Figure 1). The best simple VVA mechanism is recommended for multi-cylinder engine evaluation (Figure 2).
- Internal EGR can reduce the engine-out HC emissions by 30% and CO emissions by 50%. It also increases the exhaust temperature. However, fuel consumption increases slightly.
- EEVO can be used to increase the exhaust temperature, however with EEVO the engine-out HC, CO, and smoke emissions deteriorate significantly if the exhaust valve opens too early. This is due to early quenching of the in-cylinder chemical reactions.
- The only benefit of combining recompression with fuel reforming is lower combustion noise at some engine operation conditions. No other benefits were observed.

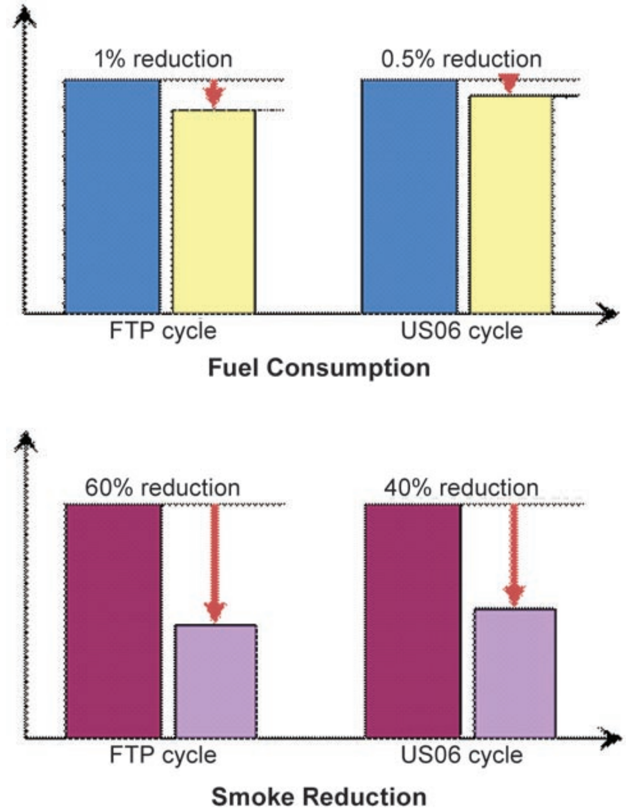

FIGURE 1. Benefits of Using LIVC in a Single-Cylinder Diesel Engine

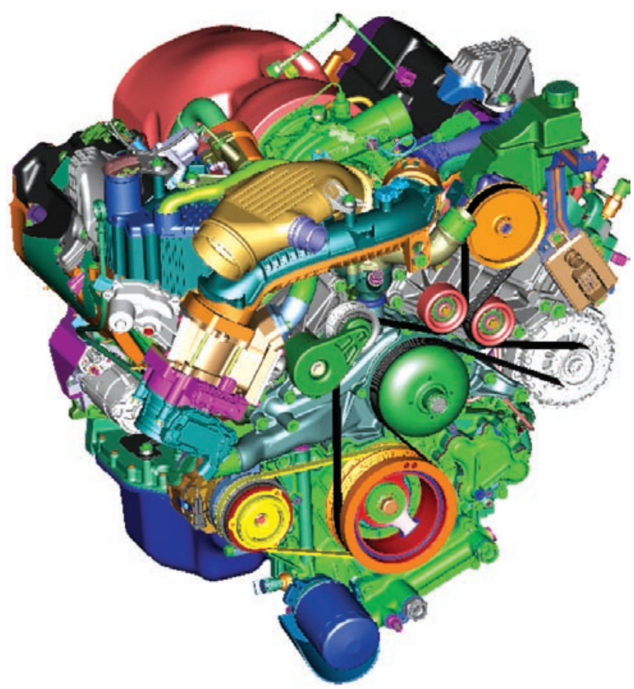

FIGURE 2. Multi-Cylinder Diesel Engine for the Next Phase of VVA Implementation

Conclusions

Significant benefits of using VVA in a diesel engine have been observed. By adopting LIVC, the low-temperature combustion region can be expanded, which improves fuel consumption and reduces smoke emissions. By increasing internal EGR, VVA can help reduce HC and CO emissions at low/idle loads. The single-cylinder engine work has created recommendations for the best way to use simple VVA mechanisms in a multi-cylinder diesel engine to achieve LIVC and increase internal EGR. The multi-cylinder engine is utilizing the recommendations from the single-cylinder work and hardware implementation has been initiated.

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II.A.23 Light-Duty Efficient Clean Combustion

Tim Frazier (Primary Contact), Tom Korb
Cummins Inc.
1900 McKinley Ave.
Columbus, IN 47201

DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Carl Maronde

Objectives

- Develop an advanced combustion system that meets Environmental Protection Agency (EPA) Tier 2, Bin 5 emissions standards while demonstrating a 10.5% improvement in fuel economy over the Federal Test Procedure (FTP) city drive cycle.
- Maintain power density comparable to that of current conventional engines for the applicable vehicle class.
- Evaluate different diesel fuel properties and ensure combustion system compatibility with commercially-available biofuels.

Accomplishments

- Developed combustion system model for the light-duty diesel (LDD) engine. A preliminary combustion system optimization, which will be validated in single-cylinder engine tests, has been completed at several steady-state points representing both the FTP75 and US06 drive cycles.
- Developed and calibrated an engine cycle simulation model for the LDD engine. The model was expanded beyond the base engine to simulate variable valve actuation (VVA) functions on both the intake and exhaust. The model has been used primarily to evaluate the relative emissions and efficiency trade-offs of VVA functions to specify and procure a multi-cylinder VVA prototype. Advanced air handling and exhaust gas recirculation (EGR) components are also being evaluated and will be used to specify and procure hardware for engine tests beginning in 2009.
- Based on analysis-led-design, we have developed preliminary engine architectures that will be studied experimentally during the next project phase. Due to the potential supplemental FTP (SFTP2) regulation, architectures have been developed for an in-cylinder solution as well as a NOx aftertreatment solution using high efficiency selective catalytic reduction (SCR).
- Cummins entered a joint development program with a VVA supplier to develop a multi-cylinder prototype VVA system for the LDD engine. Specification of system functionality and conceptual design phases are complete and detailed component design has begun.
- Cummins' project partner, BP, has initiated a fuels market research program to study the type and properties of diesel fuels that are on the market today and are predicted to be on the market in the next several years. Results will be used to determine whether statistically significant differences in fuel properties that affect performance can be detected and used to optimize engine performance depending on the type of fuel being burned.

Future Directions

The first phase of the project, Applied Research, has been focused heavily on analysis-led-design. During the next phase of the project, Advanced Development, the emphasis on simulation will be reduced and experimental development and validation will become the primary focus. During 2009, we expect to:

- Conduct single-cylinder engine experiments to optimize the combustion recipe and investigate NOx/brake specific fuel consumption trade-offs to determine what emissions compliance strategy enables the greatest improvement in fuel efficiency. Investigate changes to the combustion system requirements that will be driven by the potential SFTP2 emissions regulation.
- Complete detailed design and procure cylinder heads to accommodate the addition of VVA valve train components.
- Experimentally validate and optimize VVA system functionality for fuel economy improvement and emissions control.
- Conduct multi-cylinder engine experiments to evaluate the potential benefits and develop algorithms for closed-loop combustion control and advanced model-based air handling controls.
- Assess suppliers of critical components for technology and commercial readiness to ensure the technologies required for the planned architecture will be available for production.

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Introduction

Light-duty vehicles account for over 60% of all transportation energy consumption in the United States. Reducing petroleum fuel use and greenhouse gas emissions will require limiting the fuel consumed in light-duty vehicle engines. Today nearly all light-duty vehicles in the United States are powered by gasoline engines. Diesel engines have significant efficiency benefits over gasoline engines, and there are opportunities to further improve the diesel combustion system. If 30% of the light truck fleet in the United States were to transition to diesel engines, fuel consumption would be reduced by approximately 90 million barrels of oil per year. When fully implemented, developments proposed in this project will enable a 10.5% efficiency improvement, increasing potential fuel savings to 119 million barrels per year. The fuel savings associated with this project would reduce greenhouse gas emissions by eliminating the production of 11 million metric tons of carbon dioxide per year.

Cummins will develop and demonstrate combustion technologies for diesel engines that realize 10.5% efficiency improvements while meeting U.S. EPA Light-Duty Emissions Standards (Tier 2, Bin 5) in a robust and cost-effective manner. The work integrates the areas of low-temperature combustion (LTC), air handling, advanced fuel systems, and closed-loop controls to support high efficiency, low-emission combustion concepts. Multiple steps are planned in the development process including analysis-led design, concept integration, advanced system development and demonstration.

Approach

The project strategy is focused on the expansion of LTC to meet project objectives. LTC will result in very low engine-out emissions while achieving high efficiency. Two modes will be evaluated to expand the LTC region: smokeless rich combustion and early premixed-charge compression ignition (PCCI). Cummins believes these two modes offer the most opportunity for efficiency improvements while maintaining extremely low engine-out emissions.

As the engine transitions to higher speed and load operation, the combustion mode will transition to lifted flame diffusion-controlled combustion. Lifted flame diffusion-controlled combustion occurs when the diffusion flame is positioned further downstream of the liquid diesel fuel compared to conventional diffusion-controlled diesel combustion. Anchoring the diffusion flame further downstream allows more air to be entrained into the combustion plume, resulting in lower equivalence ratios in the region of first stage reactions. The overall consequence is lower soot formation as the engine transitions from lower-load PCCI combustion to high-load engine performance.

Although the details are not yet finalized, the potential SFTP2 regulation proposes to mandate tailpipe-out emissions levels over the aggressive US06 drive cycle that are similar in magnitude to the levels required for the light-load FTP75 urban drive cycle. This represents a significant risk for an in-cylinder NOx solution since the US06 drive cycle produces significant high-load, high-speed engine operation. As a result, both in-cylinder and advanced SCR solutions are being considered.

Results

The first phase of the project, Applied Research, has been focused primarily on analysis-led-design. Combustion models have been used to analyze and optimize the combustion recipe. Engine cycle simulation models have been used to evaluate VVA, air handling and EGR components and to investigate preliminary architecture options. Control algorithms and software have been developed and tested in the software simulation environment. Based on this work, preliminary engine architectures have been developed for both in-cylinder and advanced SCR solutions.

The preliminary architectures are designed to improve fuel efficiency by focusing on four main areas; closed-cycle efficiency improvements, air handling/EGR systems, advanced controls, and aftertreatment. The major contributors to closed-cycle efficiency improvements include expansion of LTC, combustion system optimization, enhanced EGR cooling, and VVA. Air handling and EGR system improvements include high-efficiency two-stage variable-geometry turbocharging (VGT), advanced low-pressure-drop EGR cooling systems, and VVA. Controls efforts are focused on closed-loop combustion control and model-based air handling controls. Both paths also include a reduction in fuel economy penalties associated with the diesel particulate filter (DPF) via reduced regeneration frequency and pressure drop.

Based on the analysis efforts, an estimate of fuel efficiency improvements for the preliminary architectures has been developed. The estimated fuel efficiency improvements for the in-cylinder solution are shown in Table 1. The efficiency improvements shown are relative to the current baseline engine which is equipped with a lean-NOx trap (LNT) NOx aftertreatment system.

As shown in Table 1, the estimated fuel efficiency improvement for an in-cylinder NOx emissions solution is 11.5%, which exceeds the project goal of 10.5%. However, the most significant risk associated with an in-cylinder solution is that it will not be capable of meeting

TABLE 1. Estimated Improvements in Fuel Efficiency for an In-Cylinder NOx Emissions Solution Relative to an Architecture Employing an LNT NOx Aftertreatment System

Category	Major Technologies	Fuel Efficiency Improvement
Closed-Cycle	Expand LTC Optimize combustion system Enhanced EGR cooling VVA	3%
Air handling/ EGR	High-efficiency two-stage VGT Low-pressure-drop EGR VVA	2%
Controls	Closed-loop combustion control Model-based air handling controls	1.5%
Aftertreatment	Elimination of LNT Reduced DPF regeneration	5%
Total		**11.5%**

the emissions requirements required by the potential SFTP2 regulation. Hence, a high efficiency SCR NOx aftertreatment solution is also being investigated. The estimated efficiency improvement for the SCR architecture, relative to the baseline LNT architecture, is similar to the in-cylinder solution. However, since the SCR solution enables high engine-out NOx over much of the drive cycle, closed-cycle efficiency improvement is expected to be slightly greater. Due to urea consumption and thermal management, efficiency improvements associated with aftertreatment are expected to be slightly less than the in-cylinder solution. During the next phase of the project, Advanced Development, efficiency improvements with be validated and optimized experimentally. A final architecture decision will be made based on the results of these experiments.

Conclusions

The first phase of the project, Applied Research, has been focused heavily on analysis-led-design. Combustion and engine cycle simulation models have been developed, calibrated and used to analyze critical components, technologies and operational strategies.

- The analyses have lead to the development of preliminary engine architectures for in-cylinder and SCR NOx solutions.
- The goal of 10.5% improvement in fuel efficiency over the FTP75 drive cycle is technically feasible but will require a careful system integration approach due to the highly transient nature of the FTP75 drive cycle.

FY 2008 Publications/Presentations

1. 2008 DEER Conference Presentation – “Light Duty Efficient Clean Combustion”, presented by Tim Frazier, 6th August, 2008.

II.A.24 Advanced Boost System Development for Diesel HCCI Application

Harold Sun (Primary Contact), Melissa Hendra
Ford Motor Company
2101 Village Road
Dearborn, MI 48214

DOE Technology Development Manager:
Ken Howden

NETL Project Manager: William Cary Smith

Subcontractors:
- Wayne State University, Detroit, MI
- ConceptsNREC, White River Junction, VT

Objectives

The overall objective is to support industry efforts of clean and efficient diesel engine development for passenger and commercial applications. More specifically:

- ConceptsNREC objectives: leads boost system design, optimization, computer-aided engineering stress analysis and fabrication of prototypes as well as flow bench test; provides turbocharger maps for various turbo technologies to support system level simulation/integration.
- Wayne State University objectives: leads computational fluid dynamics (CFD) analysis and analytical validation of various turbocharger concepts designed by ConceptsNREC.
- Ford Motor Company objectives: leads system integration, cascade system requirement, boost system development design target, validation and demonstration of fuel economy improvement of light-duty diesel engine performance on engine test bench.

Accomplishments

Aerodynamic design, CFD validation and structure analysis of the turbocharger was completed. However, based on the findings from flow bench testing, further design iterations will be needed.

Prototype fabrication and flow bench validation of the advanced boost system was partially pulled up to validate some of the design concepts and analyses:

- Aerodynamic design, CFD and structure analyses of mixed flow turbine was completed. A total of 12 compressor design iterations were made for optimal performance.
- A production turbocharger was fitted with a mixed flow turbine to fit into the existing variable-nozzle turbine structure. Six design iterations of the turbine have been carried out to make sure the turbine meets design targets and that the structure and low/high cycle fatigue performance meet design guidelines. The detailed mechanical design of the mixed flow turbine was completed.
- Numerical evaluation of one of the dual volute compressor advanced compressor concept was completed. The results were presented at the Diesel Engine Emissions Reduction (DEER) conference.
- A turbine design review has been conducted at ConceptsNREC. One of the major turbocharger suppliers participated in the design review to make sure the turbine design is consistent with typical turbine design requirements for durability/reliability and manufacturability.
- The meanline one-dimensional (1-D) analysis of the variable geometry compressor (VGC) was completed and GTPower engine performance simulation based on the VGC was very promising. However, the VGC CFD validation and structure analyses will be delayed mainly due to the extremely challenging targets as well as the uncertainties in meanline compressor prediction and steady-state CFD simulation software, especially near compressor surge conditions.
- To address the uncertainties in turbocharger analyses, it was decided that one turbocharger configuration be fabricated and flow bench tested to support the design and numerical analyses. This prototype turbocharger, a mixed flow turbine with ultra-low solidity diffuser vane compressor (C9) but without casing treatment, was fabricated. However, two speed lines (70,000 and 108,000 rpm) were obtained on the flow bench before the turbocharger had a catastrophic failure due to overloading on the thrust bearing (Figures 1 and 2).
- The preliminary flow bench test data was encouraging on the turbine side. The preliminary data indicated that the mixed flow turbine achieved

FIGURE 1. A Mixed Flow Turbine Wheel was Fabricated as Well as Ultra-Low Solidity Airfoil Diffuser Vane Compressor

FIGURE 2. Catastrophic Failure of the First Prototype Turbocharger due to Overloaded Thrust Bearing

predicted efficiencies and showed improvement over the current production turbocharger (Figure 3), even though the test did not extend to the low speed ratio area we had planned. Of course, most importantly, the preliminary data showed reasonable agreement between 1-D meanline prediction and three-dimensional (3-D) CFD simulation which will facilitate future turbine design and analyses. The result on the compressor side is not as good as we anticipated (Figure 4). The cause of the less than expected efficiency is still under investigation.

- Since the prototype compressor did not include casing treatment, the compressor did not show the required operational range. Also, the location of peak compressor efficiency shifted to the high flow area, which was exactly predicted by CFD on the C9 compressor wheel. For this reason, the C12 compressor was designed and fabricated. But unfortunately, due to the turbocharger failure, C12 did not have a chance to be tested.

Future Directions

- Evaluation of the low-speed flow bench data as well as the failure mode of the prototype turbocharger will continue.
- Revisit the compressor and turbine design based on this preliminary flow bench test data and make improvements in simulation and further design iterations, if necessary.
- Conduct further flow bench testing on the C12 compressor wheel with three different casing treatments once the replacement turbine wheel is fabricated in two months.

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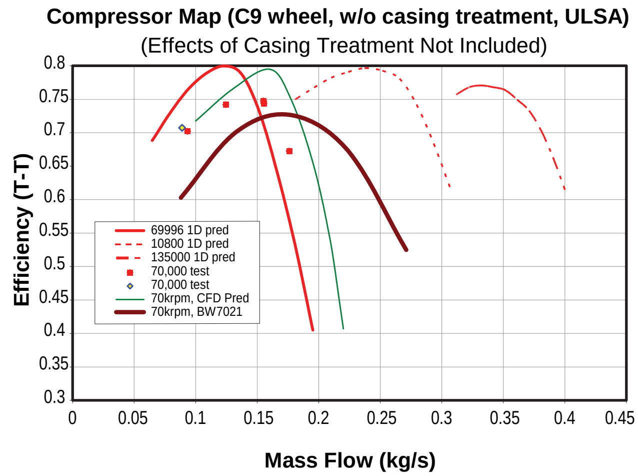

FIGURE 3. Turbine Efficiency Meanline Prediction vs. Flow Bench Test at 70,000 RPM (ULSA - ultra-low solidity airfoil)

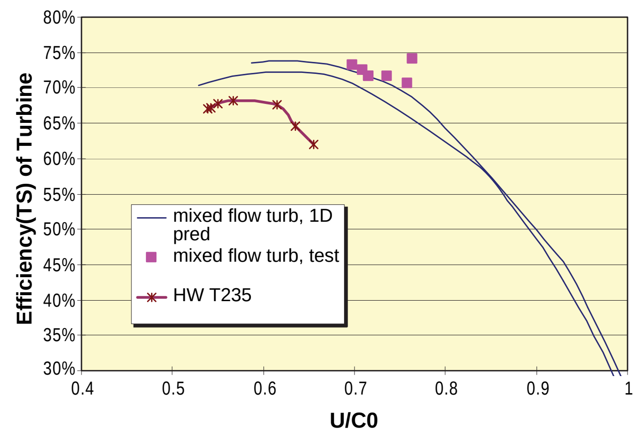

FIGURE 4. Compressor Efficiency 1-D and 3-D CFD vs. Flow Bench Test at 70,000 RPM

Introduction

Diesel homogeneous charge compression ignition (HCCI) and low temperature combustion (LTC) have been recognized as effective approaches to dramatically reduce diesel emissions. However, high levels of exhaust gas recirculation (EGR) are needed to achieve homogeneous or partially homogeneous mode combustion, which often drives the compressor and turbine into less efficient or even unstable operational areas.

This project will focus on complete and optimal system solutions to address boost system challenges, such as efficiency degradation and compressor surge, etc, in diesel combustion/emission control system development to enable commercialization of advanced diesel combustion technologies, such as HCCI/LTC.

Approach

There are several boosting concepts that have been seen in the literature and will potentially be helpful to extend the operation range with decent efficiency. They are primarily single-stage turbochargers so that they are cost-effective, have small package space, small thermal inertia while providing enough EGR that is required by advanced combustion concepts such as HCCI/LTC.

This project will particularly focus on the following:

- Compressor variable inlet guiding vane – by varying the air rotational flow direction at the compressor inlet to have a better alignment with compressor blades, the compressor can work at a smaller mass flow without surge or stall.
- Similarly, an optimized casing treatment on the compressor housing can also re-align the re-circulated air flow to extend the surge margin.
- Variable geometry compressor – an optimized airfoil diffuser can push the surge line to lower flow rates on the compressor map, often at the expense of efficiency in off-peak operation and possibly reduce full-flow capacity. A variable vane at the compressor diffuser area can maintain high compressor efficiency at a wide range of operation.
- Dual sequential compressor volute/outlet – a bifurcated volute that has a dual outlet and can be opened sequentially to match air exit velocity to compressor vane geometry. This method is an alternative design concept that is simpler, more economical and potentially more durable than the variable geometry compressor mentioned above since it has only one moving part: a switching valve.
- A mixed flow turbine is an attractive option to improve efficiency on the turbine side. Current turbine efficiency at light-load and low speed is substantially lower than its peak efficiency. This study will focus on high turbine efficiency at lower speed ratios to improve EGR pumping capacity and vehicle fuel economy on customer driving cycles.

The above technologies will be fully investigated with well-validated numerical simulation methods before the prototypes are built, and flow bench tested. The final optimized turbocharger system will be demonstrated on an engine dynamometer in terms of emissions, fuel economy and performance improvement.

Results

Figure 5 shows the predicted improvement of efficiency and operational range via variable compressor diffuser vane angle. When the engine operates at LTC modes where heavy EGR is required, the compressor provides decent efficiency with sufficient surge margin; while at the rated power condition when the engine

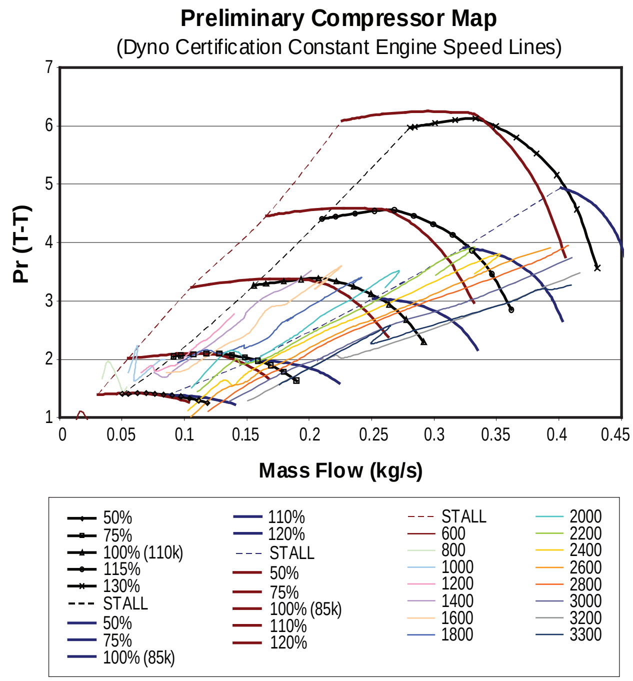

FIGURE 5. Compressor Operation Map with Variable Diffuser Vane Predicted by ConceptsNREC COMPAL

operates in the conventional combustion mode, large flow capacity is available to meet high power outputs. This 1-D prediction was carefully validated with 3-D CFD analyses, which was not precisely supported by the preliminary flow bench test on one of the vane positions (Figure 4). The cause of the discrepancy is under investigation.

During the correlation between 3-D CFD and flow bench data, it was found that the widely used mixing plane method (interfacing the rotating flow field and the flow field between stationary diffuser vanes while using single-flow passage CFD to represent the full compressor) can predict the compressor efficiency fairly well when there are no noticeable flow separations at the impeller exit. When the flow condition approaches either surge or choke, i.e. there exist noticeable flow separations; the CFD tends to over predict the mass flow even if the simulation numerically converges. In those off-peak efficiency areas, a full-flow passage CFD is recommended for future CFD analyses.

The 1-D meanline analysis of mixed flow turbine shows improved efficiency that met the design target (Table 1). The current mixed wheel design reduced the secondary flow losses therefore the turbine efficiency is improved. This mixed turbine wheel has a larger flow capacity than conventional radial flow turbines so the turbine can be downsized which further improves efficiency at part-load as well as transient response. The preliminary flow bench test data (Figure 3) at 70,000 rpm showed that the 1-D prediction of turbine

TABLE 1. Prediction vs. Design Target of Mixed Flow Turbine

Operating condition	A	B	C
Target	0.64	0.69	0.72
CFD prediction	0.700	0.733	0.747
Rotor tip clearance correction	0.012	0.012	0.012
Nozzle clearance correction	0.012	0.01	0.005
Volute loss estimate	0.01	0.01	0.01
Net predicted efficiency	0.658	0.701	0.72

efficiency is reasonably accurate. Figure 3 also indicates that the mixed flow turbine maintains high efficiency to a wider speed ratio area, i.e. the mixed flow turbine can better utilize the pulsation flow out of diesel exhaust than conventional radial flow turbines. Due to unexpected failure of the turbocharger, we did not complete the test at lower speed ratios and the high wheel speed area where even higher turbine efficiency is expected.

The turbocharger failure during the flow bench test was not design related, based on limited information available so far. It was due to an improperly designed cold-flow turbocharger test. In order to have sufficient power to drive the compressor, the cold-flow turbine had to be pressurized to a much higher level than it was designed for. As a result, the thrust loading far exceeded the limit that the thrust bearing inside the center housing of the production turbocharger can take.

Conclusions

The first round of design, analysis and flow bench test made limited achievements. Even though the flow bench test was interrupted due to turbocharger failure, the test data from two speed lines still provided valuable correction/validation for the compressor and turbine design and analysis which will guide the future design optimization for better efficiency and wider flow range. The first round exercise focused on compressor blade, diffuser vane and mixed flow turbine design optimization. The next step will focus on using fewer moving parts in the compressor to achieve the widest operation range with minimal efficiency penalty.

FY 2008 Publications/Presentations

1. DEER 2008 conference poster.
2. SAE 2009-01-0985, "Numerical Investigation of Advanced Compressor Technologies to Meet Future Diesel Emission Regulations".
3. SAE 2009-01-0936, "Numerical Study of Ultra Low Solidity Airfoil Diffuser in an Automotive Turbocharger Compressor".

Patents Issued

1. Improve compressor surge margin with active casing treatment (pending).

II.B.1 Fundamental Studies of NOx Adsorber Materials

Do Heui Kim, Ja Hun Kwak, Janos Szanyi, and Chuck Peden (Primary Contact)
Institute for Interfacial Catalysis
Pacific Northwest National Laboratory (PNNL)
P.O. Box 999, MS K8-93
Richland, WA 99352

DOE Technology Development Manager:
Ken Howden

Objectives

- Develop a practically useful fundamental understanding of oxides of nitrogen (NOx) adsorber technology operation.
- Focus on chemical reaction mechanisms correlated with catalyst material characterization.
- Actively participate in the Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) lean-NOx trap (LNT) subgroup, and transfer the developing fundamental understanding to industry via this CLEERS activity.

Approach

- Utilize state-of-the-art catalyst characterization and testing facilities in the Institute for Interfacial Catalysis at PNNL, including:
  - Synchrotron temperature programmed X-ray diffraction (XRD): catalyst structural changes.
  - Transmission electron spectroscopy (TEM)/energy dispersive X-ray (EDX) and scanning electron microscopy (SEM) microscopies: catalyst morphological changes.
  - X-ray photoelectron spectroscopy (XPS): oxidation state and relative surface concentrations.
  - Fourier transform infrared (FTIR) and solid-state nuclear magnetic resonance (NMR) spectroscopies: catalyst reaction mechanisms.
  - Temperature-programmed desorption (TPD)/thermal gravimetric analysis (TGA): surface chemistry.
  - Lab Reactor: performance measurements, kinetics and mechanisms.
- Participate as an active member of the CLEERS subgroup on LNTs.

Accomplishments

- In prior work, the morphology of barium oxide (BaO)/alumina (Al_2O_3) LNT materials was shown to be remarkably dynamic during NOx storage and reduction. A "monolayer'" of $Ba(NO_3)_2$ forms on the alumina surface in addition to large "bulk" $Ba(NO_3)_2$ particles.
- These different morphologies were also found to display dramatically different behavior with respect to NOx removal temperature, formation of a deactivating high-temperature $BaAl_2O_4$ phase, and temperature requirements of desulfation.
- *In this past year, the specific structures associated with the monolayer phase have been studied with both experiments and computational modeling.* Ultra-high resolution transmission electron microscopy (TEM) at the High Temperature Materials Laboratory (HTML) at Oak Ridge National Laboratory (ORNL) confirmed that initially BaO monomers dispersed on the γ-alumina support surface by anchoring to penta-coordinated Al sites (discussed below).
- The results from this combined experimental and computational study has allowed us to unambiguously determine the nature of "surface" and "bulk" nitrates that were identified in our prior studies and that we have shown to be important in determining the optimum practical behavior of Ba-based LNT catalysts.
- Using a one-of-a-kind very high field NMR instrument at PNNL, the role of specific surface sites on the γ-alumina catalyst support surface in its high temperature stability to phase transformation has been determined (discussed below).
- Computational studies to understand the relative performance of all alkaline earth oxide storage materials have been carried out.
- Numerous publications (nine), invited talks (eight), and other presentations (six) have resulted from this project in the past year (see below list).
- The principle investigator on this project (Chuck Peden) co-edited a special issue of the prestigious journal, Catalysis Today on Catalytic Diesel Emission Control.

Future Directions

- Continue studies of carbon dioxide (CO_2) and water (H_2O) effects on BaO morphology changes and NOx storage properties:
  - Ba-loading studies.

    – Are water-induced morphology changes reversible? If so, how?

- Detailed characterization (e.g., FTIR, TEM) of the roles (especially with respect to deactivation) and material properties of promoter species (such as ceria).
- Initial studies of interactions between multiple emission control devices (e.g., how to optimize LNT regeneration for ammonia [NH_3] production if a downstream urea selective catalytic reduction [SCR] catalyst system is present).

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Introduction

One of the key challenges facing the catalysis community is the elimination of harmful gases emitted by internal combustion engines. In particular, the reduction of NOx from an exhaust gas mixture that contains an excess amount of oxygen is difficult. Traditional three-way catalysts do not work under lean conditions because the concentrations of the reductants (CO and hydrocarbons) are greatly reduced by their oxidation with O_2 on the noble metal components of these catalysts. Therefore, new approaches to NOx reduction have been considered in the last decade. In spite of all the efforts to develop new emission control technologies for lean NOx reduction, only limited applications have been achieved. One of the most promising technologies under consideration is the NOx adsorber catalyst (aka NOx storage/reduction, NSR, or LNT) method. This process is based on the ability of certain oxides, in particular alkaline and alkaline earth oxide materials, to store NOx under lean conditions and release it during rich (excess reductant) engine operation cycles. Since the original reports on this technology from Toyota in the mid `90s [1], the most extensively studied catalyst system continues to be based on BaO supported a high surface area Al_2O_3 material [2].

Our project is aimed at developing a practically useful fundamental understanding of the operation of the LNT technology especially with respect to the optimum materials used in LNTs. As noted above in the summary Accomplishments section, we have made significant progress in a fairly wide-array of areas. For the purposes of this report, we briefly highlight progress in two areas: studies of i) the effect of Ba-loading and water on the formation and stability of $BaAl_2O_4$; and ii) the effects of water on BaO morphology and NOx uptake.

Experimental Details

Catalyst Preparation and Characterization

In a microcatalytic reactor system, LNT performance is evaluated in a fixed bed reactor operated under continuous lean-rich cycling. Rapid lean-rich switching is enabled just prior to the elevated temperature zone (furnace) where the LNT materials are contained in quartz tubing. After removing water, the effluent of the reactor can be analyzed by mass spectrometry and by a chemiluminescent NOx analyzer. For a typical baseline performance testing, the sample is heated to a reaction temperature in flowing He, the feed switched to a 'lean-NOx' mixture containing oxygen and nitric oxide (NO), as well as CO_2 and/or H_2O. After an extended period (15 minutes or more), multiple rich/lean cycles of 1 and 4 minute duration, respectively, are run and NOx removal performance is assessed after at least three of these are completed. In the LNT technology, the state of the system is constantly changing so that performance depends on when it is measured. Therefore, we obtain NOx removal efficiencies as "lean conversion (4 minutes)", which measures NOx removal efficiencies for the first 4 minutes of the lean-period.

The BaO/Al_2O_3 LNT catalysts were prepared by the incipient wetness method, using an aqueous $Ba(NO_3)_2$ solution (Aldrich) and a γ-alumina support (200 m^2/g, Condea) to yield nominal 2, 8 and 20 wt% BaO-containing samples, dried at 125°C and then 'activated' via a calcination at 500°C in flowing dry air for 2 h. State-of-the-art techniques such as solid-state NMR [3], XRD, XPS, TEM/EDS, FTIR, Brunauer, Emmett, Teller/pore size distribution, and temperature programmed desorption/reaction (TPD/TPRx), available at PNNL and at the ORNL/HTML, were utilized to probe the changes in physicochemical properties of the catalyst samples. The time-resolved X-ray diffraction (TR-XRD) experiments were carried out at beam line X7B of the National Synchrotron Light Source, at Brookhaven National Laboratory. The detailed experimental set-up and protocol have been discussed elsewhere [4,5].

Results

In prior years' reports, we have described studies that determined the cycle of morphology changes for BaO/Al_2O_3 NSR catalysts using synchrotron TPD, FTIR, TR-XRD, TEM and EDS. The results showed that large $Ba(NO_3)_2$ crystallites are formed on the alumina support material during its preparation by an incipient wetness method using an aqueous $Ba(NO_3)_2$ solution. A large fraction of the alumina surface remains Ba-free after this procedure. Upon thermal treatment, these large $Ba(NO_3)_2$ crystallites decompose to form nanosized BaO particles. In fact, we propose that a thin BaO film (monolayer) forms on a portion of the alumina support, and the BaO nanoparticles are located on top of this interfacial BaO layer. During room temperature NO_2 uptake, nanosized (<5 nm) $Ba(NO_3)_2$ particles form, and these particles are stable at room temperature. Heating the material to higher temperature (300°C) in the presence of NO_2 results in the formation of larger $Ba(NO_3)_2$ crystals (~15–30 nm). At still higher temperatures, as $Ba(NO_3)_2$ decomposes, the nano-sized BaO particles reform. These LNT material morphological changes during operation are summarized in Figure 1. We have also previously described a number of important practical consequences of these cyclic morphology changes. In particular:

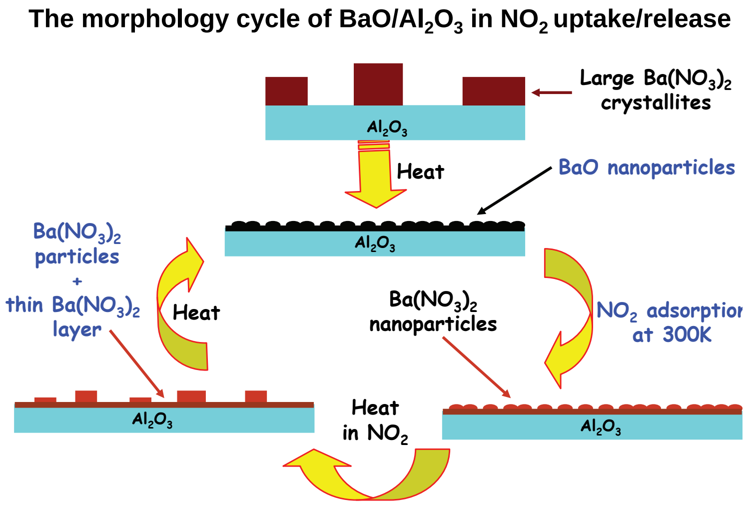

FIGURE 1. Schematics of the cycle of morphology changes taking place during NO_2 uptake and release on BaO/Al_2O_3 NOx storage/reduction materials.

- From TPD experiments, the "monolayer" morphology is found to decompose at lower temperature in vacuum and in a reducing atmosphere than "bulk" nitrates [5,6],
- "Monolayer" Ba-phase is also easier to 'de-sulfate' [7],
- Formation of a high-temperature (deactivating?) $BaAl_2O_4$ phase requires BaO coverages above 1 monolayer [8], and
- The morphology model at least partially explains relatively small use of Ba species (often <20%) in storing NOx during typical lean-rich cycling [9].

We have more recently studied the effects of water [11-12] and/or CO_2 (manuscripts in preparation) on these morphology changes.

In this year's report, we highlight two other aspects of our recent studies; the first is related to the stability of the LNT support material, γ-alumina, with the second concerning NO_2 adsorption of the monolayer Ba-phase on the surface of the γ-alumina support material.

Penta-coordinated Al^{3+} ions on γ-Al_2O_3 as nucleation sites for phase transitions and for loading of catalytic phases: studies using ultra-high magnetic field ^{27}Al MAS NMR and aberration-corrected TEM

In a recently published paper [3], we reported the first observation of preferential anchoring of an impregnated catalytic phase (BaO) onto penta-coordinated Al^{3+} sites on the surface of γ-Al_2O_3, and briefly described this work in last year's report [13]. For example, Figure 2 shows ultra-high resolution (HR) TEM image obtained at the HTML at ORNL. This image, of a 2 wt% BaO/γ-Al_2O_3 sample, shows isolated monomeric BaO species on the alumina surface (see areas "B" and "C" in the figure). Line scans "1" and "2" confirm that these adsorbed 'molecules' are single atoms that are isolated from one another. Interestingly, there are large patches of the surface where there are no BaO monomers present (indicated by "A" in the figure), a result consistent with the fact that penta-coordinated Al^{3+} sites should only be present on ~15-20% of the γ-Al_2O_3 surface. On the basis of these results, the possibility that penta-coordinated Al^{3+} ions on the γ-Al_2O_3 surface generally serve as anchoring sites for catalytically important materials (possibly both oxides and metals) is intriguing. One of the main reasons that γ-Al_2O_3 is used so commonly as a catalyst support material is its ability to form and stabilize active centers (metal and metal oxide particles) with high dispersion. As we have recently noted [3], our recent studies have shown that BaO, the active NOx storage phase in the LNT technology, initially anchors to these coordinatively unsaturated, pentahedral Al^{3+} sites. This is in excellent agreement with our previous observation that well dispersed BaO nano-particles formed upon the thermal decomposition of a $Ba(NO_3)_2$ precursor loaded onto the γ-Al_2O_3 surface [5]. Recently, we have shown that such γ-Al_2O_3 surface sites also impact the stability of this important catalyst support material [14].

In this recent work, the structural stability of γ-Al_2O_3 was investigated by a combination of XRD and high resolution solid state ^{27}Al MAS NMR at an ultra-high magnetic field of 21.1 tesla. XRD measurements (Figure 3a) show that γ-Al_2O_3 undergoes a phase transition to θ-Al_2O_3 during calcination at 1,000°C for 10 h. The formation of the θ-Al_2O_3 phase is further confirmed by ^{27}Al MAS NMR (Figure 3b); additional ^{27}Al peaks centered at 10.5 and ~78 ppm were observed in samples calcined at this high temperature. Both the XRD and NMR results indicate that, after calcination at 1,000°C for 10 h, the ratio of the θ-Al_2O_3 phase to the total alumina in samples modified by either BaO or La_2O_3 is significantly reduced in comparison with γ-Al_2O_3 (XRD

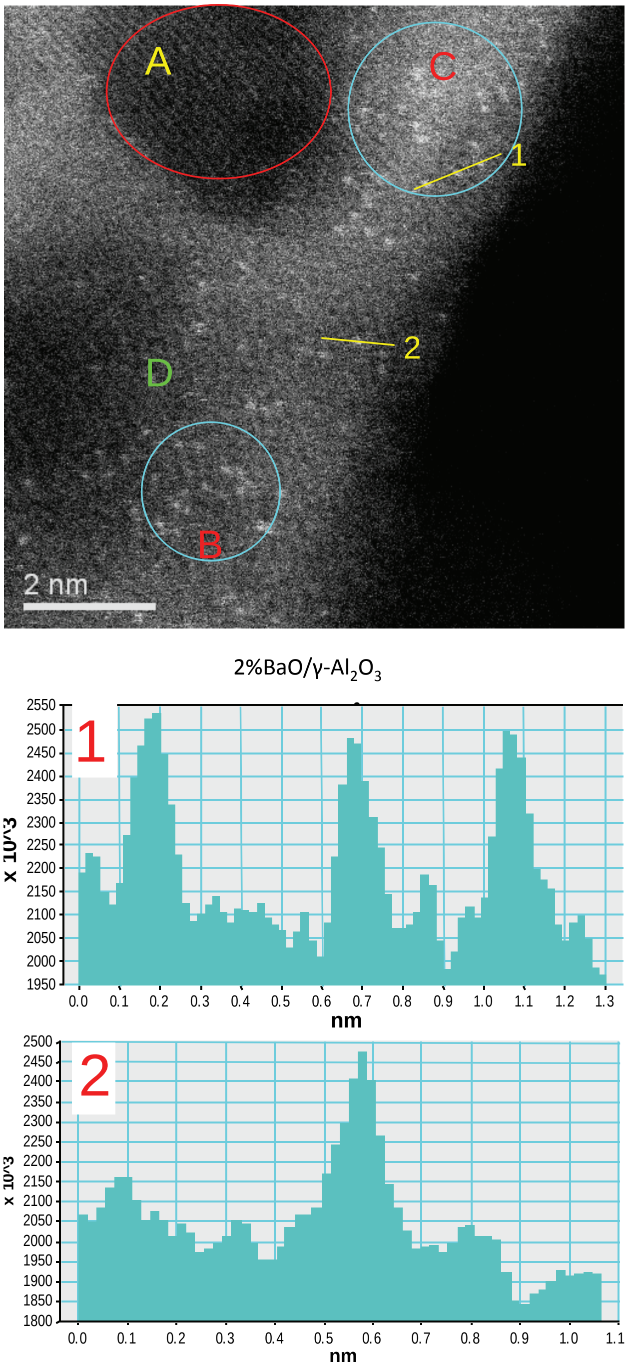

FIGURE 2. (a) HR-scanning transmission electron microscopy image obtained from a 2 wt% $BaO/\gamma\text{-}Al_2O_3$ catalyst. (b) Line scans of intensity for two positions indicated in the TEM image.

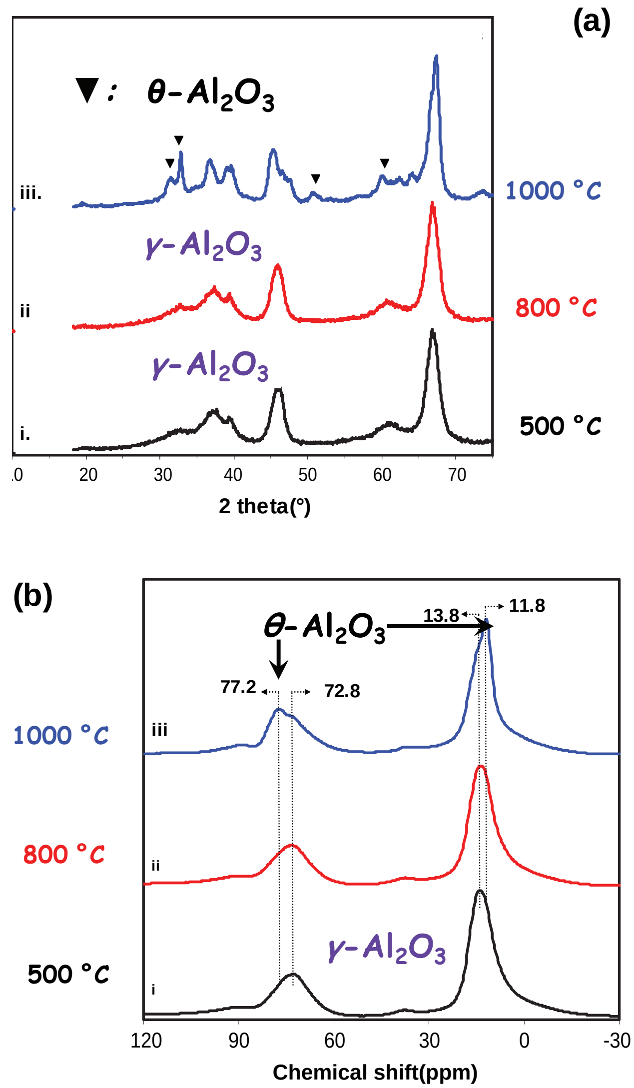

FIGURE 3. XRD patterns (a), and solid state ^{27}Al MAS NMR spectra (b) of $\gamma\text{-}Al_2O_3$ samples calcined at (i) 500°C for 2 h, (ii) 800°C for 2 h, and (iii) 1,000°C for 10 h.

data for the La_2O_3-doped material before and after high temperature calcination are shown in Figure 4a). ^{27}Al MAS NMR spectra (Figure 4b) revealed that the reduction in the extent of $\theta\text{-}Al_2O_3$ formation was highly correlated with the reduction in the amount of penta-coordinated aluminum ions, measured after 500°C calcination, in both BaO- and La_2O_3-modified $\gamma\text{-}Al_2O_3$ samples. Thus, these results strongly suggest that the penta-coordinated aluminum ions, present exclusively on the surface of $\gamma\text{-}Al_2O_3$, play a critical role in the phase transformation of $\gamma\text{-}Al_2O_3$ to $\theta\text{-}Al_2O_3$. The role of the modifiers, in our case BaO or La_2O_3, is to convert the penta-coordinated aluminum ions into octahedral ones, thereby improving the thermal stabilities of the samples [14].

NOx uptake on alkaline "surface" and "bulk" Ba phases supported on $\gamma\text{-}Al_2O_3$: experimental and computational studies

The special role of the interface between the active catalytic phase (metal or metal oxide) and the oxide support in determining the properties of practical catalysts has long been recognized [15]; however, it is still very poorly understood in most systems. The way the active phase is anchored onto the support surface

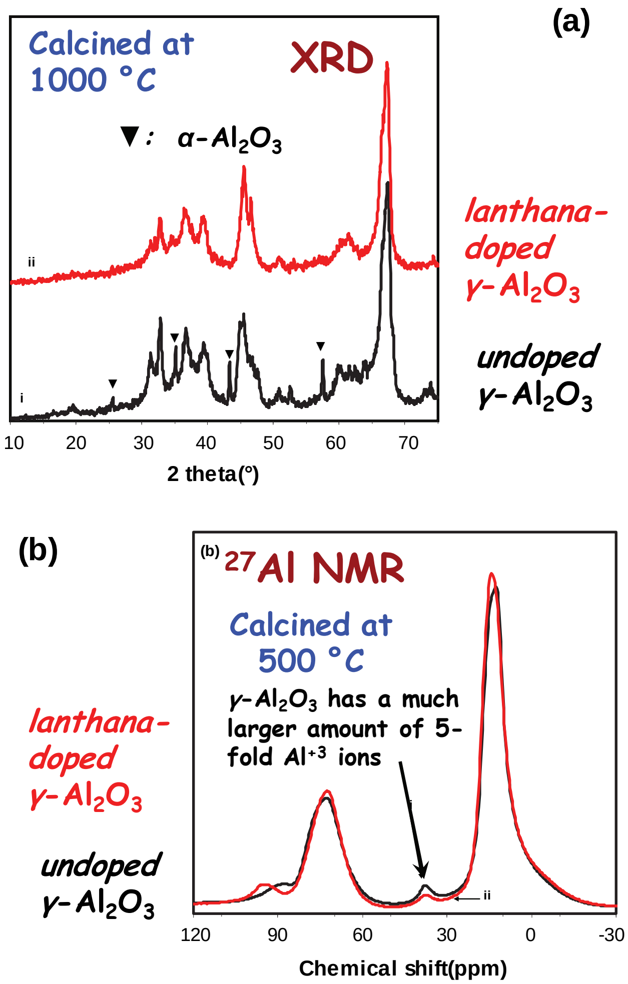

FIGURE 4. XRD patterns (a) after calcined at 1,000°C for 10 h, and solid state ^{27}Al MAS NMR spectra (b) after calcined at 500°C for 2 h of γ-Al_2O_3-150 (black), and La_2O_3/Al_2O_3 (red) samples.

may be especially important when the active phase is very highly dispersed. In such systems, the active oxide is likely anchored to some special sites of the support, and we may expect significant modifications in the chemical properties of these active centers by the underlying oxide support. Investigating the properties of these very highly dispersed active centers, however, is experimentally very difficult, and requires a concerted effort of both experimental and theoretical methods.

Very recently, we have reported the importance of a strong interaction between the BaO storage and alumina support materials in determining the adsorption mechanism of NO_2 [3]. Furthermore, the existence of two different types of nitrate species on BaO/γ-Al_2O_3-based NOx storage/reduction systems has been evident in TPD, FTIR and ^{15}N solid state NMR studies [16]. Based on the results of these spectroscopic characterizations, we concluded that "surface" and

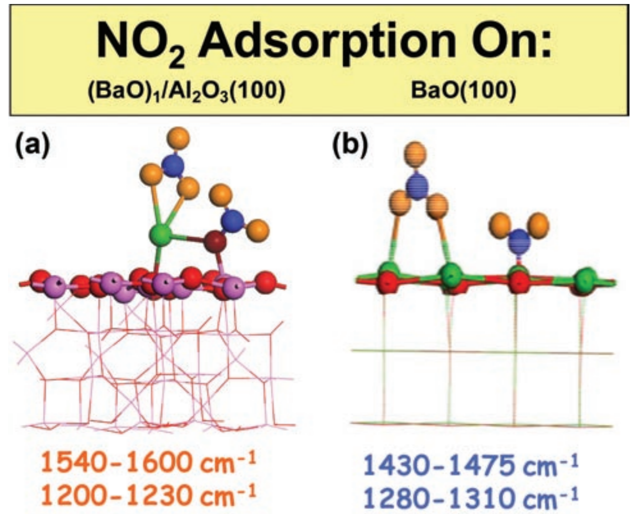

FIGURE 5. Optimized structures of nitrates formed on: a) BaO monomers on the γ-Al_2O_3(100) surface; and b) a bulk BaO(100) surface (blue: N; gold: O in NOx; green: Ba; dark red: O in BaO monomer; magenta: $Al^{3+}{}_{penta}$; and red: O atoms on the BaO(100) and γ-Al_2O_3(100) surfaces).

"bulk" Ba-nitrate species form when BaO/γ-Al_2O_3 NO_x storage materials were saturated with NO_2.

The nature of the bulk $Ba(NO_3)_2$ species on the γ-Al_2O_3 support is reasonably well understood, and its spectroscopic properties (infrared vibrational frequencies of the nitrates) have been accurately predicted by density functional theory (DFT) calculations [17]. On the other hand, no clear understanding has been developed on the nature of the so called "surface nitrates". Very recently, we have reported the results of a combined experimental and DFT investigation in which we set out to understand the role of the interaction between BaO and γ-Al_2O_3 in the NO_2 uptake process at low BaO loadings, and the characteristics of the "surface" nitrate species thus formed [18].

First-principles DFT slab calculations were used to investigate adsorption, clustering and overlayer formation of BaO on γ-Al_2O_3 surfaces [19]. Multiple stable adsorption configurations were identified for adsorbed BaO monomers and $(BaO)_2$ dimers on both (100) and (110) surfaces of γ-Al_2O_3. These structures were similar to those observed in the HR-TEM data (e.g., see Figure 2) and, thus, used to calculate stable structures of NOx on these models for "surface" Ba-nitrate species. The optimized structures of nitrates on a BaO monomer over the γ-Al_2O_3(100) surface are shown in Figure 5a, where we also list the ranges of calculated vibrational frequencies for a number of possible stable structures. Similarly, Figure 5b shows a calculated stable structure and range of vibrational frequencies for NOx adsorption on a bulk BaO(100) surface.

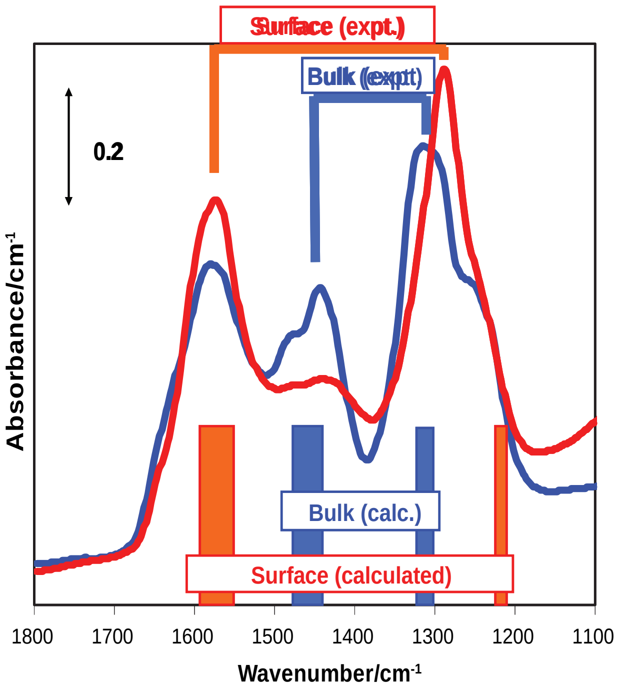

FIGURE 6. FTIR spectra obtained from an 8 wt% BaO/γ-Al_2O_3 sample after NO_2 saturation at 300 K (blue) and subsequent annealing at 600 K (red). The calculated infrared vibrational frequencies for the nitrate species formed are displayed as well.

Two infrared spectra recorded from an 8 wt% BaO/γ-Al_2O_3 after saturation with NO_2 at 300 K (both surface and bulk nitrates are present) and subsequent heating to 600 K (mostly surface nitrates are present) are shown in Figure 6, together with the vibrational frequency ranges our calculation predicted for nitrates bound to $(BaO)_x$ on γ-Al_2O_3 (red columns) and BaO(100) (blue columns). The agreement between the experimentally measured frequencies and the DFT predictions for both "surface" and "bulk" BaO-bound nitrates is excellent. This clearly indicates that two different forms of nitrates on the alumina support.

The results of our recent study [18], in conjunction with our prior work on both model and supported BaO/γ-Al_2O_3 NO_x storage systems, allows the unambiguous identification of the different nitrate species that we earlier identified as "surface" and "bulk" nitrates. Bulk nitrates can be envisioned as nitrates formed on the surfaces and in the bulk of BaO particles, while surface nitrates are the ones that from on alumina-supported $(BaO)_x$ species (monomers, dimers, and/or possibly somewhat higher x values) that are bound to penta-coordinated Al^{3+} sites. The properties of these very small $(BaO)_x$ units are fundamentally different from those of the bulk BaO particles. Their strong interaction with the alumina surface alters their chemical properties in their reaction with NO_2, thus altering their spectroscopoic characteristics.

This combined experimental and theoretical study clearly illustrates the power of such a concerted effort to unravel the interactions of NOx molecules with oxide (mixed oxide) surfaces. The results of these combined studies have allowed us to develop a clear understanding of the nature of both the surface and bulk types of nitrates on the BaO/γ-Al_2O_3 NOx storage system, a subject actively debated in the literatures for some time.

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FY 2008 Presentations

Invited

1. Peden, C.H.F. "Fundamental Studies of Catalytic NOx Vehicle Emission Control." Invited Presentations made by Chuck Peden at the following locations:

- Korea Institute of Energy Research, Daejon, South Korea, November 2007.
- Argonne National Laboratory, Argonne, IL, December 2007.
- Northwestern University, Evanston, IL, January 2008.
- Annual DOE/EE/OVT Peer Review, February 2008.

2. Peden, C.H.F. "The Use of Ultrahigh Field NMR Spectroscopy to Study the Surface Structure and Catalytic Properties of Poorly Crystalline γ–Al_2O_3." Invited Presentations made by Chuck Peden at the following locations:

- Annual Meeting of the Philadelphia Catalysis Club, Newark, DE, May 2008.
- 14th International Congress on Catalysis, Seoul, South Korea, July 2008.
- 236th American Chemical Society National Meeting, Philadelphia, PA, August 2008.

3. Peden CHF. "The Nanoscience of Next Generation Automobile Emission Control Catalysts." Invited Presentation made by Chuck Peden at the European Science Foundation Conference on "Nanotechnology for Sustainable Energy", Ötz Valley, near Innsbruck, Austria, June 2008.

Contributed

1. Peden CHF. "Fundamental Studies of NOx Adsorber Materials at PNNL." Presented by Chuck Peden at the 10th DOE CLEERS Workshop, Dearborn, MI, May 2008.

2. Kwak JH, JZ Hu, DH Kim, J Szanyi, and CHF Peden. "The Use of Ultra High-Field Nuclear Magnetic Resonance Spectroscopy to Study the Surface Structure of Poorly Crystalline γ-Al_2O_3 Surfaces." Presented by Chuck Peden at the AVS 54th International Symposium, Seattle, WA, November 2007.

3. Yi CWW, JH Kwak, CHF Peden, CM Wang, and J Szanyi. "Strong Interaction between BaO and Al_2O_3 in NOx Storage Materials: Correlation between Model and High Surface Area Catalysts." Presented by Janos Szanyi at the 54th AVS, Seattle, WA, November 2007.

4. Yi CWW, JH Kwak, CHF Peden, and J Szanyi. "Ba-Containing Al_2O_3 NOx Storage Materials: Correlation between the Model and High Surface Area Catalysts." Presented by Cheol-Woo Yi at the 235th ACS National Meeting, New Orleans, LA, April 2008.

5. Kwak JH, JZ Hu, DH Kim, CHF Peden, and J Szanyi. "Nucleation on and stability of γ-Al_2O_3 surfaces: the special role of penta-coordinated Al^{3+} sites." Presented by Janos Szanyi at the 5th International Conference on Environmental Catalysis, Belfast, Ireland, September 2008.

6. Yi CWW, JH Kwak, CHF Peden, and J Szanyi. "Understanding practical catalysts using a surface science approach: the importance of strong interactions between BaO and Al_2O_3." Presented by Janos Szanyi at the 5th International Conference on Environmental Catalysis, Belfast, Ireland, September 2008.

FY 2008 Publications

1. Epling, W.S.; Nova, I.; Peden, C.H.F. "Preface: Special Issue on 'Catalytic Control of Emissions from Diesel-Powered Vehicles." *Catalysis Today* **136** (2008) 1-2.

2. Verrier, C.; Kwak, J.H.; Kim, D.H.; Peden, C.H.F.; Szanyi, J. "NOx uptake on alkaline earth oxides (BaO, MgO, CaO and SrO) supported on γ-Al_2O_3." *Catalysis Today* **136** (2008) 121-127.

3. Epling, W.S.; Peden, C.H.F.; Szanyi, J. "Carbonate Formation and Stability on a $Pt/BaO/Al_2O_3$ NOx Storage/Reduction Catalyst." *Journal of Physical Chemistry C* **112** (2008) 10952-10959.

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8. Mei, D.; Ge, Q.; Szanyi, J.; Peden, C.H.F. "A First-Principles Analysis of NO_x Adsorption on Anhydrous γ-Al_2O_3 Surfaces." *Journal of Physical Chemistry C*, submitted for publication.

II.B.2 Mechanisms of Sulfur Poisoning of NOx Adsorber Materials

Do Heui Kim, George Muntean,
Chuck Peden (Primary Contact)
Institute for Interfacial Catalysis
Pacific Northwest National Laboratory (PNNL)
P.O. Box 999, MS K8-93
Richland, WA 99354

DOE Program Manager: Ken Howden

Cooperative Research and Development Agreement (CRADA) Partners:
- Randy Stafford, John Stang, Alex Yezerets, Neal Currier - Cummins Inc.
- Hai-Ying Chen, Howard Hess - Johnson Matthey

Objectives

- Develop and apply characterization tools to probe the chemical and physical properties of oxides of nitrogen (NOx) adsorber catalyst materials for studies of deactivation due to sulfur poisoning and/or thermal aging. Utilize this information to develop mechanistic models that account for NOx adsorber performance degradation.
- Develop protocols and tools for failure analysis of field-aged materials.
- Provide input on new catalyst formulations; verify improved performance through materials characterizations, and laboratory and engine testing.

Accomplishments

Three major thrusts this year:

- Promotional effects of H_2O treatment on fresh and thermally aged Pt-BaO/Al_2O_3 lean-NOx trap (LNT) catalysts:
  - We observed that a simple liquid water treatment applied to fresh and thermally aged Pt(2 wt%)-BaO(20 wt%)/Al_2O_3 LNT catalysts at room temperature induces morphological and structural changes in the barium species, resulting in the increase in the NOx uptake.
- Effect of sulfation levels on the desulfation behavior of pre-sulfated Pt-BaO/Al_2O_3 LNT catalyst:
  - In the previous work, our group [1] has reported that desulfation processes for sulfated Pt-BaO/Al_2O_3 LNT materials show a strong dependence on barium loading and, moreover, occur more facilely over at lower loadings by using a combination of various characterization techniques.
  - By using the similar approaches, we found that the sulfur species at low sulfur loading are less likely to be removed as H_2S and have more tendency to be transformed to sulfide species (as BaS) on the material, thus demonstrating the significant effect of sulfation levels on the desulfation behavior of LNT materials.
- Excellent sulfur resistance of Pt-Ba/CeO_2 LNT catalysts:
  - Besides their superior intrinsic NOx uptake properties, we found that ceria-based catalysts have a) much higher sulfur tolerance and b) excellent resistance against Pt sintering when they are compared to the widely used alumina based catalysts.

Five public presentations and five manuscripts have been cleared for release by CRADA partners.

Future Directions

- Further refine function-specific measures of ‘aging’:
  - More detailed studies to verify that techniques such as NO_2 temperature programmed desorption (TPD) and hydrogen temperature programmed reaction (TPRX) are providing information content suggested by studies to date.
  - Some effort still to identify new approach to unravel some key unknowns (*e.g.*, role of precious metal/storage material ‘contact’).
- Validate most-suitable function-specific measures on samples incrementally ‘aged’ under realistic conditions.
- Apply the developed techniques to the commercial fresh and “aged” samples in the monolith form:
  - Find the optimized regeneration condition by using developed reaction protocol.
  - X-ray photoelectron spectroscopy (XPS), sulfur X-ray absorption near edge spectroscopy (XANES), time resolved X-ray diffraction (TR-XRD) studies to follow the changes of sulfur species with sulfation/desulfation.
  - Use the technique with the spatial resolution such as scanning electron microscopy (SEM)/energy dispersive X-ray (EDX) and XPS to focus on the distribution of sulfur with sulfation/desulfation.

- Continue to improve mechanistic understanding of sulfur removal processes:
  - Investigate the role of Pt during desulfation.
  - Identify important desulfation intermediates.
  - Effects of sulfur concentration on Pt accessibility and barium phase changes.

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Introduction

The NOx adsorber (also known as the LNT) technology is based upon the concept of storing NOx as nitrates over storage components, typically barium species, during a lean-burn operation cycle and then reducing the stored nitrates to N_2 during fuel-rich conditions over a precious metal catalyst [2]. This technology has been recognized as one of the most promising approaches for meeting stringent NOx emission standards for diesel vehicles within the Environmental Protection Agency's 2007/2010 mandated limits. However, problems arising from either or both thermal and SO_2 deactivation must be addressed to meet durability standards. Therefore, an understanding of these processes will be crucial for the development of the LNT technology.

This project is focused on the identification and the understanding of the important degradation mechanism(s) of the catalyst materials used in LNTs. 'Simple' and 'Enhanced Model' Pt/BaO/Al_2O_3 samples were investigated. In particular, the changes in physicochemical properties related to the reaction performances of these LNT materials, due to the effects of high temperature operation and sulfur poisoning, are the current focus of the work. By comparing results obtained on 'Simple Model' Pt/BaO/Al_2O_3 with 'Enhanced Model' materials, we try to understand the role of various additives on the deactivation processes. We now move on to the real commercial sample which is being used in a Dodge Ram truck with a Cummins diesel emission control system. However, the results about the 'commercial sample' will not be covered in this report. We further note here that while project progress for the entire year is summarized in the "Accomplishments" section, we present below more detail about results obtained in this last year in three specific areas: i) promotional effect of H_2O treatment on NOx storage over fresh and thermally aged LNT catalysts, ii) effects of sulfation levels on the desulfation behavior of pre-sulfated LNT catalysts, iii) excellent sulfur resistance of Pt/BaO/CeO_2 LNT materials.

Approach

In a microcatalytic reactor system, LNT performance is evaluated in a fixed bed reactor operated under continuous lean-rich cycling. Rapid lean-rich switching is enabled just prior to the elevated temperature zone (furnace) where the LNT materials are contained in quartz tubing. After removing water, the effluent of the reactor can be analyzed by mass spectrometry and by a chemiluminescent NOx analyzer. For a typical baseline performance testing, the sample is heated to a reaction temperature in flowing He, the feed switched to a 'lean-NOx' mixture containing oxygen and NO, as well as CO_2 and/or H_2O. After an extended period (15 minutes or more), multiple rich/lean cycles of 1 and 4 minute duration, respectively, are run and NOx removal performance is assessed after at least three of these are completed. In the LNT technology, the state of the system is constantly changing so that performance depends on when it is measured. Therefore, we obtain NOx removal efficiencies as "lean conversion (30 minutes)", which measures NOx removal efficiencies for the first 30 minutes of the lean-period. In addition, material treatments such as SO_2 aging, and post mortem catalyst characterizations were conducted in the same test stand without exposing the catalyst sample to air. We have established a reaction protocol, which evaluates the performance of samples after various thermal aging and sulfation condition. In this way, we could identify optimum de-sulfation treatments to rejuvenate catalyst activities.

State-of-the-art catalyst characterization techniques such as XRD, XPS, transmission electron spectroscopy (TEM)/energy dispersive spectroscopy (EDS), Brunauer, Emmett and Teller (BET)/pore size distribution, and TPD/TPRX were utilized to probe the changes in physicochemical properties of the catalyst samples under deactivating conditions; *e.g.*, thermal aging and SO_2 treatment. Specifically, hydrogen TPRX, in situ sulfur K-edge XANES (X-ray absorption near edge spectroscopy) and TR-XRD (time-resolved X-ray diffraction) methods were used extensively to quantify the levels, speciation and phase of sulfur on the model adsorber material (Pt-BaO/Al_2O_3 and Pt-BaO/CeO_2) as a function of desulfation process.

Results

Promotional Effects of H_2O Treatment on Fresh and Thermally Aged Pt-BaO/Al_2O_3 LNT Catalysts

A simple liquid water treatment applied to fresh and thermally aged Pt(2 wt%)-BaO(20 wt%)/Al_2O_3 LNT catalysts at room temperature induces morphological and structural changes in the barium species as followed by XRD and TEM analysis. During the water treatment, liquid water sufficient to fill the catalyst pore volume is brought into contact with the samples. It was found that irrespective of the original barium chemical state (highly dispersed BaO or crystalline $BaAl_2O_4$), exposing the sample to this liquid water treatment promotes the formation of $BaCO_3$ crystallites (about 15–25 nm of its size) without changing the Pt particle size as demonstrated in XRD and TEM. Such transformations of the barium species are found to significantly promote NOx uptake from 250°C to 450°C as shown in Figure 1. All three H_2O-treated samples (1b) show higher NOx uptake for short-term and long-term performance compared with their non-treated counterparts (1a). The increase in the NOx uptake for the water-treated samples can be attributed to an enhanced Pt-Ba interaction through the redistribution of barium species. These results provide useful information for the regeneration of aged LNT catalysts since water is plentiful in the exhaust of diesel or lean-burn engines.

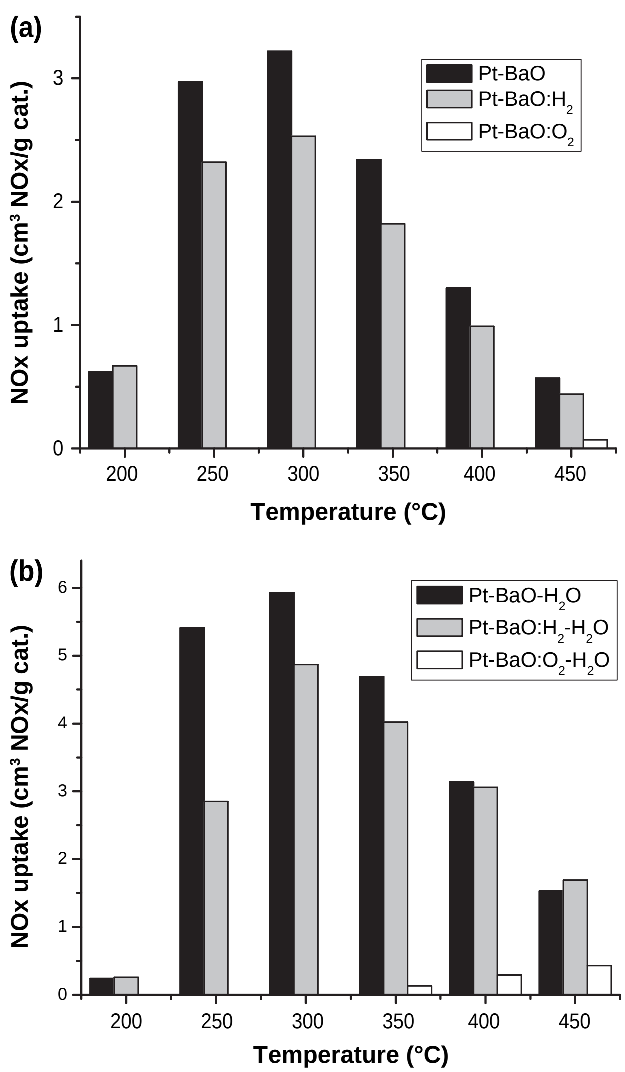

FIGURE 1. Comparison of NOx uptake as a function of temperature up to 20% breakthrough of the inlet NO concentration for over Pt-BaO/Al_2O_3, Pt-BaO/Al_2O_3–H_2 (thermally aged with H_2) and Pt-BaO/Al_2O_3-O_2 (thermally aged with O_2) samples (a) and their water-treated samples (b).

Effect of Sulfation Levels on the Desulfation Behavior of Pre-Sulfated Pt-BaO/Al_2O_3 LNT Catalyst

Our group [1] has reported that desulfation processes for sulfated Pt-BaO/Al_2O_3 LNT materials show a strong dependence on barium loading and, moreover, occur more facilely over at lower loadings by using a combination of the hydrogen TPRX, TEM with EDS, sulfur K-edge XANES, and in situ TR-XRD. This study aims at investigating the desulfation with H_2 as a function of sulfur loading. Thus, pre-sulfated Pt(2 wt%)-BaO(20 wt%)/Al_2O_3 with various sulfur loading (S/Ba = 0.12, 0.31 and 0.62) were prepared and investigated by using combined hydrogen TPRX, XPS, in situ sulfur K-edge XANES and synchrotron TR-XRD techniques. It was found that the amount of H_2S desorbed resulting from the desulfation is not proportional to the amount of initial sulfur loading based on hydrogen TPRX results as shown in Figure 2. Especially, in situ sulfur K-edge XANES and TR-XRD results showed that the sulfur species loaded initially, i.e. at lower sulfur loading, have a tendency to be transformed to BaS phase and remain in the catalyst, rather than being removed as H_2S from the catalyst. On the other hand, the sulfur species deposited exceeding some level (at least S/Ba = 0.31) was desorbed as the form of H_2S, thus the relative portion of the residual sulfide species is much less than that of the sample with low sulfur loading. Unlike the sample with high sulfur loading (S/Ba = 0.62), H_2O did not promote the desulfation over the sample with S/Ba of 0.12, implying that the formed BaS species originating from the low sulfur loading are more stable against

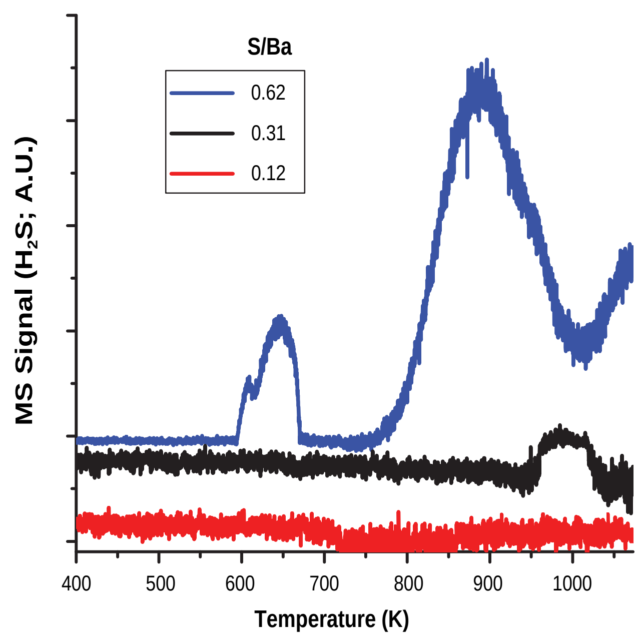

FIGURE 2. H_2 TRPX spectra for Pt-BaO/Al_2O_3 with different sulfation level, in which is described as S/Ba of 0.12, 0.31 and 0.62.

H_2O. It can be concluded that the sulfur species at low sulfur loading are less likely to be removed as H_2S and have more tendency to be transformed to sulfide species (as BaS) on the material, based on the various characterization results.

Excellent Sulfur Resistance of Pt/BaO/CeO_2 LNT Materials

We investigated the NOx storage behavior of Pt-BaO/CeO_2 catalysts, especially in the presence of SO_2. High surface area CeO_2 (~ 110 m^2/g) with a rod like morphology was synthesized and used as a support. The Pt-BaO/CeO_2 sample demonstrated slightly higher NOx uptake in the entire temperature range studied compared with Pt-BaO/γ-Al_2O_3. More importantly, this ceria-based catalyst showed higher sulfur tolerance than the alumina-based one as shown in Figure 3. The time of complete NOx uptake was maintained even after exposing the sample to ~3 g/L of SO_2. The same sulfur exposure, on the other hand, eliminated the complete NOx uptake time on the alumina-based NO_x storage catalysts. As seen in Figures 4a and 4b TEM images show no evidence of either Pt sintering or BaS phase formation during reductive de-sulfation up to 600°C on the ceria-based catalyst, while the same process over the alumina-based catalyst (Figures 4c and 4d) resulted in both a significant increase in the average Pt cluster size and the agglomeration of a newly-formed BaS phase into large crystallites. XPS results revealed the presence of about five times more residual sulfur after reductive de-sulfation at 600°C on the alumina-based catalysts in comparison with the ceria-based ones. All of these results strongly support that, besides their superior intrinsic NOx uptake properties, ceria-based catalysts have a) much higher sulfur tolerance and b) excellent resistance against Pt sintering when they are compared to the widely used alumina-based catalysts.

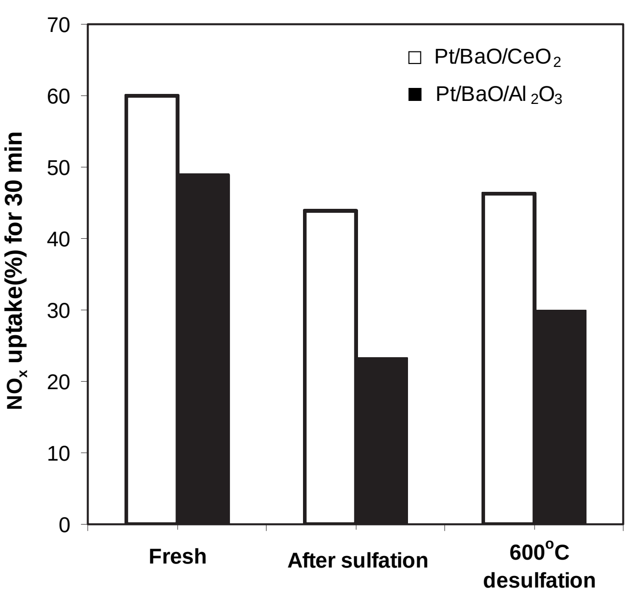

FIGURE 3. NOx Uptake (%) for 30 min over Pt-BaO/CeO_2 and Pt-BaO/Al_2O_3

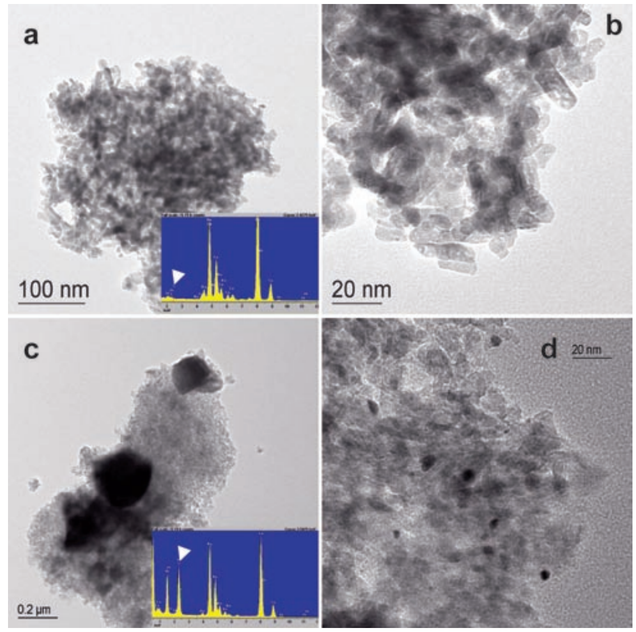

FIGURE 4. TEM Images for Pt-BaO/CeO_2 (a,b) and Pt-BaO/Al_2O_3 (c,d) after De-Sulfation at 600°C

Conclusions

PNNL and its CRADA partners from Cummins Inc. and Johnson Matthey have carried out a project to study the mechanisms of deactivation of the materials proposed for use in LNTs arising from thermal aging and SO_2 poisoning. Results demonstrate that water treatment promoted the NOx uptake significantly for the fresh and thermally aged LNT materials. By using in situ characterization techniques, we can figure out that the sulfur species at low sulfur loading is less likely to be removed and has more tendency to be transformed to BaS. We found that the CeO_2-supported LNT catalyst has better intrinsic NOx uptake in addition to the much higher sulfur tolerance and the resistance against Pt sintering than alumina-supported counterparts. In overall, these approaches are expected to give invaluable information to overcome the critical stability issues in LNT catalysts.

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II.B.3 Characterizing Lean-NOx Trap Regeneration and Desulfation

James Parks (Primary Contact),
Vitaly Prikhodko, Mike Kass, Shean Huff
Oak Ridge National Laboratory (ORNL)
2360 Cherahala Boulevard
Knoxville, TN 37932

DOE Technology Development Manager:
Ken Howden

Objectives

- Establish relationships between exhaust species and various lean-oxides of nitrogen (NOx) trap (LNT) regeneration strategies.
- Characterize effectiveness of in-cylinder regeneration strategies.
- Develop stronger link between bench and full-scale system evaluations.
- Provide data through Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) to improve models. Use models to guide engine research.

Accomplishments

- Developed LNT regeneration strategy based on Premixed Charge Compression Ignition (PCCI) combustion mode for use at low loads.
- Demonstrated low temperature desulfation (onset at ~300°C) of a Ce-based LNT formulation on a bench flow reactor, and characterized the NOx performance.
- Characterized the impact of precious metal loading on LNT performance as a function of temperature on a bench flow reactor.

Future Directions

- Analyze the regeneration process in a hybrid LNT-selective catalytic reduction system.
- Study LNT catalysis for lean gasoline applications.

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Introduction

As part of the Department of Energy's strategy to reduce imported petroleum and enhance energy security, the Office of Vehicle Technologies has been researching enabling technologies for more efficient diesel engines. NOx emissions from diesel engines are very problematic and the U.S. Environmental Protection Agency emissions regulations require ~90% reduction in NOx from light- and heavy-duty diesel engines in the 2004-2010 timeframe. One active research and development focus for lean-burn NOx control is in the area of LNT catalysts. LNT catalysts adsorb NOx very efficiently in the form of a nitrate during lean operation, but must be regenerated periodically by way of a momentary exposure to a fuel-rich environment. This rich excursion causes the NOx to desorb and then be converted by precious metal catalysts to harmless nitrogen. The momentary fuel-rich environment in the exhaust occurs 2-4 seconds for every 30-90 seconds of normal lean operation (depending on operating conditions). The rich exhaust can be created by injecting excess fuel into the cylinder or exhaust, throttling the intake air, increasing the amount of exhaust gas recirculation (EGR), or through some combination of these strategies. The controls methodology for LNTs is very complex, and there is limited understanding of the how all of the competing factors can be optimized.

While LNTs are effective at adsorbing NOx, they also have a high affinity for sulfur. As such, sulfur from the fuel and possibly engine lubricant (as SO_2) can adsorb to NOx adsorbent sites (as sulfates). Similar to NOx regeneration, sulfur removal (desulfation) also requires rich operation, but for several minutes, at much higher temperatures. Desulfation intervals are much longer, on the order of hundreds or thousands of miles, but the conditions are more difficult to achieve and are potentially harmful to the catalyst function. Nonetheless, desulfation must be accomplished periodically to maintain effective NOx performance. There is much to be learned with regard to balancing all the factors in managing LNT NOx control performance, durability, and sulfur tolerance.

The objective of this project is to understand the complex chemistry that occurs during the regeneration processes for LNTs through experiments conducted on a full-size engine-LNT catalyst system; supplemental research in a more controlled experiment is also conducted on a bench flow reactor for comparison. Different strategies for introducing the excess fuel for regeneration can produce a wide variety of hydrocarbon and other species. Specific regeneration strategies were developed for this project by operating the engine with net rich air-to-fuel ratios; such "in-cylinder" techniques utilize throttling to reduce air flow and extra fuel injection pulses during the combustion event to increase fueling. A primary focus of this work is to examine the effectiveness of various regeneration strategies in light of the species formed and the LNT formulation since the combined chemistry of the exhaust produced by the regeneration strategy and the chemistry of the LNT catalyst dictate performance.

Approach

A 1.7-L Mercedes-Benz common rail engine and motoring dynamometer have been dedicated to this activity. The engine is equipped with an electronic engine control system that provides bypass of the original equipment controller for stand-alone control of the engine. The controller is capable of monitoring and controlling all the electronically controlled parameters associated with the engine (i.e., fuel injection timing/duration/number of injections, fuel rail pressure, turbo wastegate, electronic throttle, and electronic EGR). The experimental setup allows for full exhaust species characterization throughout the catalyst system. This includes the measurement of key reductants such as hydrogen (H_2), carbon monoxide (CO), and hydrocarbons as well as NOx and potential nitrogen-based byproducts such as ammonia (NH_3) at five locations within the LNT system. A full set of analyzers is applied to sample the various species; analysis techniques include: chemiluminescence for NOx, Fourier transform infrared spectroscopy for NH_3, magnetic sector mass spectrometry for H_2, nondispersive infrared analysis for CO, and flame ionization detector analysis for hydrocarbons.

Results

In Fiscal Year 2008, experiments were conducted on both the diesel engine platform and bench flow reactor. A main component of the engine studies was the development of a regeneration strategy for use during PCCI combustion. Specifically, a type of PCCI combustion known as High Efficiency Clean Combustion (HECC) has been used in companion projects (specifically the project "Efficient Emissions Control for Multi-Mode Lean DI Engines") to demonstrate low emissions (NOx and particulate matter) with fuel efficiency comparable to more conventional diesel combustion modes. HECC utilizes high EGR rates and advanced fuel injection timing with high injection pressures. Strategies were developed to enable the transition to rich combustion from HECC.

Bench flow reactor experiments were conducted on two LNT catalyst formulations. A Ce-based formulation was studied based on reports from Honda about the low temperature performance associated with Ce-based LNTs [1]. CeO_2 was added to a Pt/alumina (Al_2O_3) model catalyst to form the Ce-based LNT; the catalyst was on a 300 cells per square inch (cpsi) cordierite substrate. The NOx reduction efficiency of the Ce-based LNT was measured as a function of temperature at a space velocity of 30,000/hr. Results are shown in Figure 1. Performance peaked at ~250°C, and the performance in general was optimal at temperatures slightly lower than typical (Ba-based) LNT formulations. After loading the Ce LNT with sulfur by flowing sulfur dioxide (SO_2) over the catalyst in an oxygen-rich environment, the catalyst was desulfated by flowing H_2 over the catalyst in an oxygen-depleted environment. Temperature Programmed Reduction (TPR) was used to determine the desulfation temperature of the catalyst. Figure 2 shows the TPR data; the S was released primarily as hydrogen sulfide (H_2S). Onset of desulfation occurred slightly below 300°C and continued until ~500°C. Sulfation of the Al_2O_3 in the catalyst may have contributed to the higher temperature S release.

The other LNT formulation examined was Ba-based which is the most common alkaline earth material used for LNTs. Four Ba-based LNT catalysts were coated with different Pt loads on 300 cpsi cordierite substrates;

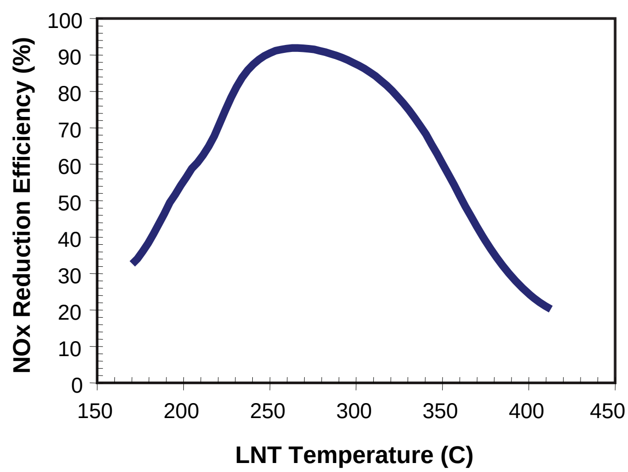

FIGURE 1. NOx Reduction Efficiency as a Function of Temperature for a Ce-Based LNT

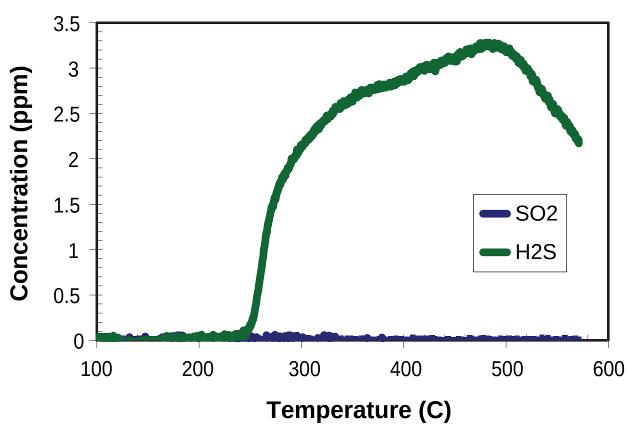

FIGURE 2. TPR Showing Desulfation of the Ce-Based LNT

the formulation was a model catalyst with Ba on Pt/Al_2O_3. The four Pt loads were 25, 50, 75, and 100 g/ft^3. The NOx reduction performance of the four Pt loaded catalysts as a function of temperature is shown in Figure 3. A reduction in Pt causes two effects: (1) an overall loss in NOx storage capacity which impacts NOx reduction performance at all temperatures and (2) a loss of performance specific to the low temperature onset of activity. This information is important as research is focused on lowering the cost of these technologies, and lower costs are needed for fuel efficient technologies to be able to penetrate the market significantly.

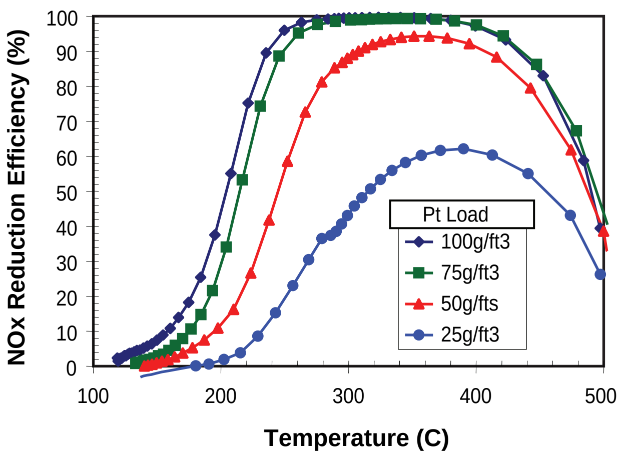

FIGURE 3. NOx Reduction Efficiency as a Function of Temperature for Four Different Pt Loadings

Conclusions

- LNT regeneration strategies can be developed that transition directly from high level EGR PCCI-type combustion modes.
- Ce-based LNTs show low temperature desulfation capabilities and have NOx reduction performance in a temperature range slightly lower than more common Ba-based LNTs.
- Decreasing the Pt load of a Ba-based LNT affects the NOx reduction performance by lowering storage capacity at all temperatures and increasing the light-off temperature indicative of the onset of performance.

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II.B.4 Development of Chemical Kinetics Models for Lean-NOx Traps

Richard S. Larson
Sandia National Laboratories
MS 9409, P.O. Box 969
Livermore, CA 94551-0969

DOE Technology Development Manager:
Kenneth Howden

Collaborators:
Kalyana Chakravarthy, Josh A. Pihl, Jae-Soon Choi, and C. Stuart Daw (Oak Ridge National Laboratory, Knoxville, TN)

Objectives

- Identify a set of elementary (microkinetic) surface reactions that can account for the observed behavior of a lean-oxides of nitrogen (NOx) trap (LNT) during a complete storage/regeneration cycle.
- Optimize the kinetic parameters associated with these reactions by matching model predictions with laboratory reactor data.
- Extend the mechanism to include reactions involving sulfur-containing species, with the aim of describing both catalyst degradation during normal operation and catalyst restoration during high-temperature desulfation.
- Use the validated reaction mechanism to suggest improvements in the usage of existing LNT materials and to help in the development of a new generation of catalysts.

Accomplishments

- Completed construction and optimization of a thermodynamically consistent reaction mechanism for the storage (both NOx and oxygen) sites on a benchmark LNT catalyst, to be used in conjunction with the previously developed precious metal mechanism.
- Modified our transient plug flow code to account for radial washcoat diffusion and evaluated the effective mass-transfer coefficients simultaneously with the kinetic parameters.
- Assembled tentative mechanisms for sulfur reactions on the precious metal, NOx storage, and oxygen storage sites on the catalyst and formulated the corresponding thermodynamic constraints.
- Using the previously adopted methodology, carried out a preliminary evaluation of the sulfation/desulfation kinetic parameters that allows qualitative reproduction of observed poisoning behavior.

Future Directions

- Complete parameter optimization for the sulfation/desulfation mechanism to allow a full quantitative description of catalyst poisoning and restoration.
- Account for the role of partial oxidation products as alternate reductant species during normal catalyst regeneration.
- Use the validated reaction mechanisms to investigate coupling between an LNT and other devices in the aftertreatment train.

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Introduction

The increasingly strict constraints being placed on emissions from diesel and other lean-burn engines require the development of a new generation of aftertreatment technologies. LNTs represent one option for achieving the stated targets with regard to NOx emissions. In an LNT, NOx produced during normal lean engine operation is trapped and stored via adsorption on high-capacity catalytic sites, and periodically this stored NOx is released and reduced to harmless N_2 on precious metal sites by imposing rich conditions for a short time. While this qualitative description is widely accepted, a detailed quantitative understanding of the underlying chemistry is not yet available. Such knowledge is needed in order to use the LNT concept to best advantage, so it is the principal goal of this project to develop an elementary reaction mechanism that describes both phases of LNT operation.

A complicating factor in the use of LNTs is that sulfur-containing contaminants in the fuel can lead to degradation in the catalyst performance over time, so periodic desulfation episodes are needed in addition to the ordinary regeneration (deNOx) excursions. Thus, a truly comprehensive mechanism must include reactions of sulfur-containing species alongside those describing storage, release, and reduction of NOx.

Clearly, a kinetics model with the ability to simulate all phases of LNT operation must account for the chemistry occurring on several kinds of catalytic sites: the metal oxide sites used to store NOx, additional oxide sites used (sometimes) for oxygen storage, and the precious metal sites involved primarily in the reduction of released NOx. While it is tempting to associate each of these kinds of sites with a particular part of the LNT cycle, it must be remembered that the desorption of NOx from the storage sites is an integral part of the regeneration process, while oxidation of NO on the precious metal sites is thought to be a key part of the storage phase. Nevertheless, it is possible to design experiments that isolate a particular subset of the chemistry, and this has been used to facilitate model development in this project. Thus, work in previous years led to a mechanism for the precious metal sites alone, and our more recent work has allowed us to complete the basic mechanism by appending reactions for the storage sites. The addition of sulfation/desulfation reactions involving all kinds of sites is then fairly straightforward if one assumes that the roles of nitrogen- and sulfur-containing species are analogous.

Approach

Our basic approach to mechanism development is to assemble a candidate set of elementary reactions, often with poorly known kinetic parameters, and then to optimize the parameters by fitting the results of reactor simulations to bench-scale experimental data provided by our collaborators at Oak Ridge National Laboratory. This process requires two principal pieces of supporting software: a reactor code to simulate flow through a single monolith channel using the proposed reaction mechanism (expressed in Chemkin format), and an optimization code to carry out the fitting process on a massively parallel machine. For the simulation of LNT cycles we have used a specially modified transient Chemkin-based plug flow code, and for the optimization we have adopted the Sandia APPSPACK code [1], which is ideally suited to this application.

As mentioned above, a mechanism for the chemistry occurring on the precious metal sites was constructed and validated in previous years. We have elected to incorporate this almost without modification into the complete mechanism; the sole exception is that the precious metal site density, which was indeterminate in the previous calculations, is now added to the list of adjustable parameters. To the (nearly) fixed precious metal mechanism is added a set of candidate reactions for the storage sites, and the unknown kinetic parameters are estimated by fitting the results (specifically, the exit gas concentrations) of full-cycle reactor simulations to the corresponding experimental data at three distinct temperatures.

As with the precious metal mechanism, a significant issue that must be addressed in the optimization process is that not all of the parameters can be varied independently if thermodynamic consistency is to be maintained. Thus, a number of well-defined relationships among the various parameters are enforced; this reduces the size of the optimization problem, but it greatly increases the programming complexity. In addition, all of the activation energies, whether varied independently or computed from thermodynamic constraints, are required for physical reasons to be non-negative. Fortunately, the resulting inequality constraints are easily handled by APPSPACK.

A further complication in simulating LNT cycles is that mass-transfer resistance within the catalyst washcoat probably cannot be ignored. A full treatment of this phenomenon would result in a transient two-dimensional reactor model, which would be computationally prohibitive in light of the large number of simulations needed for parameter optimization. Thus, we have elected to adopt a one-dimensional lumped-parameter description of the washcoat: At each axial position and for each gas-phase species, the actual radial concentration profile is replaced by a single average concentration value, and reaction rates are evaluated at this internal value rather than at the concentration in the bulk gas. Transport within the washcoat is then described in terms of a set of adjustable mass transfer coefficients.

Results

Our attempt to develop a mechanism describing all phases of normal LNT operation has been completed. As noted above, this involved adding to the precious metal submechanism a set of reactions describing storage of both NOx and oxygen, each on its own type of site. The submechanism for the baria (NOx storage) phase involves six kinds of surface species, namely empty sites and adsorbed oxygen atoms, carbonates, hydroxides, nitrites, and nitrates. In addition, there is a so-called bulk nitrate to represent the slow storage sites suggested by experimental observations. The first step in the proposed reaction scheme is the dissociative adsorption of oxygen. Reaction of gas-phase NO_2 with an oxygenated site then yields a surface nitrate; to accord with experiment, analogous storage of NO is not allowed. CO_2 and H_2O can displace NO_2 from surface nitrates to form carbonates and hydroxides, respectively, and CO_2 and H_2O can also displace each other. Gas-phase NO can reduce a surface nitrate to form a nitrite, but actual storage of NO can occur only after conversion to NO_2 on the precious metal sites. Formation of nitrites can also occur via surface decomposition of nitrates or spillover from adjacent precious metal sites. Finally, surface nitrates can be converted to the bulk form (and vice versa, as all reactions are treated as reversible). By contrast, the submechanism for the ceria (oxygen storage) phase is much simpler, consisting of just a single adsorption step.

As noted above, the kinetic parameters for the storage phases are evaluated by fitting transient plug flow simulations involving the complete mechanism to experimental data for complete LNT cycles. Because the surface site densities for the various phases are not known with any accuracy, they are also treated as adjustable parameters. However, they are first mathematically decoupled from the reaction rate terms (as opposed to the capacity terms) in the conservation equations, in much the same way that the activation energies are decoupled from the rate constants. This greatly facilitates the optimization process.

APPSPACK is used to fit the model to data for a benchmark long cycle at three temperatures (200°C, 300°C, and 400°C) simultaneously. The experimental [2] and simulated results at 200°C are shown in Figures 1 and 2, respectively, while the corresponding results at 400°C are shown in Figures 3 and 4. Given the relative crudeness of the mass transfer model and the use of independently-derived precious metal parameters, the agreement is overall quite good. At 200°C there is an obvious problem with the underprediction of N_2O, which may be due to imperfections in the precious metal chemistry; in any case, reproducing experimental results at these relatively low temperatures is usually difficult. There are also some minor discrepancies at 400°C, but the size of the NOx puff at the start of regeneration and the timing of the various breakthrough events, in particular, are reproduced very well.

In keeping with our stepwise approach to mechanism development, a framework for describing sulfation and desulfation has been constructed by appending sulfur-specific reactions to the completed mechanism for normal LNT operation, which is now regarded as fixed. Because the expanded mechanism has not yet been used to fit experimental data quantitatively, it almost certainly contains some reactions that will ultimately prove to be unimportant. On the other hand, it is already simpler than the storage/regeneration mechanism in one sense, namely that it involves sulfates but not sulfites, the latter not being observed experimentally.

The sulfur-specific reactions involve the same surface phases defined previously and follow the general pattern already established for nitrogen-containing species. Thus, on the precious metal sites, there are adsorptions of the three new gas-phase molecules (SO_2, SO_3, and H_2S), stepwise surface decompositions of the adsorbates, oxidations of surface H_2S fragments by adsorbed oxygen, and reductions of surface SOx fragments by adsorbed H and CO. There is also a route for H_2S formation via a carbonyl sulfide intermediate,

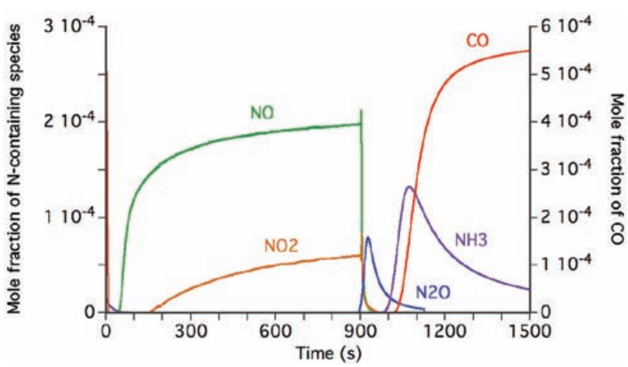

FIGURE 1. Experimental outlet concentrations for a benchmark long storage/regeneration cycle at 200°C [2].

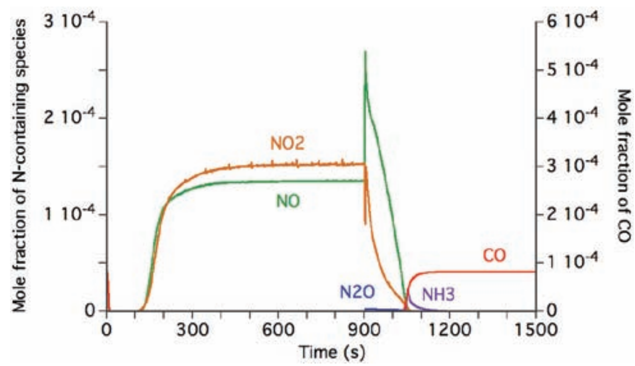

FIGURE 3. Experimental outlet concentrations for a benchmark long storage/regeneration cycle at 400°C [2].

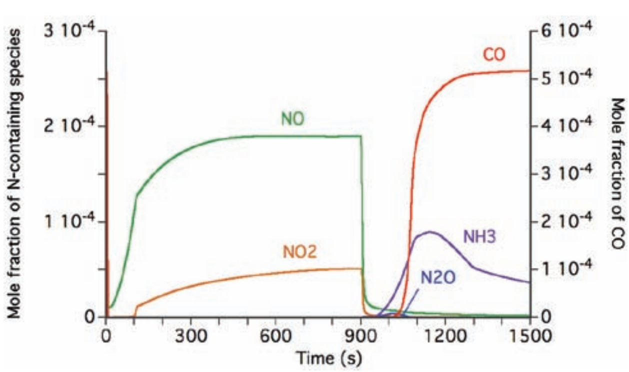

FIGURE 2. Simulated outlet concentrations for a benchmark long storage/regeneration cycle at 200°C.

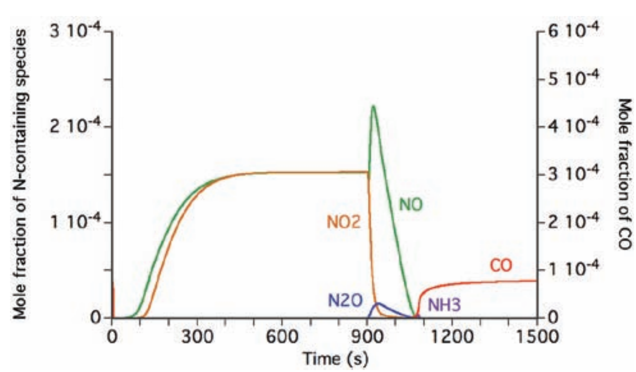

FIGURE 4. Simulated outlet concentrations for a benchmark long storage/regeneration cycle at 400°C.

analogous to the isocyanate pathway for ammonia formation. On the baria storage sites, there are candidate processes for sulfate formation involving reaction of SO_3 with surface oxides, carbonates, hydroxides, nitrates, and nitrites. Finally, there is the possibility of SO_3 spillover from the precious metal sites and formation of sulfates on the ceria sites nominally used for oxygen storage.

Because the new sulfur-containing species compete for sites and engage in chemistry on all of the surface phases, numerous effects on LNT operation are possible. However, the phenomena of most interest from a practical point of view are the progressive degradation in NOx storage capacity and the change in selectivity of N_2 over undesirable regeneration products such as NH_3 and N_2O. Here we show how our proposed mechanism, with kinetic constants not yet adjusted to fit experimental data quantitatively, can nevertheless produce the right kind of behavior. Figures 5 and 6 show the results of simulations very similar to that of Figure 2, the basic difference being that the feed during the lean period now contains 10 ppm of SO_2 in addition to the other components. As a result of sulfate storage (largely irreversible at this temperature), the state of the catalyst is no longer the same at the beginning and end of a given cycle, and the NOx storage capacity progressively degrades. Figures 5 and 6 show the exit gas compositions for the first and fifth of these cycles, respectively, and the changes are evident. SO_3, which is produced from the inlet SO_2 via oxidation on the precious metal sites, is adsorbed so strongly that it begins to appear in the exit gas only during the fifth cycle, after the slip of NOx has increased dramatically. Needless to say, a good deal remains to be done before the sulfation/desulfation mechanism is in its final form, but the framework now in place should allow a satisfactory result to be achieved in a straightforward manner.

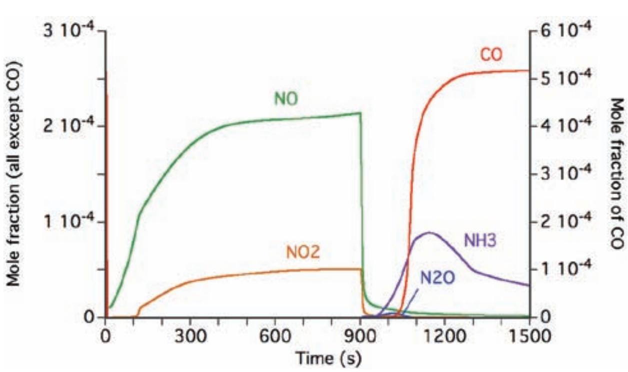

FIGURE 5. Simulated outlet concentrations for the first storage/regeneration cycle at 200°C with SO_2 added to the lean phase feed.

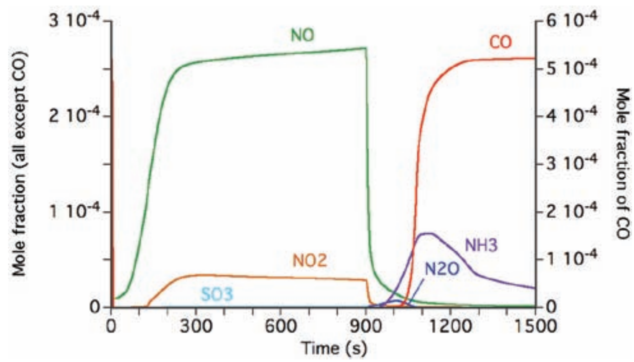

FIGURE 6. Simulated outlet concentrations for the fifth storage/regeneration cycle at 200°C with SO_2 added to the lean phase feed.

Conclusions

- The behavior of an LNT over a complete storage/regeneration cycle can be simulated quite well with an elementary reaction mechanism involving independently derived kinetic parameters for the precious metal sites of the catalyst.
- Mass transfer resistance in the washcoat appears to be an important factor, and the difficulty in accounting for it correctly may be a significant source of error in the model.
- A sulfation/desulfation mechanism constructed by analogy with the NOx reactions can reproduce observed behavior qualitatively, but adjustment of the rate parameters to achieve quantitative agreement is needed.

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2. J.A. Pihl, M.S. Thesis, University of Wisconsin–Madison, 2005.

FY 2008 Publications/Presentations

1. R.S. Larson, J.A. Pihl, V.K. Chakravarthy, T.J. Toops, and C.S. Daw, “Microkinetic Modeling of Lean NOx Trap Chemistry under Reducing Conditions,” *Catal. Today* **136**, 104–120 (2008).

2. R.S. Larson, “Benchmark Reaction Mechanisms and Kinetics for Lean NOx Traps,” DOE Office of Vehicle Technologies Annual Merit Review Meeting, Bethesda, Maryland, February 25, 2008.

3. R.S. Larson, J.A. Pihl, V.K. Chakravarthy, and C.S. Daw, “Microkinetic Modeling of Lean NOx Trap Storage and Regeneration,” Eleventh CLEERS Workshop, Dearborn, Michigan, May 13, 2008.

II.B.5 NOx Abatement Research and Development CRADA with International Truck and Engine Co./Navistar Inc.

Todd J. Toops (Primary Contact) and Josh A. Pihl
Oak Ridge National Laboratory (ORNL)
2360 Cherahala Boulevard
Knoxville, TN 37932

Cooperative Research and Development Agreement (CRADA) Partner:
Navistar, Inc., Vadim Strots, Brad Adelman, Ed Derybowski, and Alan Karkkainen

DOE Technology Development Manager:
Ken Howden

Objectives

- Explore leading edge engine and emissions control technology.
- Enable compliance with emissions regulations while maintaining or improving overall engine efficiency.
- Specific approach for 2007-2010 includes bench-scale emissions control research and development and model development.

Accomplishments

- Established fully-automated bench-scale flow reactor at ORNL.
- Developed protocol that provides the critical transient and steady-state model parameters for selective catalytic reduction (SCR) catalysts.
- Implemented a subset of the protocol on commercial-intent SCR catalyst.
- Coordinated modeling efforts with Michigan Technical University (Michigan Tech).

Future Directions

- Complete model development and protocol optimization.
- Evaluate model parameters with aged catalysts.
- Investigate effects of hydrocarbons (HCs) and SO_2 on model parameters.
- Navistar is interested in expanding effort to incorporate combustion efficiency.

Introduction

Heavy and light-duty emissions standards call for significant reductions in oxides of nitrogen (NOx) emissions by 2009-2010. Many emissions control strategies currently being implemented on vehicles rely on urea-SCR to meet the requirements. To effectively implement this system engine manufacturers are relying on on-board controls for both the engine operation and the emissions control system. While some of the underlying SCR chemistry is understood, the specific parameters that are essential for accurate emissions control strategies are not well known. Furthermore, new catalyst formulations are continuously being delivered to the manufacturers and therefore, the parameters need to be constantly updated. Therefore, our industrial partner, and the diesel engine manufacturing industry in general, has a need for a systematic approach to evaluating SCR catalysts under realistic exhaust conditions. This effort focuses on meeting this need by developing and implementing an evaluation protocol in conjunction with modeling efforts in Professor Gordon Parker's group at Michigan Tech. The ultimate goal of this effort is to determine the most critical parameters of the model and to then optimize the protocol, and thus minimize the experimental efforts for new catalyst formulations.

Approach

Efforts during this year focused on developing a systematic evaluation protocol that will cover the typical operating range of an SCR catalyst. The protocol is developed for evaluations in a bench-core flow reactor and relies on NH_3 rather than urea for NOx reduction. To perform the protocol in an efficient manner it is necessary to utilize a reactor system that is fully automated, and therefore, a portion of the effort this year has been geared towards establishing this capability at ORNL. The data generated during the SCR catalyst evaluation is analyzed and incorporated into modeling parameters at Michigan Tech. This model is used by Navistar and implemented into control strategies. The catalysts used in this study have been provided to Navistar through a major catalyst supplier.

Results

In a joint effort, ORNL and Navistar have established an evaluation protocol that will reproduce several key conditions that occur during a typical drive cycle. This protocol is schematically portrayed in Figure 1. The first step establishes identical surface

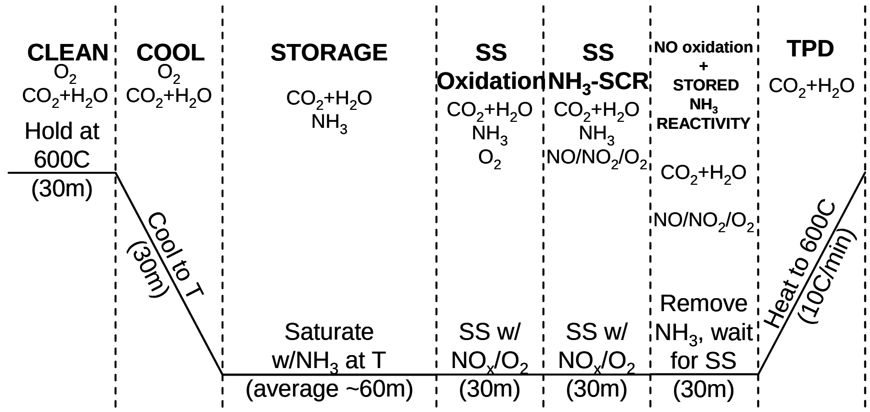

FIGURE 1. Schematic of SCR Evaluation Protocol (Protocol is designed to be implemented at evaluation temperatures [T] of 150 to 600°C; TPD: temperature programmed desorption.)

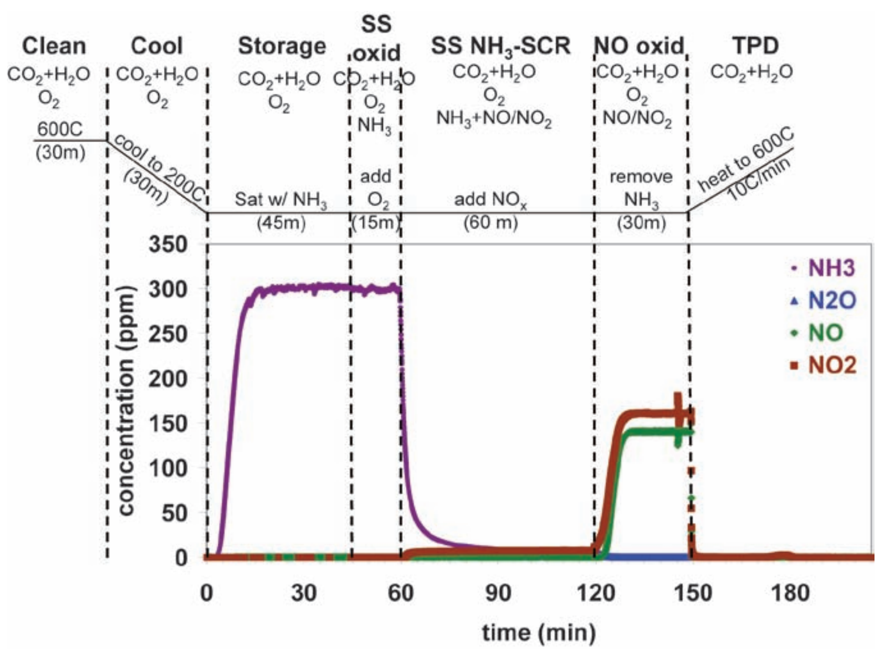

FIGURE 2. Sample Profile of Protocol Operated at an Evaluation Temperature of 200°C

conditions for each sample and condition by holding the sample at 600°C under oxidizing conditions. The sample is then cooled to the temperature of interest; there are 12 targeted temperatures between 150°C and 600°C. A key parameter in the model will be measuring how much NH_3 can adsorb on the sample at a given temperature. This is important since the SCR catalyst will be able to accommodate some over-injection of urea, but it will be important for the onboard control strategy to know how much NH_3 is available in this adsorbed state and how reactive is this ammonia. Obtaining this understanding is the goal of the next four steps. The storage step describes total number of available sites, the steady-state (SS) oxidation step describes the reactivity of NH_3 for direct oxidation with O_2, the SS NH_3-SCR step relates the important NOx reduction activity, and the stored-NH_3 reactivity step relates the reactivity of the NH_3 that is remaining on the catalyst. The final step of the protocol returns the catalyst to its initial condition while recording what species are desorbing. Throughout these steps, gases are being turned on and off and transients are being recorded.

This protocol is intended to be operated at 12 temperatures between 150 and 600°C, 3 gas hourly space velocities (GHSVs) between 30,000 and 90,000 h^{-1}, and a wide range of concentrations of NO, NO_2, and NH_3. An example of the gas concentration profile using a production-intent SCR catalyst during the protocol is shown in Figure 2. The reactor conditions used in this example are 200°C, a GHSV of 60,000 h^{-1}, and NH_3 and NOx concentrations of 300 ppm, when applicable. These results are analyzed to obtain the parameters listed in Tables 1-4. These parameters as well as the rate of change observed in transitioning from one step to the next are key contributions to the model that is under development at Michigan Tech. Data has been collected at 200, 300 and 400°C which have lead to initial model results in Figure 3.

To completely execute the protocol that has been outlined above will require approximately 500 hours of experimental effort. This is a large investment of time even and if it was necessary to have a research staff member with the instrument the entire time, we would not be able to accomplish the goals with the available funding. Therefore, we have established an automated bench flow reactor system that meets all of ORNL's stringent safety guidelines and operated unattended. Having this capability will enable the protocol to be carried-out after normal work hours and on the weekends.

TABLE 1. NH_3 Storage and Reactivity

	µmol/g monolith
NH_3 stored	109
NO reacted	36
NO_2 reacted	33
NOx reacted	69

TABLE 2. Steady-State SCR Reactivity

species	inlet (ppm)	outlet (ppm)	conversion
NH_3	301.4	298.9	0.8%

TABLE 3. Steady-State NH_3 Oxidation

species	inlet (ppm)	outlet (ppm)	conversion
NH_3	301.4	6.0	98%
N_2O	0	1.2	--
NO	140.6	0	100%
NO	160.6	7.6	95.3%
NOx	301.2	7.6	97.5%

TABLE 4. Total Release of Adsorbed Species During the TPD

	µmol/g monolith
NH_3	0.05
N_2O	0
NO	0
NO_2	0.5

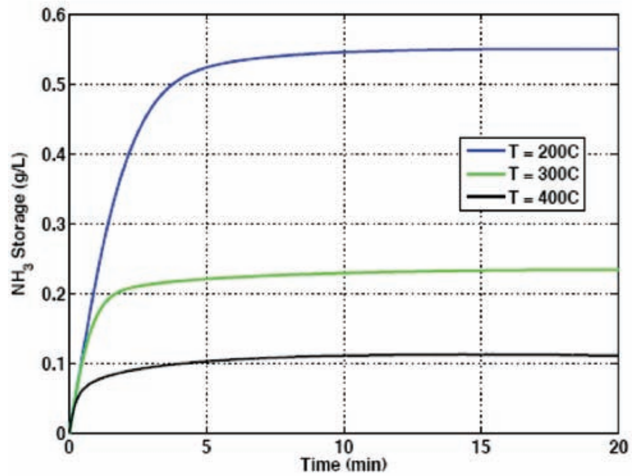

FIGURE 3. Transient NH_3 Storage Model Results from Michigan Tech at 200, 300, and 400°C

Conclusions

To accurately capture all of the SCR behavior that is necessary for efficient diesel emissions control systems, both steady-state and transient data is necessary. A protocol has been developed to evaluate SCR catalysts and develop model parameters that will be critical for ITEC/Navistar on-board controls. Efforts are under way but there has not been enough experimentation yet to offer any firm conclusions regarding new understanding of the underlying SCR chemistry. A new fully-automated system has been established at ORNL that allows unattended operation that will be essential for efficient execution of the protocol.

Presentations

1. J.A. Pihl, T.J. Toops, "ITEC CRADA-Advanced Engine/Aftertreatment System Research and Development", DOE-Advanced Combustion Engine Program Annual Merit Review, Crystal City, VA, February 2008.

II.B.6 Fundamental Sulfation/Desulfation Studies of Lean NOx Traps, DOE Pre-Competitive Catalyst Research

Todd J. Toops (Primary Contact) and
Josh A. Pihl
Oak Ridge National Laboratory (ORNL)
2360 Cherahala Blvd.
Knoxville, TN 37932

DOE Technology Development Manager:
Ken Howden

Objectives

- Provide a better understanding of the fundamental deactivation mechanisms that result during desulfation of lean NOx traps (LNTs).
- Investigate methods for improving performance and/or durability of LNTs.

Approach

- Conduct pre-competitive LNT research.
- Study deactivation and regeneration mechanisms fundamentally.
- Coordinate efforts with other projects to maximize knowledge findings.
- Investigate materials changes that can improve performance and desulfation behavior.

Accomplishments

- Demonstrated 8-13% improvement in LNT performance at 200 and 300°C and lowered the initial desulfation temperature by 50°C through small-scale exploratory catalysis research.
  - Ca dopant was added to BaO storage phase to influence behavior.
- Identified axial location of sulfur within a wash-coated core and how the strength of the sulfate bond varied axially.
- Presented efforts at 14th International Congress on Catalysis, 5th International Conference on Environmental Catalysis, 11th Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Workshop, and 2008 DOE Vehicle Technologies Merit Review.
- Published paper in Catalysis Today.

Future Directions

- Identify distinct phases on which sulfur is adsorbing in commercial gasoline direct injection catalyst.
- Correlate performance improvements from exploratory catalysis research to materials changes and investigate durability.

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Introduction

Under future vehicle regulations, the efficiency of a diesel engine powertrain will be correlated to the efficiency of the catalyst system since a fuel penalty is sustained to achieve the emissions requirements. Therefore, it is essential to have an efficiently functioning catalyst system in conjunction with a diesel engine. This project pursues two paths to achieve this goal while focusing primarily on LNT technologies. The first path focuses on establishing a fundamental understanding of the underlying LNT chemistry to improve the accuracy of computer simulations used to design, develop, and control LNT aftertreatment systems. This includes identifying the roles of the catalytic phases of commercial-intent LNTs, elucidating reaction pathways, and determining the fate of sulfur in the catalyst. This effort is closely tied to the CLEERS kinetics activities and serves as a complementary research mechanism. Essentially, the microreactor and diffuse reflectance infrared Fourier-transform spectroscopy (DRIFTS) reactor capabilities developed under this project are used to answer specific questions that arise from bench-scale reactor research performed under the "CLEERS LNT Kinetics and Multi-Lab Diesel Emissions Reduction Activities" project or by collaborators on other DOE-funded projects.

The second path, which is more in line with the traditional, exploratory role of this project, is aimed at making modifications to the LNT catalyst with the goal of either improving the performance or lowering the required desulfation temperature. This effort is possible due to a winning proposal at ORNL's Center for Nanophase Materials Science (CNMS), a Department of Energy Basic Energy Sciences national user facility. CNMS synthesizes the LNT catalysts to our specification and fully characterizes the samples. We then evaluate the LNTs under typical operating conditions, and work to correlate performance changes to material properties. In taking this multi-pronged approach to studying LNT fundamentals, we are able to make the biggest impact in the most areas while operating within the current funding constraints.

Approach

Our first approach to LNT fundamentals is in support of CLEERS kinetics activities. Model catalysts are studied to obtain a base understanding of the catalyst components, and then that knowledge is applied to more complex commercial-intent LNTs. For instance, during the past year specific questions have been raised about the location of the sulfur on the LNT catalyst after several sulfation and desulfation cycles. This was specifically of interest on the commercial-intent LNT that is serving as the reference catalyst for the CLEERS-LNT focus group. The core samples studied in the CLEERS kinetics project were sectioned following a sulfation step and were analyzed for sulfur content and sulfate bond strength using a temperature-programmed microreactor technique. This approach utilizes the unique capabilities and expertise developed in previous years of this project, i.e. the barrel-ellipse DRIFTS reactor and the differential microreactor.

Our second approach investigates the effects of material modifications to the LNT catalyst on NOx reduction performance and desulfation temperature. The performance of an LNT catalyst is strongly dependent on the relative stabilities of nitrates and sulfates on the catalyst surface. La, Ca, and K dopants were introduced into the BaO lattice to measure the effects on performance and desulfation. The dopants were chosen with a range of properties (see Table 1) to affect the BaO lattice spacing and/or the number of oxygen vacancies. The resulting changes in the storage material should, in turn, impact the stability of stored nitrates and sulfates, as measured by NOx conversions and desulfation temperatures.

Results

To understand the axial location and relative bond strength of trapped sulfur on a commercial-intent catalyst, a sulfated catalyst core was sectioned into four parts and a temperature-programmed reduction (TPR) was performed on the individual sections (SXN). The catalyst temperature was ramped to 1,000°C in an attempt to achieve complete sulfur removal. The resulting desulfation profiles are shown in Figure 1. The front section of the LNT, SXN1, contains the highest concentration of sulfur, and a significant amount of this sulfur is released at relatively low temperatures, below

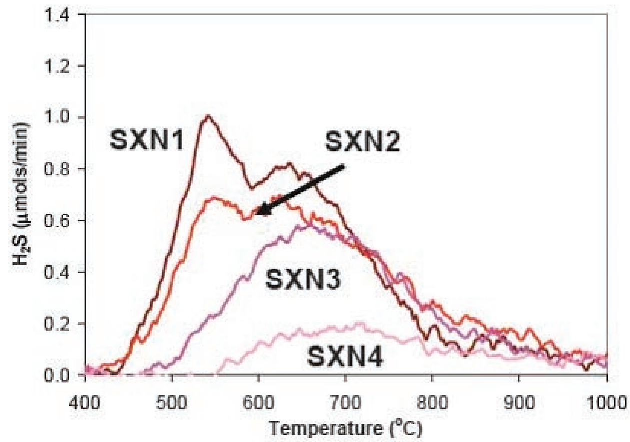

FIGURE 1. Temperature programmed de-sulfation profiles for the four sections (SXN) of sulfated commercial-intent LNT catalysts; ramped at 5°C/min. Flow conditions: 30k h^{-1}, 1% H_2, 5% H_2O, 5% CO_2, in Ar.

500°C. SXN2 shows a similar profile as SXN1, but there is noticeably less total sulfur in this portion. SXN3 and SXN4 demonstrate significantly different release profiles, which confirm that the sulfur reaching the back portion of the catalyst is only stored on the most stable sites. Deconvolution of the release profiles suggest that there are up to four different sulfate bond strengths being removed from this catalyst. These four sulfates are likely to correlate to the four phases that are known to exist on the commercial-intent LNT: Al_2O_3, CeO_2-ZrO_2, $MgAl_2O_4$, and BaO. In the CLEERS kinetics project much effort has gone into determining how sulfur is impacting the specific reactions that occur within the LNT, i.e. NOx storage and reduction (NSR), water-gas-shift reaction, and the oxygen storage capacity (OSC) reaction. Results from the bench reactor suggest that the NSR reaction is inactive in the front half of the sulfated catalyst, but the OSC reactions take place throughout the catalyst core. These results guide the TPR data and suggest that the most stable sulfur is adsorbed on the BaO phases which are responsible for NSR, and that the less stable sulfates are stored on the CeO_2-ZrO_2 phase that is responsible for OSC reactions.

As an example of the DRIFTS support that is provided to the CLEERS kinetics project, results investigating sulfur coverage on Pt are discussed. Pt and the other Pt-group metals are key catalytic components that promote several reactions occurring in LNTs. DRIFTS can be used to identify how much surface Pt is available for these reactions using CO as a probe molecule. Using this concept, a series of experiments was performed to determine when, and if, S is bound to Pt. Lean phase SO_2 was introduced to the system followed by exposure to a rich "desulfation" gas mixture. Since the temperature in the DRIFTS reactor could not exceed 600°C, only partial sulfur removal was achieved, but the temperatures were high enough to mobilize the

TABLE 1. Storage Material and Dopant Properties

	Ba	Ca	K	La
Covalent Radius (Å)	1.98	1.74	2.03	1.69
Valence	+2	+2	+1	+3

sulfur on the surface. Figure 2 shows the peak area that quantitatively indicates active Pt sites at 300°C. The initial value, 0 on the chart, is recorded before any sulfur is introduced at 300°C. The red bar at 300°C is recorded after exposing the LNT to "desulfation" gases at 300°C, i.e. without any heat treatment. The sample was then heated to 400°C under rich conditions and cooled to 400°C. The active Pt is indicated by the red bar at 400°C. This is substantially lower than the initial value, and indicates that after heating to 400°C some sulfur is released from the oxide phase and blocks the Pt surface. A simple oxidation step at 300°C removes much of this sulfur and active Pt sites are once again obtained. Heating to higher temperatures results in nearly complete poisoning of the Pt active sites under rich conditions; however, the surface can be recovered at 300°C with a brief lean period. These results indicate that during the rich-phase removal of sulfur, the Pt is covered with sulfur and becomes inactive. This is a very important finding since it is commonly thought that sulfur forms a stable sulfate under typical operating conditions, and that its only impact is in reducing total storage sites. These results suggest that under typical operating temperatures, as low as 400°C, sulfur is mobile on the surface of the catalyst and can move from one phase to another phase, i.e. from ceria to Pt and potentially to Ba.

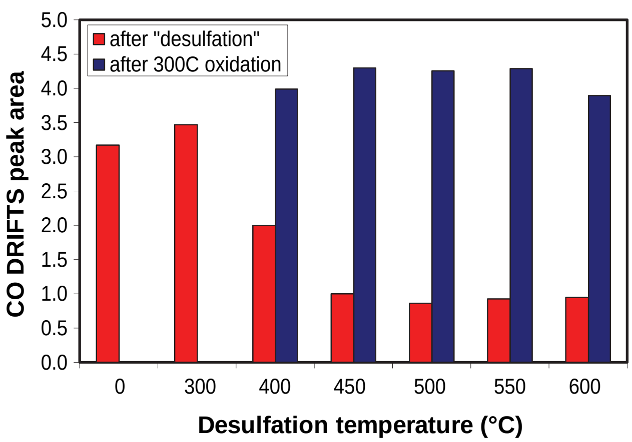

FIGURE 2. Measured peak area of the Pt-CO infrared absorbance, which is a direct indication of active Pt sites. The spectra are all recorded at 300°C either directly after cooling from the desulfation temperature (■ after "desulfation"), or after a brief oxidation period at 300°C (■).

While this year there have been significant efforts in support of the CLEERS kinetics project, the LNT-dopant work with the CNMS is more in line with the exploratory efforts that have been a hallmark of this project. The goal of this approach is to understand how storage material dopants affect LNT performance and desulfation. The LNT catalysts were synthesized in a stepwise fashion. The Pt was dispersed on commercial-grade γ-Al_2O_3 using H_2PtCl_6 and the incipient wetness technique was applied to obtain a 1.5 wt% loading. Wet impregnation of nitrate salts was then used to add the storage phase, with 5% mol of the Ba being substituted with Ca, K, or La. The specific final catalyst compositions, Brunauer, Emmett and Teller surface areas are listed in Table 2 along with measured performance at 200-400°C. The Ca-doped material shows a significant increase in performance at 200 and 300°C, while also maintaining high conversion at 400°C. Conversely, both the K- and La-doped LNT catalysts show moderate decreases in performance at 200 and 400°C while matching the Ba-only performance at 300°C.

Following the performance measurements, the samples are then sulfated to 5.5 mg S/g_{cat} and desulfated to 1,000°C. Figure 3 shows the impact of the dopants on the desulfation behavior. The Ba, K+Ba, and La+Ba all show similar desulfation behavior, with moderate differences in desulfation onset and peak release temperatures (see Table 2) indicating that sulfates on the K+Ba and La+Ba are slightly more stable than those on the undoped Ba. The Ca+Ba catalyst, on the other hand, demonstrates a markedly different bimodal desulfation behavior with desulfation onset occurring 50°C before the undoped Ba catalyst. Although the peak release temperature is higher than the Ba-only sample, the significant amount of less stable sulfur released before 550°C is very beneficial to the overall desulfation behavior of an LNT catalyst.

These results suggest that the electronic manipulation of the storage phase does not have a positive effect on the performance or desulfation characteristics of the LNT catalyst; however, introducing metals with the same valence but different radii can benefit both the NOx performance and desulfation. Additional experimentation and characterization are being performed on the fresh and desulfated LNT catalysts to understand the physical impact of the

TABLE 2. Catalyst Composition, Initial Surface Area, NOx Conversion and Desulfation Temperature

Catalyst	Pt (wt %)	Ba (mol %)	Dopant (mol %)	Surface Area (m^2/g)	Initial NOx conversion 200°C	300°C	400°C	Desulfation T onset	peak
Pt/Al_2O_3	1.5%	-	-	133	-	-	-	-	-
Ba-only	1.1%	20%	0%	77	24%	81%	75%	550°C	700°C
Ca+Ba	1.1%	19%	1%	79	37%	89%	75%	500°C	790°C
K+Ba	1.1%	19%	1%	78	5%	78%	62%	590°C	760°C
La+Ba	1.1%	19%	1%	80	29%	80%	65%	565°C	740°C

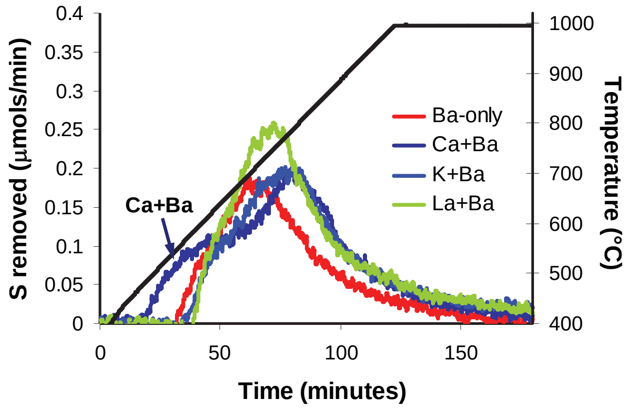

FIGURE 3. Desulfation profiles for the series of LNT catalysts. Flow conditions: 70k h^{-1}, 0.7% H_2, 1.2% CO, 5% H_2O, 5% CO_2, in Ar.

dopants on the BaO and their durability. Specifically, lattice spacing, surface area, pore size distributions, and elemental analysis will be evaluated.

Conclusions

- Distinct sulfate strengths are observed in the sulfated commercial catalyst and these vary in axial location. The sulfation progresses in a sequential fashion with the most stable sulfates forming first and the least stable sulfates forming last.
- Under typical operating temperatures, as low as 400°C, sulfur is mobile on the surface of the LNT and can move from one phase to another phase, i.e. from ceria to Pt and potentially to Ba.
- Electronic manipulation of the storage phase, through addition of K (+1) or La (+3), does not have a positive effect on the performance or desulfation characteristics of the Ba (+2)-based LNT catalyst.
- Introducing Ca, a metal with the same valence as Ba, but a different radius, benefits both the NOx performance and desulfation behavior.

FY 2008 Publications/Presentations

1. T.J. Toops and J.A. Pihl, "Sulfation of Model K-based Lean NOx Trap while Cycling Between Lean and Rich Conditions", Catalysis Today 136 (2008) 164.

2. J.-S. Choi, W.P. Partridge, J.A. Pihl, T.J. Toops, M.J. Lance, C.E.A. Finney, V.K. Chakravarthy, C.S. Daw, "Correlation between spatiotemporal distribution of reactions and global performance of a commercial lean NOx trap catalyst at varying sulfation stages", oral presentation at the 5th International Conference on Environmental Catalysis, Belfast, United Kingdom, August 31-September 3, 2008.

3. J.A. Pihl, T.J. Toops, "DRIFTS Investigation of Sulfation of Model Lean NOx Trap", poster presentation at the 5th International Conference on Environmental Catalysis, Belfast, United Kingdom, August 31-September 3, 2008.

4. J.-S. Choi, W.P. Partridge, J.A. Pihl, T.J. Toops, "Fundamental studies of commercial lean NOx trap performance, sulfation and desulfation: postmortem characterization", poster presentation at the 14th International Congress on Catalysis, Seoul, South Korea, July 2008.

5. J.-S. Choi, W.P. Partridge, J.A. Pihl, T.J. Toops, M.J. Lance, C.E.A. Finney, V.K. Chakravarthy, and C.S. Daw, "Experimental studies of LNT sulfation and desulfation with the Umicore reference catalyst", oral presentation at the DOE CLEERS (Crosscut Lean Exhaust Emissions Reduction Simulations) Focus Group Teleconference, April 10, 2008.

6. J.-S. Choi, W.P. Partridge, J.A. Pihl, M. Lance, L. Walker, C. Finney, K. Chakravarthy, V. Prikhodko, C.S. Daw, T.J. Toops "ORNL Research on LNT Sulfation and Desulfation: CLEERS LNT Kinetics and Multi-Lab Diesel Emissions Reduction Activities (8746) and Pre-Competitive R&D on LNT Mechanisms (8744)", DOE- Office of Vehicle Technologies Annual Merit Review, Bethesda, MD, February 2008.

7. T.J. Toops, J.A. Pihl, "Sulfation and Desulfation Studies of Model Lean NOx Traps", 2007 National Meeting of the American Institute of Chemical Engineers, Salt Lake City, UT, November 2007.

II.B.7 NOx Control and Measurement Technology for Heavy-Duty Diesel Engines

Bill Partridge[1] (Primary Contact), Jae-Soon Choi[1], Jim Parks[1], Neal Currier[2], Alex Yezerets[2], Mike Ruth[2], Mike Cunningham[2]
[1]Oak Ridge National Laboratory (ORNL),
[2]Cummins Inc.
2360 Cherahala Blvd.
Knoxville, TN 37932

DOE Technology Development Manager:
Ken Howden

Objectives

- Improve diesel engine-catalyst system efficiency through detailed characterization of chemistry and degradation mechanisms.
- Work with industrial partner to develop full-scale engine-catalyst systems to meet efficiency and emissions goals.

Accomplishments

- Develop diagnostic for rapid, on-engine measurements of oil dilution by fuel.
- Apply oil-dilution diagnostic to investigate performance of development engine at Cooperative Research and Development Agreement (CRADA) partner's facility:
  - Improved engine calibration points identified.
  - Dedicated instrument for integrated development applications at Cummins delivered via separate funds-in project.
- Enable SpaciMS ammonia (NH_3) measurement capability.
- Ammonia formation and utilization within (oxides of nitrogen [NOx] storage/reduction [NSR]; a.k.a. lean-NOx [LNT]) catalysts during regeneration studied and clarified:
  - First direct experimental evidence of fast NH_3 generation and intermediate-NH_3 regeneration pathway.
  - Provided detailed data necessary to better understand and model NH_3 chemistry.
  - Provided detailed data necessary to develop improved NH_3-management protocols; e.g., via formulation tuning, active control, design and modeling.
- Investigate NSR-catalyst sulfation/desulfation kinetics. Improve desulfation protocol design basis by clarifying roles and sulfation/de-sulfation kinetics of catalyst components. (Joint activity between Cummins-ORNL CRADA and the Cross-Cut Lean Exhaust Emissions Reduction Simulations Focus Groups.)

Future Directions

- Quantify engine-system dispersion and mitigation strategies.
- Develop methods for in situ, on-engine-system assessment of catalyst state.
- Investigate selected nitrogen-selectivity issues related to LNT regeneration and hybrid catalyst systems.

Introduction

Diesel engine technology has advanced significantly over the last decade. Modern diesels utilize advanced injector technology to enable multiple injections of fuel per combustion cycle. Precise control of injection timing allows optimization of efficiency and emissions. Advanced fuel injectors also allow extra fuel to be injected during select combustion events to generate fuel-rich exhaust for management of the catalyst system. Unfortunately, this additional fuel injection can lead to fuel-spray impingement on the cylinder wall, subsequent fuel build-up in the engine oil, and ultimately durability issues such as cylinder-wall scuffing. The engine system must be carefully calibrated to manage the engine-catalyst system without compromising durability. Typical methods for assessing fuel-in-oil (FiO) require off-line measurement, which typically take days. A real-time on-engine FiO diagnostic is needed to allow the engine calibration space to be rapidly swept with sufficient resolution to identify optimum operation points. The CRADA team has developed and applied such a real-time on-engine diagnostic.

LNT catalysts are a candidate technology for diesel engine NOx emissions abatement. Unfortunately, these catalysts are susceptible to being poisoned (i.e., deactivated) by exposure to sulfur. In practice, high-temperature desulfation events are performed to release trapped sulfur from, and reactivate the catalyst. Improved understanding of the detailed sulfation/desulfaiton chemistry is needed to develop control strategies, and optimize efficiency and fuel-penalty of these devices. These catalysts can also emit ammonia which is an undesirable emission. However, hybrid catalyst systems are also being considered, where it may be desirable to cause the LNT catalyst to generate ammonia for the purpose of NOx reduction over a downstream selective catalytic reduction catalyst. Detailed understanding of the ammonia formation and utilization roles in LNT catalyst is necessary to appropriately design and control these catalyst systems for optimum efficiency with minimum fuel penalty.

Approach

Laser-induced fluorescence (LIF) spectroscopy is used to rapidly measure the fuel dilution of oil in situ on an operating engine. A fluorescent dye, commercially available and suitable for use in diesel fuel and oil systems, is added to the engine fuel. The LIF spectra are monitored to detect the growth of the dye signal relative to the background oil fluorescence; fuel mass concentration is quantified based on a known sample set. The diagnostic is based on fiber optic probes for excitation light delivery and fluorescence collection; this allows flexibility of sampling location in the engine oil system, and could even be implemented in the cylinder-wall oil film where oil dilution is highest. A low cost 532-nm laser diode is used for excitation. Spectrally resolved fluorescence detection is effected via small fiber-coupled spectrometers. The diagnostic is portable.

Catalyst-related chemistry is studied on a laboratory bench reactor using model and fully formulated catalysts and application of conventional and advanced diagnostics. Notable is application of spatially resolved capillary inlet mass spectrometer for real-time intra-catalyst measurements of transient species distributions. This allows the detailed timing and sequence of the various reactants, intermediates and products to be quantified, and provides unmatched insights into catalyst chemistry.

Results

Oil Dilution Measurements: A LIF technique for rapid in situ measurement of the fuel dilution of oil in a diesel engine has been demonstrated. The technique utilizes a fluorescent dye, commonly sold for diesel and oil leak detection, to provide increased sensitivity to the fuel dilution rate. Fiber optic probes enable the technique to be conveniently employed on an engine platform. Measurements of fuel dilution during lean-rich cycling of the engine for LNT regeneration were performed; rich operation was enabled by intake throttling and additional in-cylinder fuel injection.

In experiments comparing the LIF technique to a standard ASTM International (gas chromatograph [GC]-based) method, dilution trends were similar (see Figure 1). The most likely explanation for the discrepancy between the two techniques is that the LIF technique is based on the dye which does not evaporate from the oil like fuel components. However, the LIF technique has greater precision and sensitivity than the GC technique which allows detection of smaller rates of dilution, and provides the real-time, fast-feedback, on-engine measurements necessary for effective system calibration development. The LIF technique is most useful as a tool to measure dilution rates so that engineers can rapidly obtain feedback for controls development. Complementary measurements with a GC technique are recommended to measure equilibrium fuel in oil levels attained through evaporation processes. In applications of the oil-dilution diagnostic to

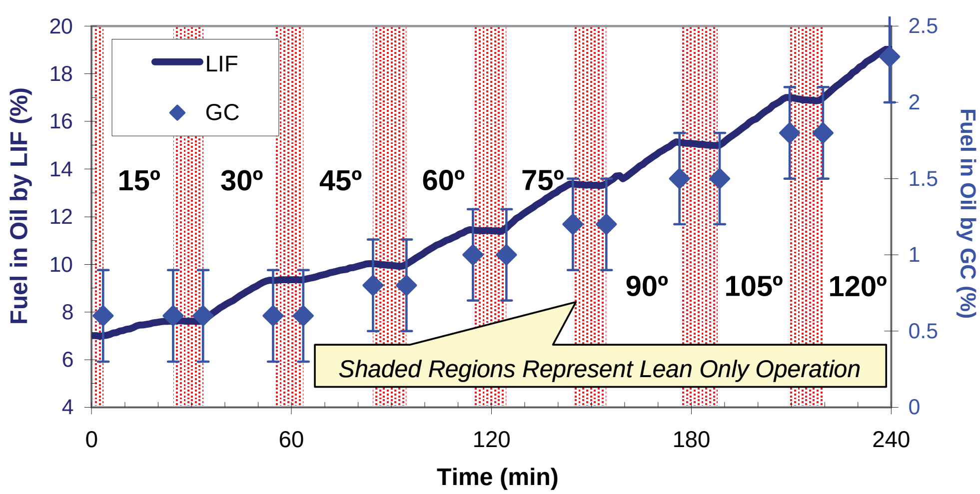

FIGURE 1. Comparison of LIF- and conventional (ASTM, GC-based) fuel in oil measurements. The shaded regions represent lean only operation. Lean-rich cycling caused fuel dilution to occur during periods between the shaded regions.

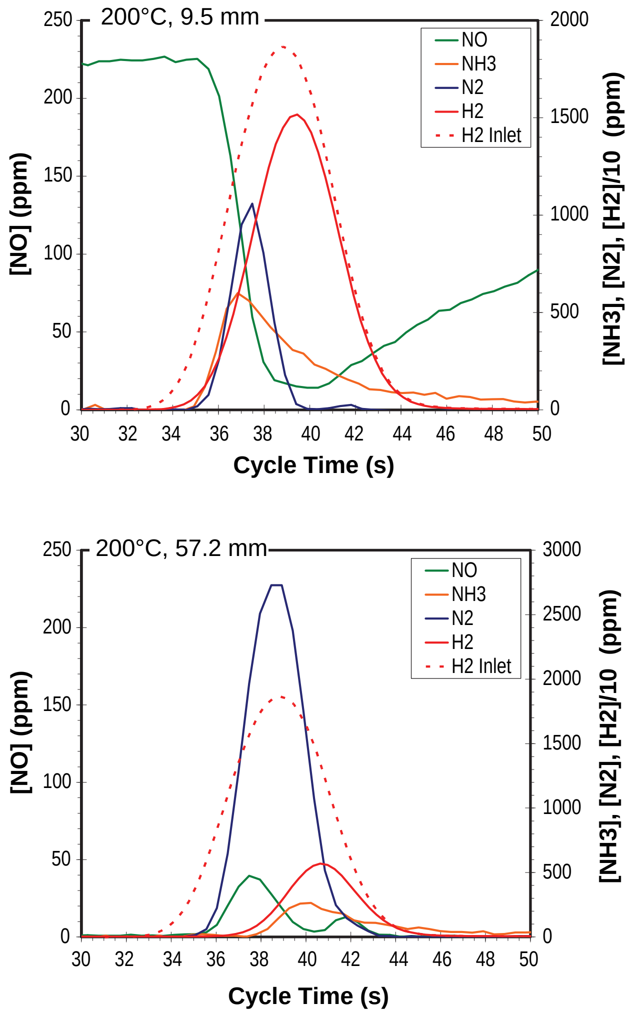

FIGURE 2. Species profiles inside the catalyst channel near the front (9.5 mm) and back (57.2 mm) of the catalyst channel. The species sequence (N_2, $H_2 \approx NH_3$) 57 mm along the catalyst channel is typical of the effluent sequence reported in the literature. Measurements at the catalyst front show that in fact NH_3 is generated on the same timescales as is N_2. However, since N_2 is inert, locally generated N_2 passes unreacted through the catalyst. In contrast NH_3 is continuously being generated and consumed in the NOx-storage region of the catalyst.

development engine systems previously hidden, more optimum operation points were identified enabling enhanced efficiency and durability (i.e., reduced costs).

Catalyst Chemistry Measurements and Insights: Previous catalyst out measurements showed a typical species sequence (N_2, $H_2 \approx NH_3$) which suggested that ammonia was generated when catalyst regeneration was near complete (see Figure 2, 57.2-mm location). Based on this broadly demonstrated behavior, the catalyst community generally understood NH_3 as generated by "slow" NOx storage sites. As shown in Figure 2 (9.5-mm location), CRADA work demonstrated that inside the catalyst NH_3 is generated on the same timescales as

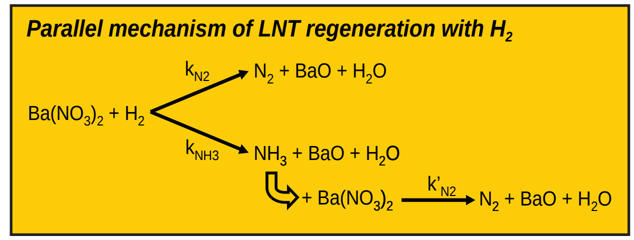

FIGURE 3. Parallel direct-H_2 (k_{N2}) and intermediate-NH_3 (k_{NH3}) regeneration pathways appear feasible. Further work is needed to determine the partitioning between the two regeneration pathways.

is N_2, and that NH_3 is utilized as a reductant; i.e., the effluent species sequence is an integral effect, and "slow" NOx sites are not practically relevant to fast cycling catalyst operation. This has direct implications on modeling, design and control of catalyst systems. Based on this improved understanding of the detailed catalyst chemistry, direct H_2 and intermediate-NH_3 regeneration pathways appear feasible (see Figure 3). Additional work is needed to better understand the partitioning between the two regeneration pathways.

Conclusions

- LIF-based oil-dilution diagnostic provides fast feedback (ca. 5 min vs. days with conventional GC method) of oil dilution significantly streamlining engine system development.
- LIF-based oil-dilution diagnostic enables finer probing of the engine operation space and identification of previously hidden high-efficiency operation points.
- Inside the catalyst NH_3 is generated on the same timescales as is N_2.
- Intra-catalyst generated NH_3 is used locally as a reductant.
- Parallel direct-H_2 and intermediate-NH_3 catalyst regeneration pathways appear feasible.

FY 2008 Publications/Presentations

Papers:

1. Jim Parks, Bill Partridge and Shawn Whitacre "Rapid In Situ Measurement of Fuel Dilution of Oil in a Diesel Engine using Laser-Induced Fluorescence Spectroscopy," Society of Automotive Engineers paper 2007-01-4108, 2007.

2. Jae-Soon Choi, William P. Partridge and C. Stuart Daw (2007). "Sulfur impact on NOx storage, oxygen storage and ammonia breakthrough during cyclic lean/rich operation of a commercial lean NOx trap," Applied Catalysis B: Environmental 77, 145–156; doi:10.1016/j.apcatb.2007.07.025.

3. Jae-Soon Choi, William P. Partridge, Josh A. Pihl and C. Stuart Daw (2008). "Sulfur and temperature effects on the spatial distribution of reactions inside a lean NOx trap and resulting changes in global performance," Catalysis Today 136, 173–182; doi:10.1016/j.cattod.2008.01.008.

Presentations:

1. Jim Parks, Bill Partridge, and Shawn Whitacre, Rapid In Situ Measurement of Fuel Dilution of Oil in a Diesel Engine Using Laser-Induced Fluorescence Spectroscopy, presented at the SAE Powertrain and Fluid Systems Conference in Chicago, IL on October 29-31, 2007.

2. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, C. Stuart Daw, "Sulfur Effects on Spatiotemporal Distribution of Reactions in a Commercial Lean NO_x Trap," AIChE National Meeting, Salt Lake City, Utah, November 7, 2007.

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4. Bill Partridge, Jae-Soon Choi, "Ammonia Formation and Utilization in Lean NOx Trap Catalysts: Experimental Determination of Reaction Pathways," 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation, University of Michigan, Dearborn, Michigan, May 13th, 2008.

5. Jae-Soon Choi, Bill Partridge, Josh Pihl, Todd Toops, Michael Lance, Charles Finney, Kalyana Chakravarthy, Stuart Daw, "Sulfation Impact on LNT Performance: Experimental Studies with Umicore CLEERS Reference Catalyst," 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation, University of Michigan, Dearborn, Michigan, May 13th, 2008.

6. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, Todd J. Toops, V. Kalyana Chakravarthy, C. Stuart Daw, "Correlation between Spatiotemporal Distribution of Reactions and Global Performance of Lean NOx Trap Catalysts," 14th International Congress on Catalysis, Seoul, Korea, July 14th, 2008.

7. Bill Partridge, Jae-Soon Choi, "Ammonia Formation and Utilization in Lean NOx Trap Catalysts: Experimental Determination of Reaction Pathways," Hanseo University, Seosan, Korea, July 21, 2008.

8. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, Todd J. Toops, V. Kalyana Chakravarthy, C. Stuart Daw, "Correlation between Spatiotemporal Distribution of Reactions and Global Performance of Lean NOx Trap Catalysts," Hyosung Corporation, Anyang, Korea, July 22, 2008.

9. William Partridge, Jae-Soon Choi, Josh Pihl, Todd Toops, Stuart Daw, "Intermediate NH3 Generation and Utilization Inside a Lean NOx Trap Catalyst," 5th International Conference on Environmental Catalysis, Belfast, United Kingdom, September 2, 2008.

10. Jae-Soon Choi, William Partridge, Josh Pihl, Todd Toops, Michael Lance, Charles Finney, Kalyana Chakravarthy, Stuart Daw, "Correlation between Spatiotemporal Distribution of Reactions and Global Performance of a Commercial LNT Catalyst at Varying Sulfation Stages," 5th International Conference on Environmental Catalysis, Belfast, United Kingdom, September 3, 2008.

Posters:

1. Jae-Soon Choi, Bill Partridge, Josh A. Pihl, and Todd J. Toops, "Fundamental Studies of Commercial Lean NOx Trap Performance, Sulfation and Desulfation: Postmortem Characterization," 14th International Congress on Catalysis, Seoul, Korea, July 17th, 2008.

Special Recognitions & Awards/Patents Issued

Awards:

1. The SpaciMS received the 2008 R&D 100 Award, which recognizes the year's most significant technological innovations. The SpaciMS was developed in the Cummins-ORNL CRADA and sponsored by DOE\EERE\Vehicle Technologies and predecessor programs. The SpaciMS R&D 100 team was ORNL, Cummins Inc., Queen's University Belfast, Hiden Analytical, and Y-12 National Security Complex. Hiden Analytical has commercialized the SpaciMS technology.

Patents Submitted:

1. US Appl. No.: 12/137,964, "Laser-Induced fluorescence fiber optic probe measurement of oil dilution by fuel," ORNL Ref. No.: 1940.0, Filed 6/13/2008.

II.B.8 Efficient Emissions Control for Multi-Mode Lean DI Engines

James Parks (Primary Contact), Shean Huff, Mike Kass, Vitaly Prikhodko
Oak Ridge National Laboratory (ORNL)
2360 Cherahala Boulevard
Knoxville, TN 37932

DOE Technology Development Manager:
Ken Howden

Objectives

- Assess the relative merits of meeting emission regulations via catalytic aftertreatment or advanced combustion for diesel engines capable of operating in multiple combustion modes ("multi-mode" engines).
- Determine the fuel efficiency of combinations of catalytic aftertreatment and advanced combustion modes.
- Characterize exhaust chemistry from advanced combustion and the resulting evolution of chemistry in catalysts for emissions control to improve the understanding of advanced engine and aftertreatment systems.

Accomplishments

- Demonstrated the benefits of advanced combustion (High-Efficiency, Clean Combustion, HECC) to enable clean diesel technologies; in conjunction with a lean-NOx trap (LNT), lower oxides of nitrogen (NOx) emissions were obtained with only slight drop in fuel efficiency as compared with conventional combustion modes.
- Achieved NOx emission levels (estimated from a steady-state data set) in the range of the U.S. Environmental Protection Agency (EPA) Tier 2 Bin 5 emission level.
- Identified two technical challenges to be addressed with HECC-related systems: low temperature CO and hydrocarbon emission control and exhaust gas recirculation (EGR) fouling.

Future Directions

- Investigate the potential to control the higher CO and hydrocarbon emissions associated with HECC by diesel oxidation catalysts.
- Research the synergies between urea-based selective catalytic reduction emission control and HECC combustion.

Introduction

New combustion regimes are being investigated as a means to increase the efficiency of, and to reduce the emissions from, diesel engines. The reduction of emissions during combustion is beneficial to the fuel efficiency of the system as a whole (engine plus emissions control system or "aftertreatment"). Specifically, lower engine-out NOx emissions can remove some burden from post-combustion emissions controls, and can thereby reduce the fuel penalty associated with NOx reduction. Although new combustion techniques have been developed that offer advantages for both engine fuel efficiency and emissions, often the techniques are not attainable over the entire range of load and speed required for market acceptance. Thus, engines designed to implement the new combustion techniques often operate in a "multi-mode" fashion where, at certain loads, the engine is operated with advanced combustion techniques and, at other loads, the engine is operated with more conventional diesel combustion. While modern control systems enable switching between the multiple modes of operation, the optimization of the system for fuel efficiency and emissions becomes more complex. One particular challenge is optimizing the size, cost, and complexity of the emissions control system. This project is aimed at understanding the complex issues of efficiency and emissions management for multi-mode engines with advanced emission control systems. Characterization of combustion exhaust chemistry and catalytic control are conducted to assist industry in the design of multi-mode engine and emission control systems.

Approach

This research has been conducted at ORNL in conjunction with ongoing engine studies. Two related projects at ORNL ("Measurement and Characterization of LNTs," and "Exploring Advanced Combustion Regimes for Efficiency and Emissions" in the Advanced Combustion Engines Program) are being leveraged with this activity. Experiments were performed on a Mercedes-Benz 4-cylinder, 1.7-liter diesel engine that has been significantly upgraded with advanced technologies (variable geometry turbocharger, high-throughput EGR, multi-injection control, etc.) to enable advanced combustion studies. The engine is operated on an engine dynamometer in ORNL's facility. All experiments were conducted at steady-state load and speed conditions which were chosen and weighted for estimating Federal Test Procedure (FTP) drive cycle emissions based on industry guidance. Low-Temperature Combustion (LTC) is a relatively new combustion mode that enables an order of magnitude reduction in NOx and particulate matter (PM) emissions through high levels of EGR. HECC is a new evolution of LTC that achieves extremely low NOx and PM emissions while maintaining low brake specific fuel consumption; HECC has comparable fuel efficiency to conventional modes [1]. HECC achieves good efficiency and emissions by coupling high levels of EGR with advanced injection timing. Although NOx and PM emissions are reduced in HECC, CO and hydrocarbon emissions increase. Formaldehyde emissions increase as well; formaldehyde is classified as a mobile source air toxic by the EPA. Thus, while the emissions control system does not need to reduce NOx and PM significantly during HECC, higher CO and hydrocarbon emission control is needed. Experiments were conducted to understand the synergies between HECC combustion and advanced aftertreatment (specifically LNT catalysis) and focused on comparing fuel efficiencies of the combined engine and emissions control system for three combustion modes: no EGR, original equipment manufacturer (OEM)-level EGR, and HECC. The LNT used for the study was provided by a member of the Manufacturers of Emission Control Association and has been used in other studies at ORNL.

Results

The light-duty diesel engine was operated in the advanced combustion mode HECC and compared to two other conventional lean combustion modes. The conventional modes included a case with no EGR ("no EGR") and OEM-level EGR ("OEM"); both of these modes used OEM injection timing and represent conventional diesel engine performance for both emissions and efficiency. The HECC combustion mode provided dramatic reductions in both NOx and PM emissions by enabling more homogeneous combustion in the engine cylinders created by advanced fuel injection timing, increased injection pressure, and high rates of EGR. However, CO and hydrocarbon emissions increased with HECC. A catalyzed diesel particulate filter and LNT catalyst were placed in the engine exhaust to enable further reduction of NOx and PM emissions. The engine was periodically operated rich to enable regeneration of the LNT. The frequency of regeneration was varied for all combustion modes to build a set of data for analysis of optimal engine and aftertreatment performance. A series of steady-state engine load and speed points used by industry groups in previous work served as a basis to estimate performance for the transient FTP drive cycle.

Figure 1 shows a graph of the performance for all three combustion modes at an engine condition of 1,500 rpm and 2.6 bar. Here each point on the curve

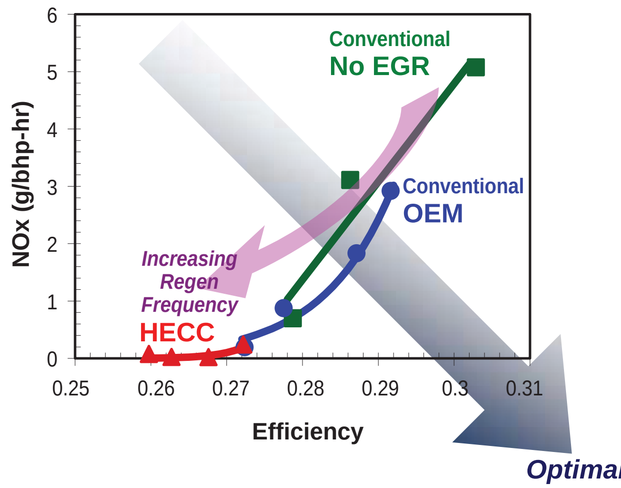

FIGURE 1. NOx Tailpipe Emissions vs. Thermal Efficiency for all Combustion Modes at 1,500 rpm and 2.6 bar brake mean effective pressure (BMEP)

represents a different regeneration frequency for each combustion mode. Data points indicated tailpipe NOx levels in g/bhp-hr and thermal efficiency. Here thermal efficiency is simply the amount of work produced by the engine per amount of fuel energy consumed, and the fuel consumption includes the higher fuel use for regeneration of the LNT. All combustion modes show that increasing the regeneration frequency of the LNT reduces tailpipe NOx but at a sacrifice of efficiency. The "optimal" regeneration frequency is somewhat subjective but can be considered as the closest data point to the lower right corner of the graph (maximum efficiency and lowest NOx emissions). The contrast in performance between HECC and the conventional modes is of most interest. Clearly, the lowest NOx levels were obtained with the HECC combustion; however, HECC gave lower efficiency at this point in comparison to the OEM and no EGR modes.

Figure 2 shows the same type of data as in Figure 1 except at an engine condition of 2,000 rpm and 2.0 bar. Here similar data curves were generated for the three combustion modes; however, at this engine condition, the HECC combustion mode produced superior performance in comparison to the no EGR and OEM cases. HECC results in much lower NOx emissions without any loss in efficiency relative to the conventional modes.

A compilation of the data at five different steady-state engine speed and load combinations was used to estimate performance over the FTP transient drive cycle. The combined NOx emission estimates in g/mile are shown in Figure 3. The lower engine-out NOx levels achieved with HECC enable the lowest NOx emission level at the tailpipe position. The U.S. EPA Tier 2 Bin 5 regulation level is shown for reference (red dashed line). Combined efficiency is shown in Figure 4. HECC did

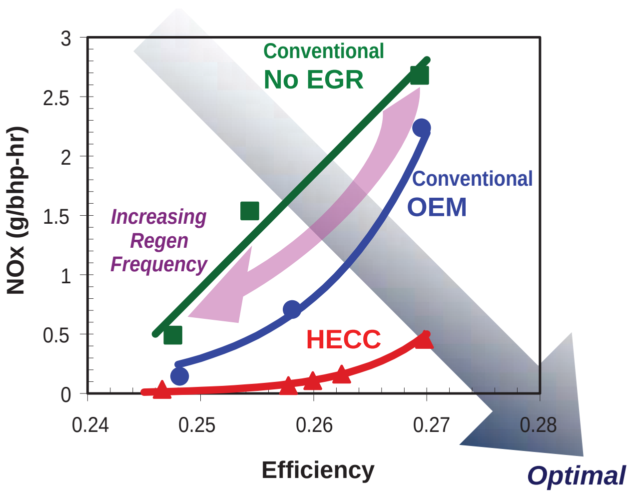

FIGURE 2. NOx Tailpipe Emissions vs. Thermal Efficiency for all Combustion Modes at 2,000 rpm and 2.0 bar BMEP

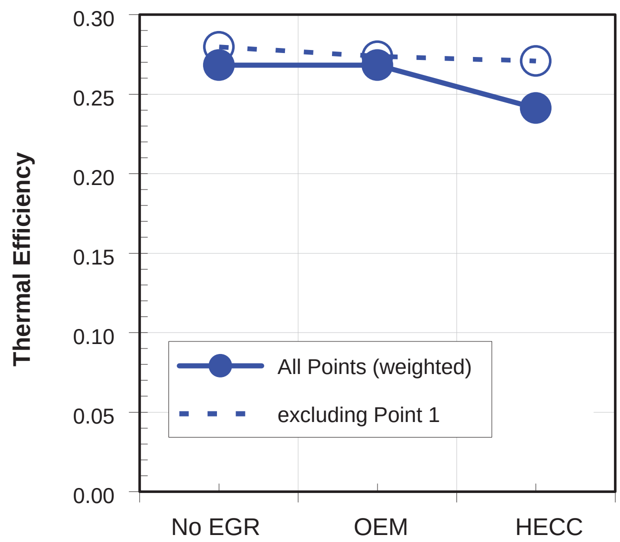

FIGURE 4. Estimated Thermal Efficiency Based on the Same Weighted Steady State Data Shown in Figure 3 for all Combustion Modes

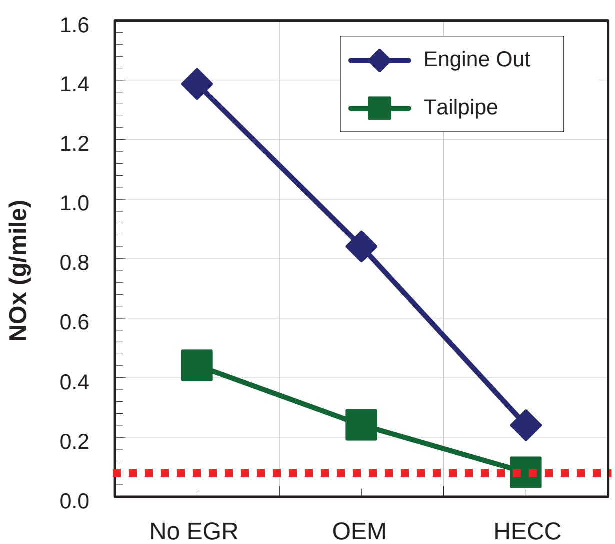

FIGURE 3. Estimated NOx Emissions for the FTP Cycle Based on Steady-State Data for all Combustion Modes

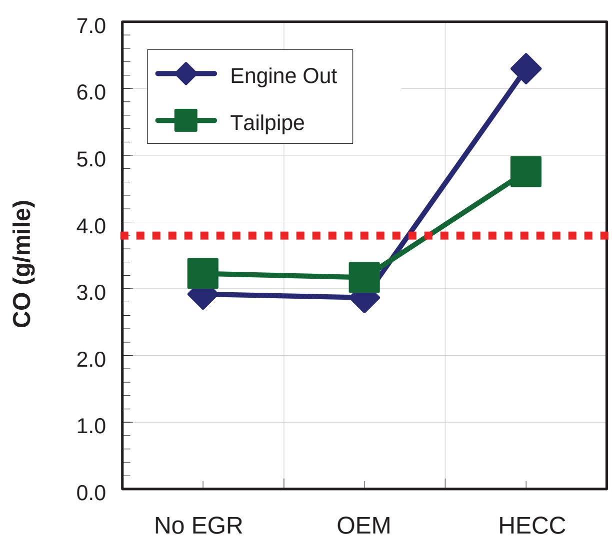

FIGURE 5. Estimated CO Emissions for the FTP Cycle Based On Steady-State Data for all Combustion Modes

show a drop in efficiency, but the efficiency decline was primarily due to the lowest load point (near idle mode) in the data set. Excluding the near idle mode point, the HECC efficiency was comparable to the conventional no EGR and OEM levels.

Figure 5 shows the CO emissions for the same data compilation as shown in Figure 4; again, the U.S. EPA Tier 2 Bin 5 regulation level is shown for reference (red dashed line). Here an increase in CO emissions is shown for HECC. The CO emissions were most problematic at the lowest load near idle point where catalyst temperatures were <150°C and too low to control the higher CO emissions produced by HECC combustion. Thus, a close-coupled diesel oxidation catalyst or better thermal management of the aftertreatment system will be needed to control these emissions under certain circumstances.

Another technical challenge identified in conjunction with the higher CO and hydrocarbon emissions is EGR fouling. The high EGR rates used for HECC coupled with the rich operation for LNT regeneration caused significant fouling of the EGR system. Mitigation of fouling will need to be addressed for commercialization of HECC.

Conclusions

- LNT aftertreatment greatly benefits from HECC operation, and the combination of HECC with LNT emission control produces the lowest NOx levels in comparison to combinations with more conventional combustion modes.
- Two technical challenges were identified that need to be addressed for commercialization of HECC: (1) higher CO and hydrocarbon emissions at low loads where catalyst temperatures cannot control these higher emissions and (2) EGR fouling that results from the high EGR rates combined with rich combustion for LNT regeneration.

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1. Jim Parks, Shean Huff, Mike Kass, Brian West, Todd Toops, and Vitaly Prikhodko, "Lean NOx Trap Catalysis: Exhaust Chemistry Related to Advanced Diesel Engines", *SAE Light-Duty Diesel Emissions Control Symposium*, Ypsilanti, MI, November 3-5, 2008.

2. E. Santillan-Jimenez, M. Crocker, J.E. Parks II, C. Salinas Martinez de Lecea, "Carbon nanotube supported metal catalysts for NOx reduction using hydrocarbon reductants", *5th International Conference on Environmental Catalysis*, Belfast, Ireland, August 31-September 3, 2008.

3. Jim Parks, Vitaly Prikhodko, Mike Kass, and Shean Huff, "Synergies of PCCI-Type Combustion and Lean NOx Trap Catalysis for Diesel Engines", *SAE Technical Paper Series* 2008-01-2493 (2008).

4. J.M.E. Storey, S.A. Lewis, J.E. Parks, J.P. Syzbist, T.L. Barone, and V.Y. Prikhodko, "Mobile Source Air Toxics (MSATs) from High Efficiency Clean Combustion: Catalytic Exhaust Treatment Effects", *SAE Technical Paper Series* 2008-01-2431 (2008).

5. Jim Parks, Shean Huff, Mike Kass, and Vitaly Prikhodko, "Synergies of High-Efficiency Clean Combustion and Lean NOx Trap Catalysts", *Proceedings of the 14th Diesel Engine-Efficiency and Emissions Research Conference* (2008).

6. Vitaly Prikhodko, Jim Parks, Shean Huff, and Mike Kass, "Impact of PCCI on LNT Performance", *11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation*, May 13-15, 2008 (2008).

II.B.9 Cross-Cut Lean Exhaust Emission Reduction Simulation (CLEERS): Administrative Support

Stuart Daw
Oak Ridge National Laboratory (ORNL)
National Transportation Research Center
2360 Cherahala Boulevard
Knoxville, TN 37932-6472

DOE Technology Development Manager:
Ken Howden

Key ORNL personnel involved in this activity are Stuart Daw, Vitaly Prikhodko, Charles Finney, and Tracy Bryant.

Objectives

Coordinate the CLEERS activity for the Diesel Cross-Cut Team to accomplish the following:

- Promote development of improved computational tools for simulating realistic full-system performance of lean-burn engines and associated emissions controls.
- Promote development of performance models for emissions control components such as exhaust manifolds, catalytic reactors, and sensors.
- Provide consistent framework for sharing information about emissions control technologies.
- Help identify emissions control research and development (R&D) needs and priorities.

Accomplishments

- Continued co-leading the CLEERS Planning Committee and facilitation of the selective catalytic reduction (SCR), lean-NOx trap (LNT), and diesel particulate filter (DPF) Focus Group telecoms with strong domestic and international participation.
- Continued co-leading the LNT Focus Group and refinement of the standard LNT materials protocol.
- Identified key R&D priorities from the CLEERS community, including coordination of a second R&D priorities survey with response from 16 DOE Diesel Crosscut Team companies and their supplier and energy company partners in 2008.
- Provided regular update reports to the DOE Diesel Crosscut Team.
- Organized 11th CLEERS workshop at the University of Michigan, Dearborn on May 13-15, 2008.
- Maintained Web site functionalities, security, and data to facilitate Web meetings and serve Focus Group interactions.

Future Directions

- Continue co-leading the CLEERS planning committee.
- Continue co-leading the LNT Focus Group and support the DPF and SCR Focus Groups as needed.
- Continue providing standard reference LNT materials and data for Focus Group evaluation.
- Issue final report on the 2008 R&D priorities survey and continue assisting in refinement of CLEERS technical priorities, especially in regard to the balance between LNT and urea-SCR R&D and synergies between these two technology areas.
- Organize and conduct the 12th CLEERS workshop in the spring of 2008.
- Expand basic data and model exchange between CLEERS and other Office of Vehicle Technologies projects.
- Continue maintenance and expansion of the CLEERS Web site.
- Continue providing regular update reports to the DOE Diesel Crosscut team.

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Introduction

Improved catalytic emissions controls will be essential for utilizing high-efficiency lean-burn engines without jeopardizing the attainment of much stricter U.S. Environmental Protection Agency emission standards scheduled to take effect in 2010. Simulation and modeling are recognized by the DOE Diesel Crosscut Team as essential capabilities needed to achieve this goal. In response to this need, the CLEERS activity was initiated to promote improved computational tools and data for simulating realistic full-system performance of lean-burn engines and the associated emissions control systems. Specific activities supported under CLEERS include:

- Public workshops on emissions control topics;
- Collaborative interactions among Crosscut Team members, emissions control suppliers, universities, and national labs under organized topical focus groups;
- Development of experimental data, analytical procedures, and computational tools for understanding performance and durability of catalytic materials;

- Establishment of consistent frameworks for sharing information about emissions control technologies; and
- Recommendations to DOE and the DOE Crosscut Team regarding the most critical emissions control R&D needs and priorities.

ORNL is involved in two separate DOE-funded tasks supporting CLEERS:

- Overall administrative support; and
- Joint development of benchmark LNT kinetics with Sandia National Laboratories and Pacific Northwest National Laboratory.

Approach

In the administrative task, ORNL coordinates the CLEERS Planning Committee, the CLEERS Focus Groups, CLEERS public workshops, and the CLEERS Web site (http://www.cleers.org). The specific activities involved include:

- Coordination of the CLEERS Planning Committee and the LNT Focus Group;
- Organization of the annual CLEERS public workshops;
- Maintenance of the CLEERS Web site;
- Preparation and presentation of status reports to the Crosscut Team; and
- Response to requests and inquiries about CLEERS from the public.

Results

The 11th CLEERS workshop was held May 13–15, 2008 at the Dearborn campus of the University of Michigan. More than 100 registrants from emissions controls suppliers, universities (both foreign and domestic), software vendors, and consultants shared experiences with experimental characterization and modeling of lean exhaust aftertreatment control systems. The meeting was structured around the three traditional emissions control technology areas (LNTs, DPFs, and SCR) and included topics related to systems integration and component interactions. The technical program and presentations are available on the Web site (http://www.cleers.org) under the 11th workshop heading. Key observations coming from the workshop include:

- Definition of global kinetics for NH_3-generation, sulfation, and desulfation of LNTs continues to be an area of great interest and progress.
- Models for LNT simulation continue to improve and have been implemented (in low-order form) into systems simulation software such as the Powertrain Systems Analysis Toolkit (PSAT).
- There is increasing interest in development of a CLEERS protocol for characterizing transient urea-SCR catalyst response (as opposed to steady-state kinetics only).
- Methods for using urea-SCR models to diagnose (on-board) the current state of catalyst NH_3 storage and hydrocarbon poisoning are becoming increasingly important.
- Publicly available DPF soot oxidation kinetics continue to be inadequate for low-temperature combustion modes and with unconventional fuels (e.g., biodiesel).
- The appropriate role of diesel oxidation catalysts (DOCs) for DPF performance continues to reflect a large diversity of opinion.

The LNT, SCR, and DPF Focus Groups have continued regular phone/Web meetings throughout the year under the new single monthly meeting format adopted in 2006. This format has continued to work well.

R&D priorities identified by the CLEERS members were updated in a second anonymous poll conducted in the spring of 2008 by New West Technologies. For 2008, the CLEERS Planning Committee made several modifications to the poll questions, specifically designed to simplify the reporting and gather information on technologies through a slightly different set of questions. Respondents were asked only to prioritize activities on an overall basis, versus prioritizing activities with respect to commercial relevance, national energy strategy, scientific importance, and suitability for national laboratory capabilities. In addition, specific mention was made in 2008 of DOCs (for 2007, these were included in a larger category of "integrated systems simulation"). Questions for 2008 were also designed to elicit more comments on the need for applications-related work. As in 2007, questionnaires were sent to 22 organizations, and respondents were asked to identify themselves as belonging to either diesel or gasoline categories.

There were a total of sixteen poll responses under the diesel category and seven under gasoline. The overall list of respondents included three engine manufacturers, three light-duty vehicle manufacturers, two heavy-duty vehicle manufacturers, four major suppliers, and two energy companies. For the diesel category, key results were:

- There was no major change in the most prominent perceived R&D needs; that is, urea-SCR and DPF simulation were still of highest priority.
- However, modeling related to on-board diagnostics for urea-SCR and DPF appeared to be growing in importance for the diesel community.

- R&D needs for DOC modeling continued to be high in priority also and were somewhat better defined than in 2007.
- Interest in hydrocarbon (HC)-SCR simulation continued but at a much lower level than urea-SCR and DPF simulation.

For the gasoline respondents, the major findings were:

- LNT simulation was still the dominant area of interest.
- Urea-SCR increased significantly in importance between 2007 and 2008.
- Interest in HC-SCR as a longer-range aftertreatment option has also continued in 2008.
- DPF technology for gasoline systems remains one of the lowest priorities.

Details of the 2008 survey have been summarized in a final report to the CLEERS Planning Committee, the DOE Diesel Crosscut Team and the CLEERS Focus Groups. This information is being used by the CLEERS Planning Committee to complete identification of gaps in the current CLEERS-related research activities both in DOE and in industry that was begun last year. It is expected that a summary of the identified gaps and corresponding recommendations will be presented to the Crosscut Team early in Fiscal Year 2009.

Conclusions

CLEERS continues to serve a central role in coordinating emissions control R&D among the Crosscut Team members and their partners. The success of CLEERS is most noticeable in the broad participation among industry, national labs, and universities in the public workshops; the strong domestic and international participation in the monthly technical focus meetings; the heavy interest in the R&D priority survey among CLEERS community; and the large number of visits to the CLEERS Web site. We expect that utilization of the CLEERS R&D gaps analysis results will provide an important new approach for improving the effectiveness of collaborative emissions control R&D among the DOE labs, universities, and industry partners.

FY 2008 Publications/Presentations

1. http://www.cleers.org

2. Michael Laughlin, Stuart Daw, and Richard Blint, "CLEERS Priorities Poll Response Analysis 2008 (Final Report to the DOE Diesel Crosscut Team)," November 7, 2008.

II.B.10 Cross-Cut Lean Exhaust Emission Reduction Simulation (CLEERS): Joint Development of Benchmark Kinetics

Stuart Daw
Oak Ridge National Laboratory (ORNL)
National Transportation Research Center
2360 Cherahala Boulevard
Knoxville, TN 37932-6472

DOE Technology Development Manager:
Ken Howden

Key ORNL personnel involved in this activity are:
Jae-Soon Choi, Bill Partridge, Stuart Daw, Kalyana Chakravarthy, Todd Toops, Jim Parks, Josh Pihl, Charles Finney, and Vitaly Prikhodko.

Objectives

Coordinate ORNL's collaboration with Pacific Northwest National Laboratory (PNNL), and Sandia National Laboratories (SNL) in the development of kinetics information needed for aftertreatment component simulation through the following:

- Provide benchmark laboratory measurements of oxides of nitrogen (NOx) reduction chemistry and reaction rates in lean-NOx traps (LNTs) under realistic operating conditions.
- Correlate laboratory measurements of LNT and selective catalytic reduction (SCR) catalysts with test-stand/vehicle studies.
- Develop and validate global chemistry and (low-order) models for LNT and SCR kinetics.

Accomplishments

- Made detailed spatially resolved capillary inlet mass spectrometer (SpaciMS), microscopy, and temperature programmed reaction measurements of model and Umicore reference LNT catalysts to resolve critical details about the impact of sulfation and desulfation on the following:
  - Ammonia production during stored NOx reduction.
  - The types of sulfates that form and their relative stabilities.
  - How axial variations in LNT in sulfur poisoning relate to overall performance.
- Utilized above information to develop a low-order LNT model capable of systems simulation studies.
- Continued diffuse reflectance infrared Fourier-transform spectroscopy (DRIFTS) measurements of the fundamental mechanisms involved in sulfur poisoning and desulfation of LNTs.
- Continued collaboration with SNL to apply the above measurements in developing a detailed kinetics model of combined LNT NOx capture and stored-NOx regeneration.
- Initiated DRIFTS studies of Umicore zeolite urea-SCR catalyst in collaboration with PNNL.
- Completed a preliminary evaluation of 3-dimensional (3D) X-ray technology for visualizing details inside catalytic monoliths.

Future Directions

- Confirm primary chemical mechanisms and kinetics of sulfation and desulfation by means of the following:
  - Complete specialized LNT sample analyses using X-ray photoelectron spectroscopy (XPS) and electron probe microanalysis (EPMA).
  - Characterize model sulfate compounds with DRIFTS and temperature programmed reaction (TPR) and compare with LNT samples.
  - Extract global Arrhenius rate parameters for sulfation and desulfation.
  - Validate LNT model performance predictions against laboratory bench-scale and engine measurements.
- Implement a combined LNT model that includes NOx capture and reduction and sulfation and desulfation in a form that can be used for systems drive cycle simulations and shared with the CLEERS community.
- Ramp up investigation of urea-SCR kinetics.
- Interface with CLEERS industry partners to determine if X-ray monitoring would be useful for diesel particulate filter (DPF) onboard diagnostics (OBD)/model validation.
- Continue identification of synergies between LNT NH_3 generation kinetics and NH_3-SCR as a potential alternative to urea-SCR NOx control.

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Introduction

Improved catalytic emissions controls will be essential for utilizing high-efficiency lean-burn engines without jeopardizing the attainment of much stricter U.S. Environmental Protection Agency emission standards scheduled to take effect in 2010. Simulation and modeling are recognized by the DOE Diesel Crosscut Team as essential capabilities needed to achieve this goal. In response to this need, the CLEERS activity was initiated to promote improved computational tools and data for simulating realistic full-system performance of lean-burn engines and the associated emissions control systems.

ORNL is involved in two separate DOE-funded tasks supporting CLEERS:

- Overall administrative support; and
- Joint development of benchmark LNT kinetics with SNL and PNNL.

Approach

In the benchmark kinetics task (covered by this report), ORNL is collaborating with SNL and PNNL to produce kinetic information for LNT and urea-SCR aftertreatment devices, both as individual and system integrated components. The results of this work are discussed with the LNT, DPF, and SCR Focus groups prior to publication to provide technical review and guidance to the labs. Specific activities involved include:

- Regular direct interactions among ORNL, PNNL, and SNL.
- Experimental measurements of LNT chemistry and reaction rates using laboratory reactors and prototype devices installed on engine test stands and vehicles.
- Analysis and reconciliation of experimental data from different sources with predictions from computer simulations.
- Publications in journals and presentations in public meetings and on the Web site.

Results

This year, LNT studies focused on dynamic bench reactor measurements of model and commercial monolith catalyst cores with SpaciMS probes during NOx capture and regeneration at varying degrees of sulfation and desulfation. In addition, samples of LNT catalyst at varying stages of sulfation were analyzed with TPR and specialized microscopy techniques (including XPS and EPMA) to characterize the physical and chemical state of the catalyst. As in previous years, this work has been extensively reported in a large number of publications and presentations referenced at the end of this report.

One key finding from the LNT experiments is that there is a strong correlation between global sulfur loading and the amount of ammonia (NH_3) slip observed from the Umicore catalyst. The global selectivity for NH_3 clearly increases with sulfur poisoning, while the selectivity for nitrous oxide (N_2O) remains almost unchanged. The rise in NH_3 slip with sulfation seems to support previous suggestions that combining LNT catalysts with NH_3-SCR catalysts might provide a way to reduce the negative impact of sulfur on NOx emissions control.

Figure 1 illustrates example TPR measurements that reveal four major types of sulfate formed in the Umicore LNT. The rate of desulfation is indicated by the sulfur concentration in the exit gas (typically as H_2S) as a function of temperature. Sulfates with lower stability (e.g., sulfates associated with ceria, alumina, and spinel) were released first; more stable sulfates (e.g., barium sulfate) were released later. Four distinct stages of desulfation were apparent for the Umicore catalyst. The differentiation of sulfur into four types was also confirmed by direct chemical analysis and DRIFTS measurements of sulfated catalyst samples.

Combining the above observations with direct SpaciMS measurements of key species, we now have a conceptual model for LNT sulfur poisoning with the following key features:

- As the catalyst is exposed to sulfur in the exhaust, a stable, plug-like sulfation front progresses axially down the monolith washcoat from the upstream end.
- NOx storage and reduction (NSR) occurs predominantly downstream of the sulfation front in a relatively short region where gas phase reductant and NH_3 concentrations change rapidly. The high NH_3 levels encountered in the NSR zone suggest that NH_3 may play a major role in NOx reduction.
- Downstream from the NSR zone, the primary chemical reactions are associated with oxygen storage and release (OSR). Any NH_3 escaping

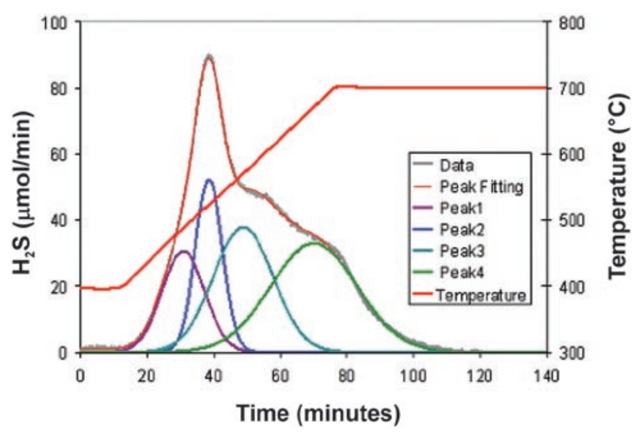

FIGURE 1. Example TPR results for a 3-inch long sulfated LNT monolith core. The sample was exposed to exhaust gas containing 1% hydrogen while the temperature was ramped to 700°C at 5°C/min. Sulfur release patterns (indicated by H_2S at the exit) imply that there were four major sulfur compounds being decomposed (represented by four smaller curves). Sulfur compounds decomposed at higher temperature are more stable and thus more difficult to remove.

the NSR zone is oxidized in the OSR zone before reaching the exit.

- As the catalyst is repeatedly sulfated and desulfated, more of the sulfur becomes concentrated in the most stable form (that is as $BaSO_4$). With repeated cycling the leading-edge sulfation zone becomes more difficult to desulfate, and the LNT gradually loses efficiency.

A simplified LNT model that includes the basic features above has been implemented in the Powertrain Systems Analysis Toolkit produced by Argonne National Laboratory. Using this model, we have been able to begin making comparisons of hybrid electric vehicles powered by stoichiometric gasoline engines versus diesel hybrid vehicles. As expected, the initial fuel efficiency of diesel hybrids is significantly better, but the introduction of lean NOx control by LNTs reduces the difference because of the additional fuel penalty for NOx and sulfur regeneration.

DRIFTS measurements of a commercial zeolite urea-SCR catalyst have been initiated in collaboration with Jonathan Male at PNNL. The specific goals are to identify important reaction intermediates (especially at low temperature) and develop models for hydrocarbon poisoning. The DRIFTS technique makes it possible to directly observe species on the catalyst surface as reactions proceed. We successfully demonstrated this year that distinctly different NH_3 storage sites are visible to DRIFTS. Example DRIFTS spectra for NH_3 accumulation on the catalyst surface are illustrated in Figure 2. We are now in the process of repeating these measurements in the presence of hydrocarbons and NOx.

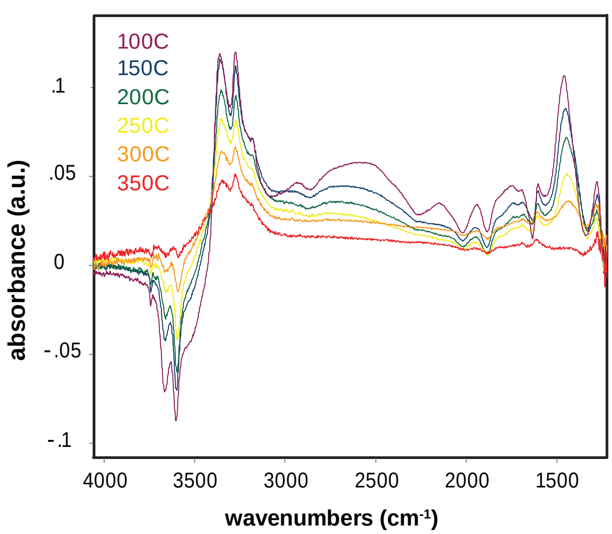

FIGURE 2. Example DRIFTS spectra for NH_3 adsorption onto the Umicore reference zeolite urea-SCR catalyst. In this case the catalyst was exposed to 300 ppm NH_3 at different temperatures. Peaks indicate the presence of specific forms of NH_3 storage. As expected, the overall level of adsorption drops strongly with increasing temperature.

From early March to May we had on-site access to an industrial X-ray machine on loan from 3D-XRAY, Ltd. This particular model, MDXi400, is capable of making detailed 3D X-ray images of catalyst monoliths up to 46 cm long by 40 cm in diameter. Machines similar to this are already utilized for monitoring industrial production quality of catalyst monoliths, so it was hoped that it might also be useful for measurements of experimental catalysts. Experiments with several 6-inch DPF monoliths in and out of the can revealed that it is possible to use this imaging technique to observe the spatial distribution and thickness of both soot and ash deposits. These results suggest that this type of X-ray instrument may be a useful method for gathering critical DPF modeling validation data as well as the basis for developing a non-intrusive DPF inspection process. Two presentations and a Society of Automotive Engineers paper covering these results have been published.

Conclusions

Closely linked laboratory experiments and collaborative modeling have improved understanding of LNT catalyst simulation and identification of opportunities for reducing the NOx control fuel penalty and improving the sulfur tolerance of LNT technology. This same approach is now being applied to urea-SCR catalysts.

FY 2008 Publications

1. Vitaly Y. Prikhodko, Ke Nguyen, Jae-Soon Choi, and C. Stuart Daw, "Axial length effects on lean NOx trap performance", *Applied Catalysis B: Environmental*, submitted.

2. Y. Ji, T.J. Toops, M. Crocker, "Effect of Ceria on the Sulfation and Desulfation Characteristics of a Model Lean NOx Trap Catalyst", *Catalysis Letters*, submitted.

3. Y. Ji, T.J. Toops, J.A. Pihl, M. Crocker, "NOx storage and reduction in model lean NOx trap catalysts studied by in situ DRIFTS", Submitted to Applied Catalysis B, October 2008.

4. T.J. Toops and J.A. Pihl, "Sulfation of model K-based lean NOx trap while cycling between lean and rich conditions", *Catalysis Today* 136 (2008) 164.

5. Richard S. Larson, Josh A. Pihl, V. Kalyana Chakravarthy, Todd J. Toops, and C. Stuart Daw, "Microkinetic modeling of lean NOx trap chemistry under reducing conditions", *Catalysis Today* 136 (2008) 104-120.

6. Yaying Ji, Jae-Soon Choi, Todd J. Toops, Mark Crocker, and Mojghan Naseri, "Influence of ceria on the NOx storage/reduction behavior of lean NOx trap catalysts", *Catalysis Today* 136 (2008) 146-155.

7. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, and C. Stuart Daw, "Sulfur and temperature effects on the spatial distribution of reactions inside a lean NOx trap and resulting changes in global performance", *Catalysis Today* 136 (2008) 173-182.

8. Y. Ji, J.-S. Choi, T.J. Toops, M. Crocker, M. Naseric, "Influence of Ceria on the NOx Storage/Reduction Behavior of Lean NOx Trap Catalysts", Catalysis Today 136 (2008) 146.

9. Y. Ji, T.J. Toops, and M. Crocker, "Effect of Ceria on the Storage and Regeneration Behavior of a Model Lean NOx Trap Catalyst", Catalysis Letters 119:3-4 (2007) 257.

10. J.-S. Choi, W.P. Partridge, and C.S. Daw, "Sulfur impact on NOx storage, oxygen storage and ammonia breakthrough during cyclic lean/rich operation of a commercial lean NOx trap", *Applied Catalysis B: Environmental* 77, 145-156 (2007).

11. C.S. Daw, "Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS): Joint Development of Benchmark Kinetics", *DOE Annual Progress Report for Advanced Combustion Engine Technologies* (2007).

12. T.J. Toops, J.A. Pihl, "Fundamental sulfation/desulfation studies of lean NOx Traps, DOE pre-competitive catalyst research", *DOE Annual Progress Report for Advanced Combustion Engine Technologies* (2007).

FY 2008 Presentations

1. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, Todd J. Toops, Michael J. Lance, Charles E.A. Finney, V. Kalyana Chakravarthy, and C. Stuart Daw, "Correlation between spatiotemporal distribution of reactions and global performance of a commercial lean NOx trap catalyst at varying sulfation stages", oral presentation at the 5th International Conference on Environmental Catalysis, Belfast, United Kingdom, August 31 – September 3, 2008.

2. William P. Partridge, Jae-Soon Choi, Josh A. Pihl, Todd J. Toops, and C. Stuart Daw, "Intermediate NH3 generation and utilization inside a lean NOx trap catalyst", oral presentation at the 5th International Conference on Environmental Catalysis, Belfast, United Kingdom, August 31 – September 3, 2008.

3. J.A. Pihl, T.J. Toops, "DRIFTS Investigation of Sulfation of Model Lean NOx Trap", poster presentation at the 5th International Conference on Environmental Catalysis, Belfast, United Kingdom, August 31 – September 3, 2008.

4. Y. Ji, V. Easterling, M. Crocker, T.J. Toops, J. Theis, J. Ura, R.W. McCabe, "Effect of Ceria on the Sulfation and Desulfation Characteristics of Lean NOx Trap Catalysts", poster presentation at the 5th International Conference on Environmental Catalysis, Belfast, United Kingdom, August 31 – September 3, 2008.

5. Finney CEA, Toops TJ, Daw CS, Zandhuis J, Fox TJ (2008). Non-destructive in-the-can x-ray measurement of soot, ash, washcoat and regeneration damage in DPFs. DEER (Detroit, Michigan USA; 2008 August 04).

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7. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, and Todd J. Toops, "Fundamental studies of commercial lean NOx trap performance, sulfation and desulfation: postmortem characterization", poster presentation at the 14th International Congress on Catalysis, Seoul, Korea, July 13 – 18, 2008.

8. Vitaly Prikhodko, Ke Nguyen, Jae-Soon Choi, and C. Stuart Daw, "Effect of length on the performance of lean NOx traps", poster presentation at the 14th International Congress on Catalysis, Seoul, Korea, July 13-18, 2008.

9. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, Todd J. Toops, Michael J. Lance, Charles E.A. Finney, V. Kalyana Chakravarthy, and C. Stuart Daw, "Sulfation impact on LNT performance: experimental studies with Umicore CLEERS reference catalyst", oral presentation at the 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation, Dearborn, Michigan, May 13-15, 2008.

10. William P. Partridge, and Jae-Soon Choi, "Ammonia formation and utilization in lean NOx trap catalysts: experimental determination of reaction pathways", oral presentation at the 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation, Dearborn, Michigan, May 13-15, 2008.

11. Vitaly Prikhodko and James E. Parks, "Impact of PCCI on LNT Performance," oral presentation at the 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation," Dearborn, Michigan, May 13-15, 2008.

12. Todd Toops and Mark Crocker, "Effect of Ceria on the Sulfation and Desulfation Characteristics of Lean NOx Trap Catalysts," oral presentation at the 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation, Dearborn, Michigan, May 13-15, 2008.

13. Kalyana Chakravarthy, "An update on Lean NOx Trap modeling in PSAT," oral presentation at the 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation, Dearborn, Michigan, May 13-15, 2008.

14. Todd J. Toops and Bruce Bunting, "Accelerated Aging of Emission Control Devices," oral presentation at the 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation, Dearborn, Michigan, May 13-15, 2008.

15. Zandhuis J, Finney CEA, Toops TJ, Daw CS, Fox TJ (2008). Non-destructive in-the-can x-ray measurement of soot, ash, wash coat and regeneration damage in DPFs. 11th DOE Crosscut Workshop on Lean Emissions Reduction Simulation (Dearborn, Michigan USA; 2008 May 12-15).

16. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, Todd J. Toops, Michael J. Lance, Charles E.A. Finney, V. Kalyana Chakravarthy, and C. Stuart Daw, "Experimental studies of LNT sulfation and desulfation with the Umicore reference catalyst", oral presentation at the DOE CLEERS (Crosscut Lean Exhaust Emissions Reduction Simulations) Focus Group Teleconference, April 10, 2008.

17. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, Michael J. Lance, Larry R. Walker, Charles E.A. Finney, V. Kalyana Chakravarthy, Vitaly Prikhodko, Todd J. Toops, and C. Stuart Daw, "ORNL research on LNT sulfation and desulfation", oral presentation at the 2008 DOE Vehicle Technologies Program Annual Merit Review, Bethesda, Maryland, February 25-28, 2008.

18. Jae-Soon Choi, William P. Partridge, Josh A. Pihl, and C. Stuart Daw, "Sulfur effects on spatiotemporal distribution of reactions in a commercial lean NOx trap", oral presentation at the American Institute of Chemical Engineers (AIChE) Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.

II.B.11 CLEERS Diesel Particulate Filter (DPF) Modeling

Mark Stewart (Primary Contact),
Darrell Herling, Gary Maupin
Pacific Northwest National Laboratory (PNNL)
P.O. Box 999, MSIN: K7-15
Richland, WA 99354

DOE Technology Development Manager:
Ken Howden

Objectives

- Develop improved modeling capabilities for diesel particulate filtration:
  - Create improved models of the local properties of the soot filter, e.g. cake permeability, density, morphology...
  - Develop improved sub-grid representations of the local soot oxidation reactions in diesel soot filters, e.g. oxidation mechanisms, detailed kinetics, global rates...
- Coordinate and lead the Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) DPF sub-team activities:
  - Provide project updates to the industry sub-team, solicit feedback, and adjust work scope accordingly.
  - Lead technical discussions, invite distinguished speakers, and maintain an open dialogue on DPF modeling issues.

Accomplishments

- Acquired, installed and tested a mini-Combustion Aerosol Standard (CAST) laboratory soot generator system.
- Developed techniques for loading individual filter walls and single channel samples with aerosolized salt particles or lab-generated soot particles for fundamental filtration studies.
- Performed energy dispersive X-ray spectroscopy (EDS) scans of fractured filter walls loaded with aerosolized salt particles to characterize particle penetration into the filter microstructure.
- Enhanced particle capture model in micro-scale filtration simulation tools and performed studies with varying capture probability.
- Obtained three dimensional X-ray scans of several filter samples (silicon carbide, catalyzed and uncatalyzed cordierite) with 1.5 micron resolution.
- Participated in monthly CLEERS teleconferences and coordinated the calls focused on DPF technology.

Future Directions

- Make improved measurements of particulate penetration into filter walls by immobilizing deposits with vaporized adhesive, potting with epoxy, and polishing wall cross-sections to a flat surface.
- Use computed tomography (CT) data to generate new DPF substrate reconstructions for pore-scale simulations.
- Compare predictions made with CT geometries to those obtained with geometries generated by stochastic reconstruction.
- Explore effects of pore structure variations (e.g. contributions of unusually large pores or cracks) in filter substrates.
- Examine effects of catalyst washcoat location and structure on flow, filtration, and regeneration.
- Conduct filter regeneration experiments in a bench-scale reactor with catalyzed filter samples loaded with lab-generated soot and soot from diesel engines.

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Introduction

Diesel engines play a central role in global transportation. Their inherent fuel efficiency makes them even more attractive as means are sought to lower carbon emissions. Increasing availability of bio-diesel adds a new dimension to the future potential of diesel engines for clean transportation. Health and climate risks associated with diesel particulates have recently led to the widespread adoption of DPFs in developed nations. While effectively removing particulates, these devices also diminish fuel efficiency through increased exhaust system back-pressure.

The project described in this report seeks to promote effective diesel particulate filter technology with minimum fuel penalty by enhancing fundamental understanding of filtration mechanisms through targeted experiments and computer simulations. The overall back-pressure of a filtration system depends upon complex interactions of particulate matter and ash with the microscopic pores in filter media. Better characterization of these phenomena is essential for exhaust system optimization.

Approach

Experimental techniques were developed to load small filter samples with aerosolized salt particles and laboratory-generated soot having controlled size distributions. While retaining the complex fractal structure of diesel soot, particles generated with laboratory systems such as the mini-CAST unit allow much better control and reproducibility than can usually be achieved with a diesel engine. Salt particles allow another level of simplification since they are roughly spherical in shape. Unlike soot, some salts are also easily distinguished from filter substrates using techniques such as EDS. This allows quantitative examination of the degree of particulate penetration into the filter wall, which is a critical factor in determining back-pressure.

Computer simulation techniques have been developed to predict the location and morphology of soot deposits within porous filter substrates by simulating the flight and deposition of individual soot particles. The lattice-Boltzmann method is used to solve for the flow field of exhaust through the filter microstructure as soot deposits form. Transport and reaction of active gaseous species during filter regeneration may also be simulated. Pore-scale simulations allow examinations of the fundamental mechanisms governing filtration efficiency and back-pressure during DPF operation.

Results

Fundamental filtration experiments were carried out with two types of filter samples. In the first type, individual channels were cut from full DPF honeycombs and loaded with particulates on their exterior surfaces by drawing gas through using a vacuum pump. In the second type, individual filter walls were similarly cut from entire filters and mounted in a plastic manifold, allowing pure wall-flow loading. Both types of samples remove complexities associated with full DPF honeycombs, such as radial mal-distribution of flow, and axial flow resistance in inlet channels.

Filtration experiments were carried out using aerosolized ammonium sulfate particles and soot particulates generated using a mini-CAST soot generating system. Both types of particulates allow a degree of control and repeatability which is very difficult to obtain when studying soot generated by actual diesel engines. Comparing filtration behavior with these two different kinds of particulates will help to quantify the affect of particle size, density, and morphology on filter performance. Another advantage of ammonium sulfate is that it can be easily washed from a filter sample using de-ionized water. Figure 1 shows the reproducibility of two filtration tests under the same experimental conditions with the same filter sample.

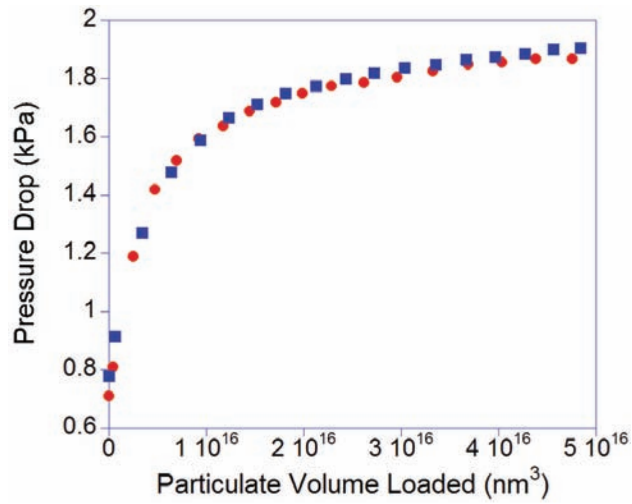

FIGURE 1. Reproducibility of Filtration Experiments with Aerosolized Salt Particles

Filters were loaded with ammonium sulfate particles, fractured, and the wall cross-sections examined using scanning electron microscopy (SEM) and EDS. EDS images indicating the location of sulfur in a cordierite filter sample were aligned and processed to yield the plot in Figure 2. Comparing line-averaged sulfur intensity to aluminum intensity gives a quantitative measure of the extent of particulate penetration into the porous filter wall. The extent to which particulates fill pore throats within the filter substrate is a major factor in overall back-pressure, and the intimacy of contact between particulates and catalyzed substrate surfaces could be important during the regeneration of some filter systems. This data also allows comparisons to the predictions made by filter models. Some shadowing was observed in the fractured samples examined. Improved results may be obtained in the future by immobilizing the particulates with a vaporized adhesive, potting with epoxy, and polishing to a flat surface [1] prior to examination.

Development of tools for pore-scale filter simulation continued in Fiscal Year 2008. Figure 3 shows soot deposits predicted by simulation of filtration with a silicon carbide substrate. Previous versions of the simulation program had assumed that particulate mass was transported in 'bundles' having a fixed diameter of 1 micron. This was done in order to allow significant deposits to be generated in reasonable time periods with limited computational resources. This simplification led to skewed filtration efficiency predictions, since capture of small particles was disproportionally affected by the interception mechanism while retaining the effect of the diffusion mechanism. The fixed 'bundle' approximation has been removed from the current version of the program. Figure 4 shows a new plot of filtration efficiency versus particle size for a simulation of filtration using cordierite. The shape of the curve agrees

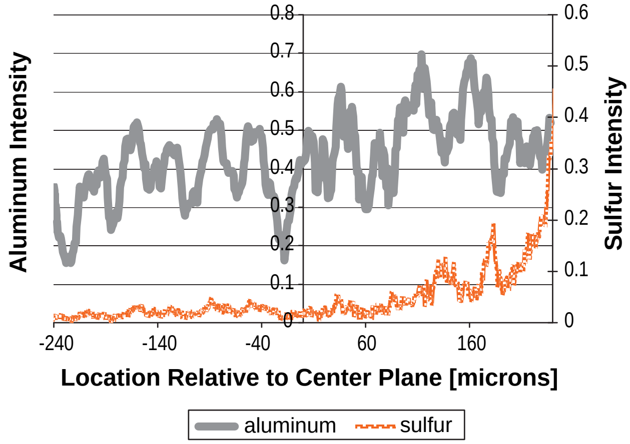

FIGURE 2. Line-Averaged Sulfur and Aluminum Intensities Indicating Penetration of Particulates Into the Filter Wall

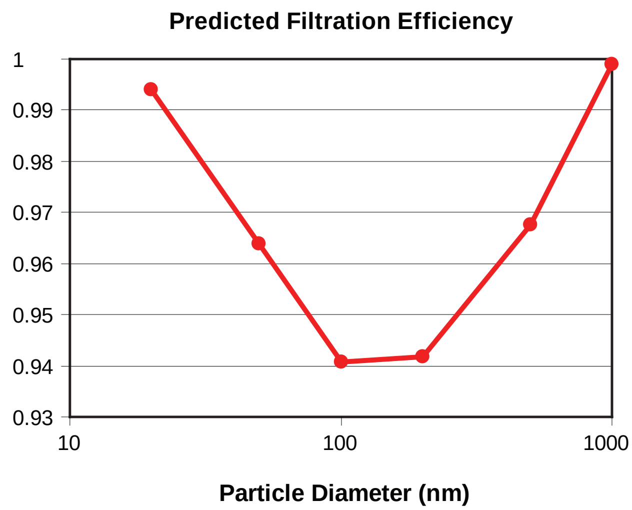

FIGURE 4. Predicted Filtration Efficiency as a Function of Particle Size

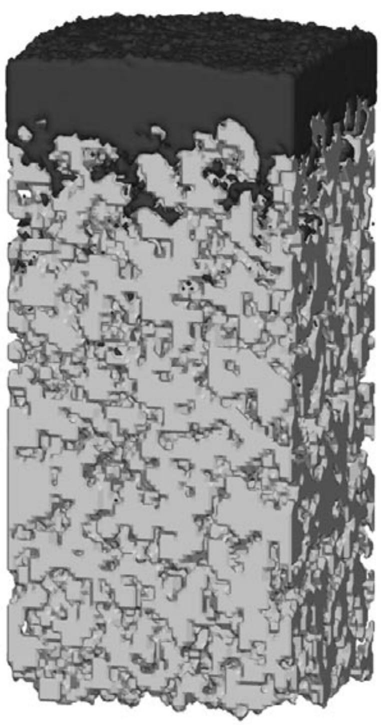

FIGURE 3. Simulated Soot Deposits in a Silicon Carbide Filter

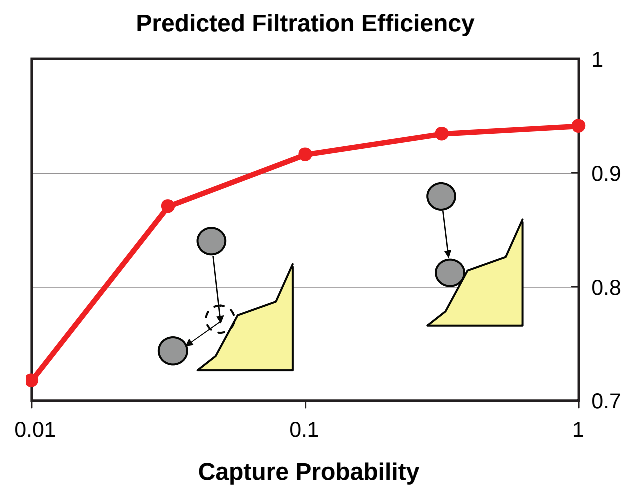

FIGURE 5. Predicted Filtration Efficiency as a Function of Capture Probability

very well with filtration experiments using aerosolized salt particles. Minimum filtration efficiencies close to 100 nm are correctly predicted, although the absolute values of efficiencies are still higher than those typically observed in experiments.

Particle contact and capture mechanics were also made more rigorous, and the ability was added to rebound particles from surfaces and deposits. This allows particle capture probabilities of less than 100% to be specified. Although instantaneous particle deposition is usually assumed for sub-micron particles [2], particle rebound has been used in the literature for simulation of realistic aerosol deposits [3]. Particle capture probability may be made to depend upon particle momentum or local shear stresses, or it could be used as an adjustable parameter to cancel artificially high filtration efficiencies caused by the particulate bundle assumption described above. Figure 5 shows a plot of initial filtration efficiency predicted for a cordierite filter versus specified capture probability. Future efforts to improve predictions will focus on more accurate three-dimensional reconstructions of substrate materials and further experimentation with particle transport and capture algorithms.

One of the primary uncertainties of the pore-scale simulations conducted to date has been the adequacy of the three-dimensional substrate reconstructions used for solid boundaries. Reconstructions based on interpolation between two-dimensional images obtained by SEM and reconstructions using stochastic algorithms have both been used. The latter technique allows volumes of any size and shape to be reconstructed from a relatively small set of two-dimensional images, but relies upon comparisons of statistical metrics such as two-point correlation or chord length distributions [4]. It is difficult to determine how close these metrics must match in order to obtain accurate predictions from simulations using the reconstructed geometries. Past experience has also shown that very fine features in substrate microstructures can have a large impact on model predictions. On the other hand, meaningful predictions for porous media also require that the domain be large enough to encompass a representative equivalent volume, or a volume large enough to average out media variations [5]. In order to address these issues, X-ray CT images were obtained for several DPF samples with voxel dimensions of approximately 1.5 microns. An example of one sample cross-section is shown in Figure 6. Geometries reconstructed from the CT data will be used for filter simulations, and the results will be compared to those using stochastic reconstructions. The data will also be used to help determine domain volume and spatial resolution required for accurate model predictions.

PNNL participates in CLEERS teleconferences, which occur at intervals of approximately one month, and coordinates the teleconferences which focus on DPF and selective catalytic reduction technology. Participants include original equipment manufacterers, universities, and other national laboratories. One benefit of hosting the monthly meeting has been the opportunity to receive feedback on the direction of specific CLEERS research activities at PNNL. In addition, presentations by various special speakers have sparked helpful and informative discussions on a variety of topics.

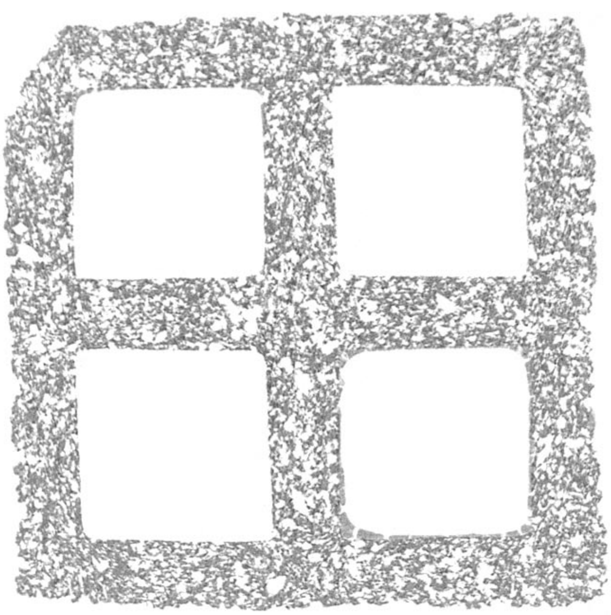

FIGURE 6. X-ray CT Image of Catalyzed Cordierite Microstructure

Conclusions

- Laboratory generated soot and aerosolized salt particles can provide controlled size distributions for fundamental filtration experiments.
- Filtration experiments with salt particles can be conducted with very good reproducibility.
- EDS may be used with filter samples loaded with salt particles in order to measure the degree of particulate penetration into filter walls.
- Pore-scale filtration simulations with realistic particle contact diameters yield efficiency trends which agree with experimental data.
- Three-dimensional CT scans can provide very detailed information about DPF structure.

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II.C.1 Variable Valve Actuation for Advanced Mode Diesel Combustion

Jeffrey Gutterman, PE
Delphi Corporation
5500 West Henrietta Rd.
PO Box 20366
Rochester, NY 14602-0366

DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Jason Conley

Subcontractor:
Electricore Inc., Valencia, CA

Objectives

- Develop an optimal, cost-effective, variable valve actuation (VVA) system for advanced low-temperature diesel combustion processes.
- Design and model alternative mechanical approaches and down-select for optimum design.
- Build and demonstrate a mechanism capable of application on running engines.

Accomplishments

- Confirmation that a single cam design did not have the required control flexibility to meet requirements.
- Three dual cam design concepts were developed and modeled.
- A dual cam design was selected from concept designs and all dynamic analyses were completed.
- An original equipment manufacturer (OEM) confirmed that the proposed dual cam design is a cost-effective and production feasible design.
- Package size was reduced to require minimal change to the OEM engine envelope.
- Advanced VVA math-based design process was introduced and design tools are now available for future modeling work.
- All of critical design analyses for high stress subcomponents including spring, bearings, gears and output rocker cam were completed.
- The mechanical actuator (cam phaser) development engineering work was completed and prints prepared.
- Cam phaser controller with proportional, integral, and derivative control capability built and tested.
- A single-cylinder device was built and installed on a free-running lab engine.
- The mechanism was tested on an engine test stand and demonstrated the capability of meeting all design requirements.
- The project was completed August 31, 2008.

Introduction

Our objective is to develop and demonstrate an optimal, cost-effective diesel VVA system for advanced, low-temperature combustion processes. Flexible control of the valve event is a significant enabler for advanced mode diesel combustion (AMDC). It is an essential factor in the control of the species and thermodynamic conditions for the combustion cycle. VVA is expected to expand the operating load and speed range of AMDC. It is also a potential tool for enhancing the effectiveness of aftertreatment catalysts. Thus, viable VVA technology is expected to help reduce the fuel consumption penalty related to extremely low emission standards.

Delphi Corporation has major manufacturing and product development and applied research and development (R&D) expertise in the valvetrain area. Historical R&D experience included the development of fully variable electro-hydraulic valvetrain on research engines as well as several generations of mechanical VVA systems for gasoline systems. A new mechanism was taken from concept stage through design, modeling, build and bench testing on a single-cylinder engine test stand.

Approach

Working with an OEM was critical to determine the mechanism motion requirement and system specifications. To speed development, significant time was spent using advanced design tools and simulations before building actual hardware. After modeling more than 200 variations of the mechanism it was determined that the single cam design did not have enough flexibility to satisfy three critical OEM requirements simultaneously, (maximum valve lift variation, intake valve opening timing and valve closing duration), and a new approach was deemed necessary.

Internal design reviews, including five with the OEM, were held and a dual-cam design was developed that had the flexibility to meet all motion requirements. The second cam added complexity to the mechanism however the cost was offset by the simplification of the actuator subsystem.

Once the design was dynamically simulated and the finite element analysis (FEA) was completed, single-cylinder hardware was built and installed on a free-running engine test stand to verify predicted performance.

The mechanism developed during the course of this investigation can be applied by OEMs to their advanced diesel engines with the ultimate goal of reducing emissions and improving fuel economy.

Results

Critical performance parameters were supplied by an OEM that had to be met before the mechanism could be applied to their engine. The previously detailed design was a single-cam device that appeared to have the potential to meet all the requirements. However, after more than 200 design iterations it became apparent that it was not possible to simultaneously meet all three critical performance requirements. The OEM wanted the intake valve opening timing to remain constant while the intake valve closing was varied more than 60 crank degrees (30 cam degrees). Simultaneously, they wanted the maximum lift to vary no more than 0.5 mm over the same range.

Maximum valve lift varied by as much as 1 mm over the entire range of valve timing thus exceeding the OEM's requirement of less than 0.5 mm. Alternative design approaches were developed to insure that the base mechanism had no variation in maximum valve lift over the entire range.

Three design approaches were proposed and detailed as shown in Figure 1.

Multiple design reviews were held and after evaluating the merits and demerits of each configuration, Design "A" was selected as the preferred approach. While a second cam was added, the mechanism allowed us to eliminate the electric motor actuator required for the single cam mechanism. Figure 2 shows an isometric view of the Design "A" herein called continuously variable valve duration (CVVD).

Once all modeling was completed the components were detailed and hardware built. Hardware was then installed on the engine stand and full dynamic testing at varying speeds and loads was performed.

FEA predicted opening cam deflection to be greater than closing cam deflection. Deflection would be at a minimum during the critical transition from opening to closing cam. The design intent was for a small step-down in lift (preferred to a step-up) at this critical transition. FEA predicted an undesirable step-up at this transition. Consideration was given to modifications to either the opening and/or closing cams in order eliminate the step-up condition. The design team chose to base cam modifications on measured test data due to the status of hardware delivery and the uncertainty of FEA predicted deflection. Data from initial testing, Figure 3, showed a step-up of approximately 0.350 mm.

Modifications were made to the opening vs. the closing cam in order to maintain maximum lift. The new cam was delivered, tested and found to only improve the

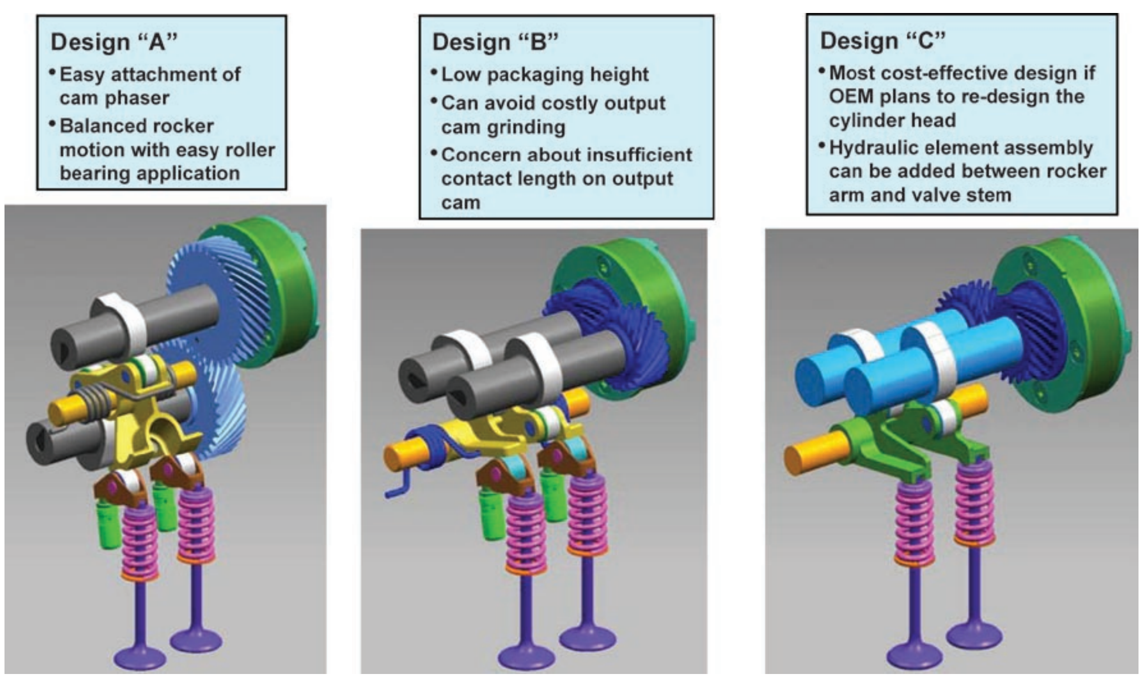

FIGURE 1. Representations of Three Design Approaches

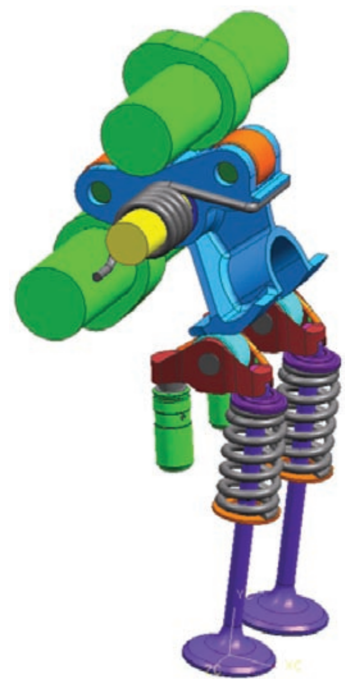

FIGURE 2. Selected Design "A" Continuously Variable Valve Duration

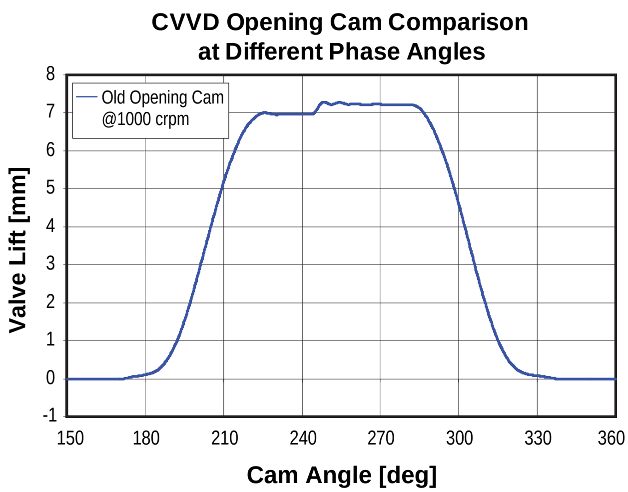

FIGURE 3. Initial Hardware Test Data Showing 0.350 mm Step-Up Transition

step-up condition. Test results on the modified opening cam, Figure 4, showed a significantly reduced step-up of 0.070 mm vs. the initial measurement of 0.350 mm.

Hardware testing indicated the transition from opening to closing cam was primarily caused by shaft deflection. Testing of second generation hardware with altered opening cam profile improved but did not eliminate the 'step-up' condition that occurs as the cam follower transitions from opening to closing cam.

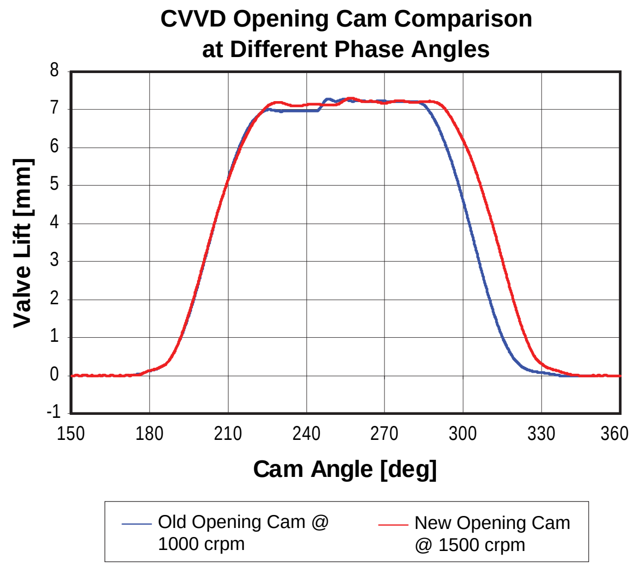

FIGURE 4. Step-Up Comparison of Initial Hardware vs. Modified Opening Cam

FEA stiffness analysis was performed and new parts were built to minimize the deflection. This hardware was tested with more improvements over previous test hardware. New hardware did not completely eliminate the step-up condition at all operating conditions. A separate design was developed in parallel (currently referred to as LM-CVVD for lost motion continuously variable valve lift) to solve the step-up condition. The LM-CVVD design eliminated the discontinuity that occurs as the cam follow transitions from opening to closing cam by maintaining follower to cam contact at all times.

The LM-CVVD design, shown in Figure 5, employs an opening and closing cam, each acting on a needle bearing follower mounted to a common output cam. Opening and closing cams are commonly referred to as input cams as they provide the oscillatory motion to the output cam. The output cam contains a third cam surface that acts through a conventional roller finger follower to provide valve lift by converting oscillatory motion provided by input cams.

Geometry for the LM-CVVD demonstration fixture was created through multiple analysis loops aimed to optimize peak loads, pressure angles, packaging, and required cam phasing authority in order to achieve required valve duration profiles and eliminate the transition steps seen in previous designs.

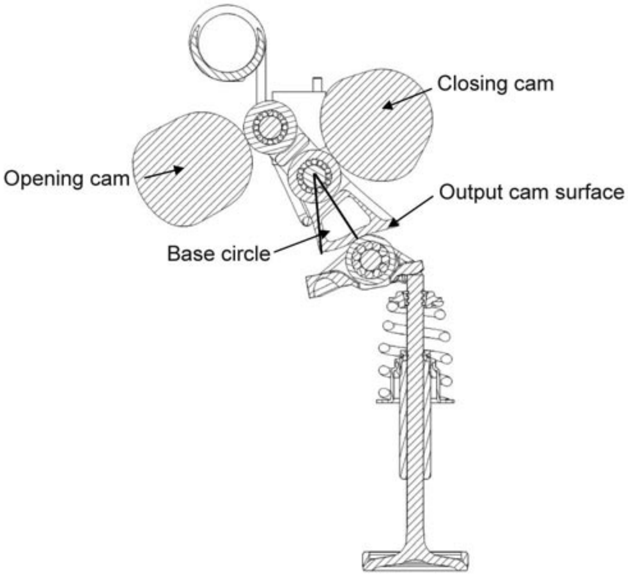

FIGURE 5. Lost Motion CVVD Design

Conclusions

- The overall design approach of the LM-CVVD mechanism satisfies the OEM's control and durability requirements.
- Design proposals to address the step-up condition in valve motion at the cam transitions point were completed and tested.
- Latest design improves but does not eliminate the step-up condition which is currently considered to be a dynamics concern.
- Valvetrain dynamic testing indicates operation consistent with typical production valvetrain systems.
- Valvetrain power consumption due to added bearings and related components is similar or slightly higher than conventional valvetrain systems.
- It is possible to achieve a smooth transition from opening to closing cams.
- However, new designs must be considered as an integral part of the engine and head assembly.
- The LM-CVVD design is a more robust configuration and will eliminate the transition discontinuity over a wider range of operation.

FY 2008 Publications/Presentations

1. DOE Vehicle Technologies Program Merit Review.
2. Design reviews were held with OEMs.

Special Recognitions & Awards/Patents Issued

Provisional Patents submitted:

1. System for Continuously Varying Engine Valve Duration.
2. Continuously Variable Valve Actuation System.
3. Electro-hydraulically actuated Variable Valve Duration System.

II.C.2 Variable Compression Ratio Engine

Charles Mendler
Envera LLC
7 Millside Lane
Mill Valley, CA 94941

DOE Technology Development Manager:
Roland Gravel

NETL Program Manager: John Jason Conley

Objective

Phase I

- Design, build and bench-test a proof-of-concept variable compression ratio (VCR) actuator system.
- Optimize the actuator system where practical within the scope of Phase I funding.

Phase II

- Optimize the actuator hydro-mechanical design and its control system.
- Installation of existing VCR engine in mule vehicle.
- Test the VCR actuator system in a mule vehicle and demonstrate low-cost, fast response and mass production practicality.

Accomplishments

- Hydraulic pressures in the actuator system were reduced by 86% through system optimization. The reduction in pressure significantly relaxes the demands that will be placed on the hydraulic system and enables cost to be reduced.
- A test rig was designed and built for evaluating actuator response. Test results indicate that compression ratio can be reduced from 18:1 to 8.5:1 in ~0.35 seconds, and increased from 8.5:1 to 18:1 in ~0.70 seconds. On average 0.074 seconds is projected to elapse for each point increase in compression ratio.
- Finite element analysis (FEA) of the Envera production-intent 4-cylinder VCR engine was conducted. Modeling results indicate that the crankcase meets all stiffness, robustness and durability requirements for mass production.

Future Directions

- Optimize the hydro-mechanical system for improved performance and manufacturability.
- Installation of existing/optimized VCR engine in mule vehicle.
- Test the VCR actuator system in a mule vehicle and demonstrate low-cost, fast response and mass production practicality.

VCR Overview

VCR is an innovative technology for improving the fuel economy of engines used in passenger cars, sport utility vehicles (SUVs) and trucks.

VCR enables the compression ratio of the engine to be changed from a diesel-like value of approximately 18:1 during normal driving conditions to approximately 8.5:1 when the engine is generating high power levels with the aid of supercharging or turbocharging. The low compression ratio permits the engine's power output to be more than doubled.

Large gains in fuel economy can be attained by replacing a large naturally aspirated engine with a small turbocharged VCR engine of similar power and torque. In some cases fuel economy can be improved by more than 50% when a large V8 engine is replaced with a turbocharged 4-cylinder engine having the same power and torque as the V8. In Figure 1 the target efficiency of the Envera 4-cylinder VCR engine is compared to the efficiency of a 4.6L V8. Most of the fuel consumed by light-duty trucks and SUVs occurs at small power levels, as indicated by the blue step curve in Figure 1. The

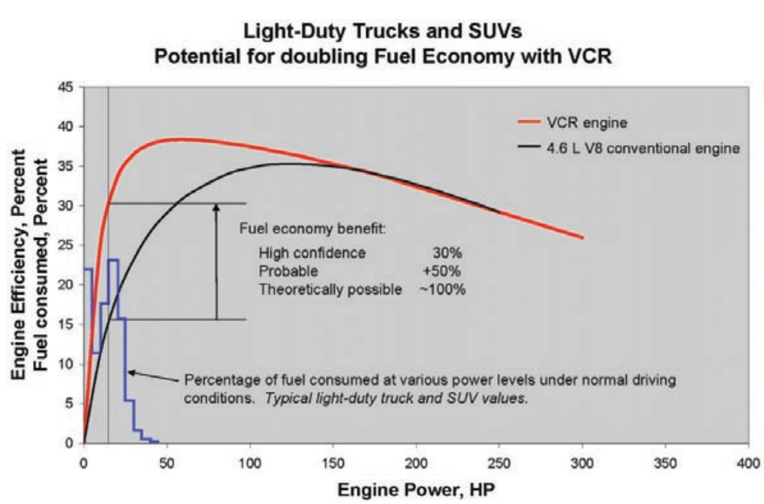

FIGURE 1. Efficiency of 4-Cylinder VCR Engine Compared to 4.6L V8

efficiency of the Envera VCR engine is double that of the V8 engine at 15 horsepower.

VCR enables turbocharged engines to attain significantly greater power levels by lowering compression ratio when the engine is under boost. Modern single and twin turbo technology provides high pressures rapidly and efficiently. Virtually all passenger car diesel engines sold in Europe are now turbocharged.

Table 1 compares the target power and torque values of the Evera 4-cylinder VCR engine to that of the Ford 4.6L V8, currently sold in the model year 2009 F-150 pickup truck. It can clearly be seen that the VCR 4-cylinder has greater power and torque than the Ford 4.6L V8.

TABLE 1. Power and Torque Compared to Ford 4.6L V8

	Power	Torque
Ford 4.6L V8	248 hp @ 4,750 rpm	294 ft lb @ 4,000 rpm
Envera VCR 4-cylinder	320 hp @ 6,000 rpm 280 hp @ 4,750 rpm	320 ft lb @ 4,000 rpm

Attaining high power levels from a small engine requires a robust VCR mechanism. Envera's VCR mechanism is exceptionally robust and reliable. Envera's VCR mechanism can support engine speeds of over 8,000 rpm. Envera's VCR mechanism has a low manufacturing cost.

At light power levels the Envera VCR engine operates at the same compression ratio setting as diesel engines, and attains similar in-cylinder combustion efficiency. The Envera VCR engine, however, has lower internal frictional losses than the diesel. The net result is that in some cases the Envera VCR engine can return higher efficiency and much greater power than a diesel engine of the same size (e.g., the same displacement). When downsizing is used, VCR engines return significantly greater fuel economy benefits.

When the benefits of improved engine efficiency attained using VCR are combined with other fuel saving technologies (hybrid drive, reduced vehicle weight, aerodynamics) the fuel economy of some light-duty trucks could be doubled.

Introduction

The current DOE/National Energy Technology Laboratory/Envera effort is directed towards reducing VCR system cost and providing a fast actuator response. The technology has three main cost areas: the VCR mechanism; the actuator system for adjusting compression ratio; and the supercharging or turbocharging hardware.

The Envera VCR mechanism comprises an eccentric carrier that holds the crankshaft of the engine. Pivoting of the eccentric carrier raises and lowers the crankshaft relative to the engine's cylinder head, and adjusts engine compression ratio. The Envera VCR eccentric carrier presently has a low cost.

A hydraulic actuator system is used to pivot the eccentric carrier. The current effort is directed towards reducing the cost of the actuator system and providing a fast actuator response. Another goal is to provide a durable compact VCR actuator design.

Prior to Phase I contract award Envera anticipated that actuator response and cost would be optimized primarily through hydraulic control circuit system design and computer software. The results of Phase I have shown, however, that hydraulic cylinder sizing and mechanical design changes are of primary importance for attaining project and commercialization objectives. Specifically, hydro-mechanical design changes realized in Phase I have resulted in an 86% reduction in projected peak hydraulic system pressure. The lower pressure will enable a simpler more robust hydraulic control circuit system to be used. In consideration of the performance gains realized in Phase I of the initiative, work is currently focused on hydro-mechanical design, system hardware, and low-cost packaging within the crankcase. The hydraulic cylinder is located vertically adjacent to engine cylinder bore 3 to provide a compact and stiff crankcase. Later in the project the optimized hardware will be procured and vehicle tested.

Approach

The current effort is directed towards the development of the actuator used for adjusting the pivot angle of the eccentric carrier. Development goals include low-cost and a fast response. At the beginning of the project mechanical loading on the VCR eccentric carrier and hydraulic system were evaluated using:

ProEngineer Wildfire 2.0	Part and mechanism assembly
MDO Extension	Dynamic force analysis
GTPower	Gas force on the piston (Prior data)
Origin 7.5	Data conversion

Dynamic loads were modeled at five conditions, from 2,000 rpm 4 bar bmep to 6,000 rpm 12 bar bmep. The 2,000 rpm 12 bar bmep condition causes the highest loading on the hydraulic system of about 2,250 psi. In Phase I of the project Envera pursued reducing the size of the hydraulic pressure spikes through system optimization. Through this effort peak hydraulic pressures have now been reduced to an estimated 314 psi, an 86 percent reduction in peak pressure. This reduction in peak pressure is a huge improvement.

A test rig was designed and built for evaluating actuator response. Test results indicate that compression ratio can be reduced from 18:1 to 8.5:1 in ~0.35 seconds, and increased from 8.5:1 to 18:1 in ~0.70 seconds. On average 0.074 seconds is projected to elapse for each point increase in compression ratio.

In consideration of the performance gains realized through geometry optimization, development work was focused on hydro-mechanical design, system hardware, and low-cost packaging within the crankcase. Figure 2 shows an Envera crankcase with integrated hydraulic actuator.

Envera ran FEA of the crankcase/cylinder head assembly. The analysis was performed using ProEngineer Mechanica software and high-performance quad-core hardware. Simulation run time was approximately 54 hours. Results were excellent. bottom-end structure is sound and stiff.

With success of the FEA, Envera anticipates using the new crankcase on the current project. The decision on whether or not to use the new crankcase will be made after successful cast, machine and assembly of the new crankcase. If problems are encountered Envera will continue with the current plan of using the existing modified Mercedes M271 VCR engine crankcase. The feasibility assessment of the new crankcase also included production of the machine drawings. The machine drawings show that the new crankcase can be mass produced using tolerances and machining operations that are compatible with low-cost mass production.

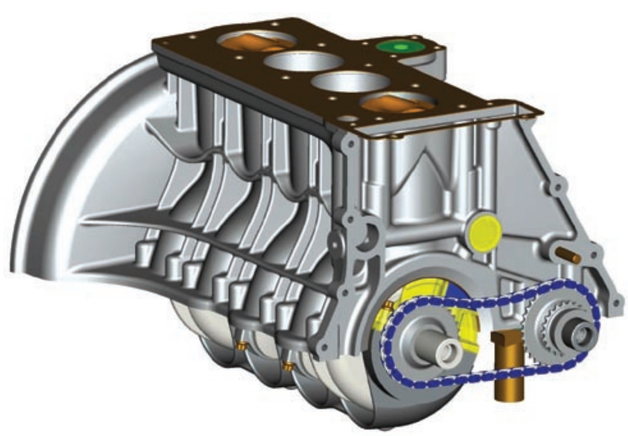

FIGURE 2. VCR Crankcase, with Hydraulic Cylinder Located Vertically next to the 3rd Engine Cylinder

Envera is currently exploring the possibility of fueling the VCR engine on compressed natural gas (CNG). There is commercial interest in CNG-fueled engines in California.

Results

Hydraulic pressures in the actuator system were reduced by 86% through system optimization. The reduction in pressure significantly relaxes the demands that will be placed on the hydraulic system and enables cost to be reduced.

A test rig was designed and built for evaluating actuator response. Test results indicate that compression ratio can be reduced from 18:1 to 8.5:1 in ~0.35 seconds, and increased from 8.5:1 to 18:1 in ~0.70 seconds. On average 0.074 seconds is projected to elapse for each point increase in compression ratio.

Conclusions

- During Phase I of the project hydraulic pressures in the actuator system were reduced by 86% through system optimization. The reduction in pressure will significantly relax the demands placed on the hydraulic actuator system.
- The fuel economy of some light-duty trucks and SUVs can be improved by over 50% with down-sized gasoline turbo-VCR engines. Stringent tail-pipe emission standards can be attained using proven catalytic converter technology. The spark-ignited VCR engine can be operated on alternative fuels such as CNG, ethanol, propane and others.
- FEA of the Envera production-intent 4-cylinder VCR engine was conducted. Modeling results indicate that the crankcase meets all stiffness, robustness and durability requirements for mass production.

II.C.3 Application of Wide Spectrum Voltammetric Sensors to Exhaust NOx Measurement

Dr. Michael Vogt
Streamline Automation, LLC
3100 Fresh Way SW
Huntsville, AL 35805

DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Aaron Yocum

Subcontractor:
University of Alabama, Tuscaloosa, AL

Objectives

- Develop engine exhaust NOx sensing element based upon gas-phase voltammetry measurement technique.
- Optimize real-time instrumentation for continuous voltammetry monitoring.
- Instrument test engine with experimental voltammetric NOx sensor.
- Demonstrate experimental sensor by gathering simultaneous data along with representative commercial NOx sensors and analyzers.

Accomplishments

The effort of the first and second quarters focused on designing and developing fabrication methods for a new NOx sensing element – one suitable for deployment in an engine exhaust stream. The investigation and effort of the third and fourth quarters focused on the design and fabrication of a miniature real-time support instrument (electronics) to couple with the new sensing element. The new instrumentation was similar enough to the core instrumentation being used for parallel defense investigations that significant cost sharing was realized and the NOx project effort was reduced. The accomplishments are as follows:

- Redesigned voltammetric NOx sensor DIP8 form factor to fit commercial/industrial fabrication process.
- Developed new fabrication method for ZrO_3 sensors.
- Developed new high-temperature lead attachment method for sensors, demonstrated on DIP8 sensors.
- Developed new multi-lithic (multiple substrate) NOx sensor design and deployment package for engine exhaust systems.
- Designed and fabricated new miniature real-time electronics support instrumentation package – to make retrofitting to existing engine controllers easier.
- Support instrumentation verification and validation in-progress.
- On-engine installation and characterization plan under development.

Future Directions

The verification and validation of the new instrument will be completed in the next quarter, and a plan for installing it and testing alongside commercial analyzers is planned. Modifications to the original calibration vs. a gas chromatograph will allow effort and time to install the new sensor on an experimental diesel engine to begin to gather real-time NOx emissions results. Bulleted description of tasks are as follows:

- Complete verification and validation of latest sensor and instrument.
- Order and secure new diesel test engine.
- Instrument test engine with verified voltammetric gas microsensor(s).
- Compare and evaluate performance against existing NOx analyzers and measurement instruments.
- Deliver example prototype sensors to Robert Bosch for commercial partner evaluation.

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Introduction

The goal of this investigation was to produce a workable nitrogen oxide (NO_2, NO, N_2O => NOx) sensor for use in diesel engine exhaust systems. The sensor would provide stable wide-band NOx concentration readings in real-time and allow for feedback to potential NOx control systems. The project focused on updating an existing experimental microsensor that came from the Department of Energy's Argonne National Laboratory. That microsensor was an all-ceramic-metallic (cermet) device which employed a new measurement technique called *gas-phase voltammetry*. The original laboratory device had been demonstrated to respond to NOx at the concentrations anticipated, but was in a form factor unsuitable for deployment in a combustion engine exhaust stream. The support electronics also were large and bench-scaled. The sensor needed to be converted to a design suitable for harsh engine environments, and the electronics needed to be miniaturized and made suitable for integration into experimental control systems. When completed, the new device would be operated on test engines, side-by-side with existing commercial NOx analyzers and measurement equipment to evaluate its performance.

Approach

The effort was divided into three stages – *sensing element redesign*, *electronic instrumentation miniaturization*, and *on-engine evaluation*. The first and second stages were both 95% completed in this first project year, and will be completed early in the next. The third stage will begin and be completed in the next project year – as the new instrumentation is available.

The sensor redesign involved changing the shape and packaging of the gas-phase voltammetry sensing element. The new design is intentionally matched to existing commercial sensors from Robert Bosch Company. The sensing phenomenon is completely different from what their own experimental NOx sensors used, but the outside shape could be made the same so as to attract the attention of their new product development research and development (R&D) laboratory. The new sensor design continues to utilize thick-film fabrication technology, but has changed the shape of the device to allow access to outside air as a reference gas. The new package also duplicates the mounting threads and space envelope of the commercial Bosch devices to allow easy interfacing. This work is 95% complete. Sensing elements have been made, and are awaiting final mounting inside of a metal housing; then they will be ready for chemical testing on a test engine.

The support electronics involved having an entirely new circuit board designed and fabricated that could use available engine electric power and implement the gas-phase voltammetry measurement methodology. There were significant challenges to overcome in miniaturizing the existing electronics, so there was significant cost sharing with other projects to produce a universal core instrument. A working prototype was delivered to our project staff in late Fiscal Year 2008, and updated in early FY 2009. The new instrument is ready and awaiting the packaged sensor to allow calibration efforts to be performed under laboratory conditions. The testing and evaluation protocols have been defined, and a new engine test plan is being drafted.

Results

The construction of the new gas-phase voltammetric NOx sensor is based upon what Streamline calls the XLSIP4 form factor (Figure 1). This is eXtra-Long Single In-line Package, with four leads (conductors). The dimensions were modeled after the Bosch LSU4 P/N 15733 Universal Planar-type Oxygen Sensor, and were intended to be easily adoptable by Bosch for packaging. The NOx sensor was a "sandwich" composed of three layers, the sensing layer, the back cover layer, and a channel layer separating the sensing and cover (Figures 2, 3, and 4). An electrolyte paste was screen-printed in between each layer and fired to cement the layers together into a durable flat device with a narrow channel running nearly all the length internally. The sensing layer had two electrodes, one on either face, and a heating element that spanned both

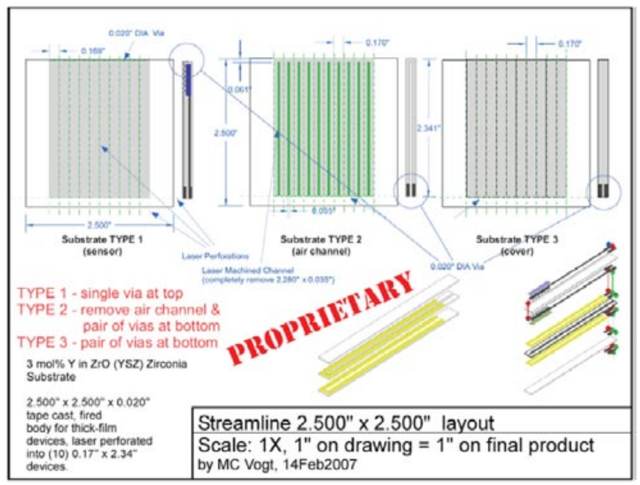

FIGURE 1. Streamline Automation XLSIP4 Voltammetric NOx Sensor

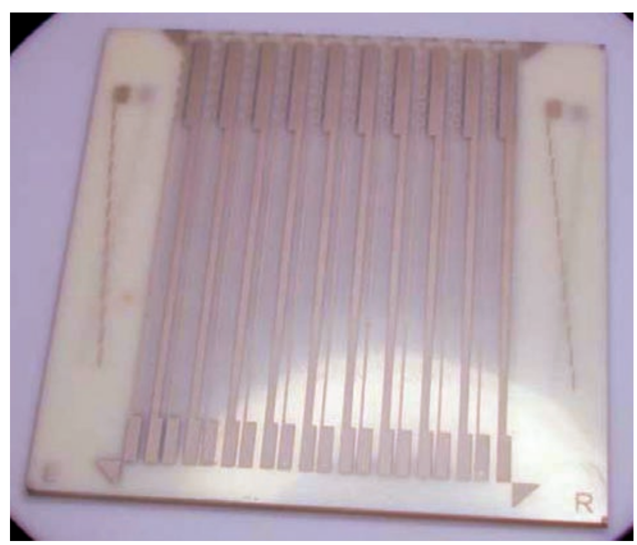

FIGURE 2. Sensing Layer Front Side

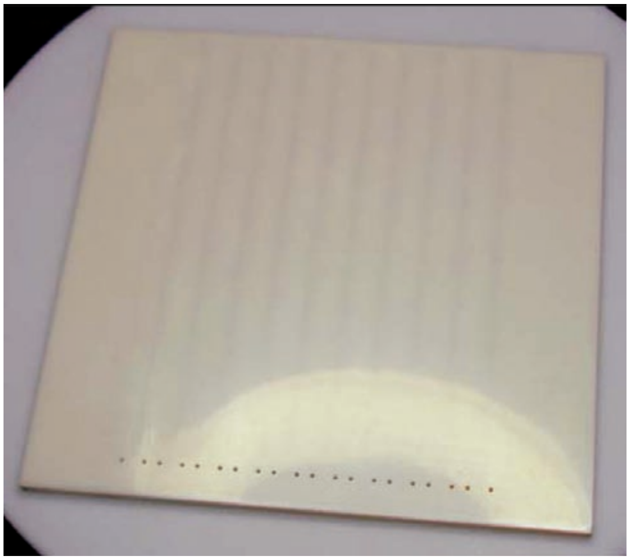

FIGURE 3. Back Cover Layer Back Side

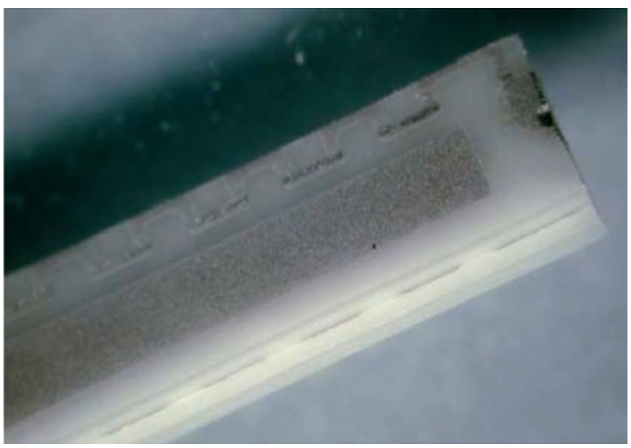

FIGURE 4. Sensor Sandwich and Cross-Over Short

faces (Figure 5). The channel provided a conduit for exposing one electrode face to the outside atmosphere as reference.

Several attempts were made before a high-quality all yttria tetragonal zirconia polycrystal (YTZP) sandwich was fired into a usable fabrication substrate. It was singulated (diced) into individual sensing elements ready for packaging.

Alternative approaches to using the smooth YTZP substrates are being explored. The same lithography and geometry can be used, but different substrates prepared – ones that either roughen up the YTZP surface (using a diamond pad) or by impregnating an Al_2O_3 substrate with yttria-stablized zirconia material through a grid of fine holes bored through the substrate by the manufacturer.

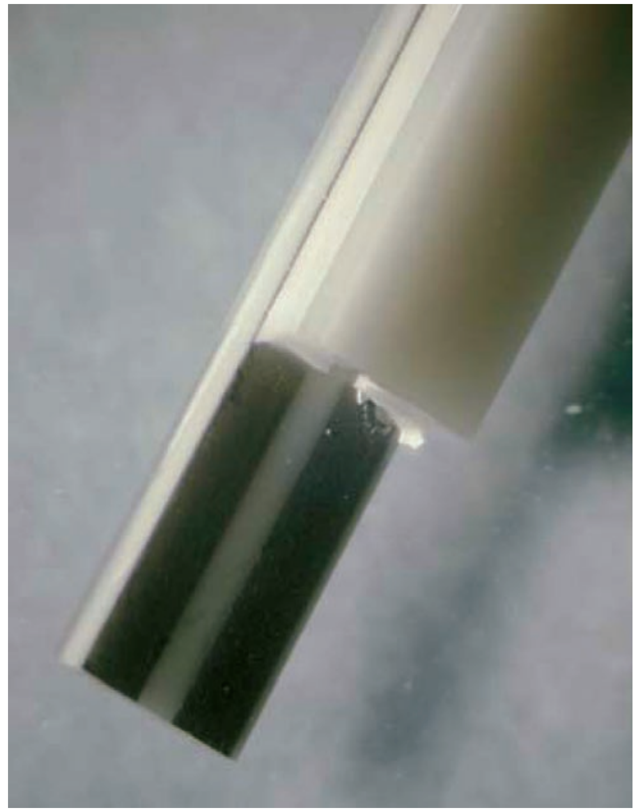

FIGURE 5. Sensor Sandwich 4-Conductor Electrode End

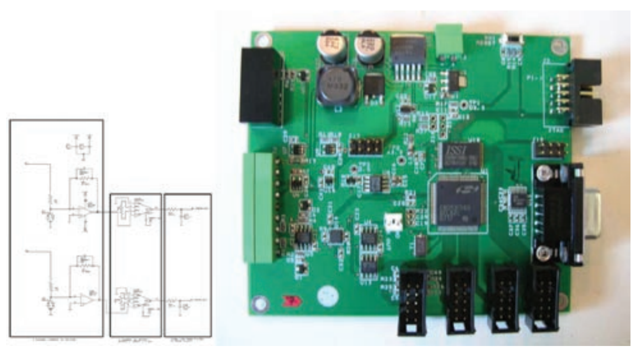

FIGURE 6. NO_XPod Module 1034 Circuit Board with Microcontroller

For this investigation, a specialized version of the Streamline core ChemPod gas-phase voltammetry measurement and support electronics was designed, and designated “NO_XPod”. The development and refinement of a satisfactory NO_XPod Module is a requirement for any additional work to develop a NOx sensor. The underlying gas-voltammetry operations must be fully-stabilized and predictable before installing the experimental sensor on-board a test engine. During July and August 2008, new NO_XPod main circuit boards were completed (Figure 6). There were flaws in the boards caused by vendor fabrication errors. Some of these flaws were very difficult to track down and correct, some were more obvious. All caused significant delays to the R&D effort and were beyond the control of the project staff to predict. When the Rev0 boards were corrected and working, the NO_XPod control software continued to be verified and along with verifying operation of components. Some experimentation was required before the boards were operational and the remainder of the NO_XPod/control software verification could be completed. When the 1034 boards were corrected, additional status light emitting diodes (LEDs) were also interfaced to form a simple but effective user-interface to the NO_XPod Module. Status LEDs showed the instantaneous condition of the foreground sensor conditioning and data management code, the background voltammetry and chemometrics code, and what gases the sensor was being exposed to. The final NO_XPod module was mounted inside an acrylonitrile butadiene styrene plastic housing produced using Stratasys/REDEYERPM rapid prototyping service.

The NO_XPod provides communications and potentiostat interface, and supports gas-phase voltammetry measurements and interfacing to the NOx sensor and test engine management system.

Conclusions

The new sensor and electronic instrumentation is now ready for laboratory and on-engine testing. The measurement performance and environmental durability will both be monitored as part of the evaluation. Final conclusions as to the effectiveness of the gas-phase voltammetry method for NOx detection in engine conditions will be addressed when that evaluation is completed.

II.C.4 Advanced Start of Combustion Sensor – Phase II: Pre-Production Prototyping

Chad Smutzer (Primary Contact) and
Dr. Robert Wilson
TIAX LLC
15 Acorn Park
Cambridge, MA 02140

DOE Technology Development Manager:
Roland Gravel

Subcontractor:
Wayne State University, Detroit, MI

Objectives

- Develop an accelerometer-based start of combustion (SOC) sensor which provides adequate SOC event capture to control a homogeneous charge compression ignition (HCCI) engine in a feedback loop.
- Ensure that the developed sensor system will meet cost, durability, and software efficiency (speed) targets.
- The Phase II objective is to have a pre-production prototype.

Accomplishments

- Three engines of same model line/different serial number installed and tested to verify engine-to-engine repeatability of the SOC sensor system (a potential drawback of accelerometer-based systems), including two dynamometer setups and one vehicle setup.
- An initial real-time version of the SOC algorithm has been developed to optimize the algorithm for accuracy and processing speed.
- Data over the operating range of interest (the expected HCCI engine operating envelope of low to medium speed, low to medium load) has been recorded.

Future Directions

- Low-temperature engine combustion will be tested to evaluate the sensor for HCCI engine operation (current data has been measured in diesel mode).
- The real-time SOC algorithm will be optimized for speed and accuracy.

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Introduction

HCCI has elevated the need for SOC sensors. HCCI engines have been the exciting focus of engine research recently, primarily because HCCI offers higher thermal efficiency than the conventional spark ignition engines and significantly lower oxides of nitrogen (NOx) and soot emissions than conventional compression ignition engines. HCCI has the potential to combine the best features of internal combustion engine technology to achieve high-efficiency and low-emission goals. However, these advantages do not come easily. It is well known now that the problems encountered with HCCI combustion center on the difficulty of controlling the start of combustion. The emergence of a durable and effective SOC sensor will solve what is arguably the most critical challenge to the viability of HCCI engine platforms. The SOC sensor could be an enabler for a new breed of engines saving 15-20% of petroleum used in transportation, while meeting or exceeding 2010 emission targets.

Approach

The objective of the Phase II research is to refine the design of the SOC sensor and algorithm into a production-ready prototype and position it for hand-off to a commercialization partner. The Phase II research will identify any potential soft spots in the algorithm and allow the team to implement and test a solution. During the Phase II effort, the team will work to make sure the processing code efficiency (response time of control system) is rapid enough that control decisions may be made and implemented. The interface with the HCCI actuation/control mechanism (variable valve actuation, fuel injection, etc.) must be rapid and robust enough to allow the control mechanisms an opportunity to change engine conditions, so as to effectively manage short transients. Phase II efforts will ensure this is the case.

Results

During Phase I of the project, data was gathered from the test engine in the vehicle and the Wayne State University engine test setup to prove the feasibility and repeatability of the SOC algorithm for select operating points. As Phase I transitioned into Phase II, the algorithm was coded to run on a real-time platform. As the second phase of the project continues, further data is actively being recorded to ensure algorithm accuracy and robustness over low to medium speed and low to medium load engine operation. Figure 1 shows the three test platforms.

Engine Test Setup at TIAX

Wayne State University Engine Test Setup

Test Engine in Vehicle

FIGURE 1. Photographs of the three engine test setups (same engine model, different serial numbers) designed to test engine-to-engine repeatability of the sensor system.

Since the effectiveness and robustness of the accelerometer-based sensor system depends on its ability to work across multiple engine blocks, installation and testing of these three similar engines was a key accomplishment.

The algorithm developed has shown promise for the detection of the SOC. Shown in Figure 2 is the pressure trace (the top plot) during the same time period as two accelerometer traces (the bottom two plots). The red circle on the pressure trace shows the calculated SOC based upon the industry standard practice of heat release analysis (an off-line laboratory approach for combustion analysis). This circle is also shown on the raw accelerometer trace next to a green circle, which is the SOC determined independently from the algorithm analyzing the accelerometer trace. The agreement between the two methods is very good, as may be seen from their close proximity.

Conclusions

- Three engine setups are being used to determine engine-to-engine repeatability of the sensor/ algorithm system, and progress to date is encouraging.
- The algorithm is being coded in a real-time embodiment and undergoing testing.
- Low-temperature combustion work will enhance the work done to date with diesel SOC detection.

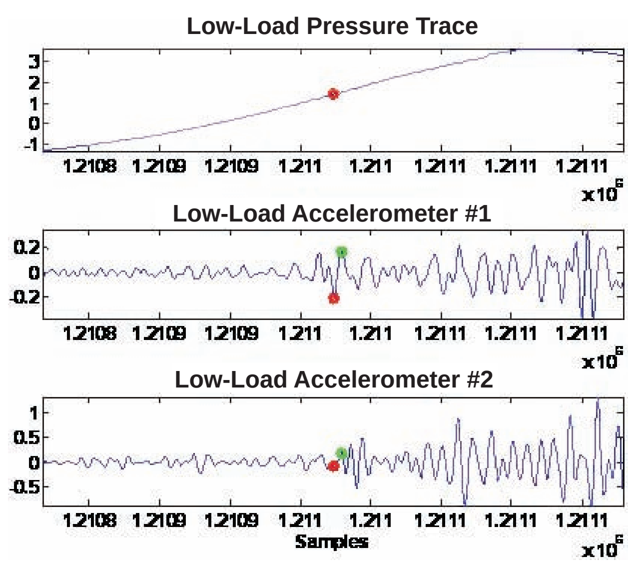

FIGURE 2. Comparison of the identification of the on-line start of combustion using the developed algorithm with the offline research-level approach.

II.C.5 The Development of a Robust Accelerometer-Based Start of Combustion Sensing System

David Mumford (Primary Contact), Jim Huang
Westport Power, Inc
1691 West 75th Ave.
Vancouver, BC V6P 6P2
Canada

DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Jason Conley

Objectives

- Development of an accelerometer-based start-of-combustion (SOC) sensing system.
- Develop a method to minimize sensor-to-sensor variation for the accelerometer-based SOC sensing system.

Accomplishments

- Exceeded initial target to achieve sensor-to-sensor variation of 0.5 crank angle degree (CA°). The average sensor-to-sensor variation over all modes has been reduced to 0.36 CA° with 98.9% confidence level.
- Exceeded the initial target to achieve total error of measured SOC timing of 0.5 CA°. The mode-averaged total error (based on one standard deviation) was reduced to 0.41 CA°.
- Extended the capability of the accelerometer-based combustion sensing system to capture not only the SOC timing but also the complete in-cylinder pressure trace.

Future Directions

- Demonstrate the accuracy of the current accelerometer-based combustion sensing system on a light-duty Cummins ISB engine.
- Demonstrate the accuracy of the current accelerometer-based combustion sensing system on a heavy-duty Cummins ISX HPDI engine.
- Demonstrate the accuracy of the current accelerometer-based combustion sensing system onboard a Class-8 truck with a Cummins ISX engine.

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Introduction

The development of modern combustion systems increasingly relies on detailed knowledge of the combustion event. As the limits of combustion are approached, tight control of combustion leads to improved emissions and higher efficiencies, while retaining and even improving engine reliability and durability.

While developing a novel homogeneous charge compression ignition (HCCI) technology for large natural gas engines, Westport found that there was no reliable cost-effective technology to monitor the combustion event. As a result, Westport began to develop a solution based on commercially-available knock sensors. While initially developed around HCCI, Westport has identified that numerous other forms of combustion (high exhaust gas recirculation [EGR] systems, homogeneous charge direct injection, etc) will require combustion sensors. This requirement is also reflected in the development of other technologies in this field. However, the potential low system cost and the lack of intrusion into the cylinder head area are significant benefits for the Westport approach.

Previous work by Westport has proven the method on two different large compression ignition gas engines. The objective of the current work is to improve robustness of this technology; particularly, to identify and reduce the sensor-to-sensor variations.

Approach

Experimental study has been carried out on a Cummins ISB 5.9L HPCR diesel engine. Accelerometer (knock sensor) data were collected under 6 of 13 European Stationary Cycle (ESC) testing modes, which cover a wide range of engine loads and speeds. After obtaining the initial signal from the sensors, physical models that describe the correlation between the sensor signal and in-cylinder pressure change were established. An algorithm was developed based on these models to obtain the timing for the SOC using the data from the accelerometers. This timing was compared with the SOC determined from the in-cylinder pressure measurement.

To further explore the potential of the sensing system, another algorithm was developed to reconstruct the in-cylinder pressure and heat release rate from the raw knock sensor data. The algorithm allows in situ compensation of sensor-to-sensor variation as well as variation of sensitivity over a wide range of operating conditions; the algorithm also compensates for variations in dynamic response of the sensors.

Results

Data have been collected using two sets of Siemens knock sensors with integrated cables on an ISB325 HPCR diesel engine. Engine tests were carried out at 6 of the 13 ESC modes covering a relatively wide range of engine operating conditions. The test conditions are summarized in Table 1. At each mode, a three-point SOC timing swing (with advanced, nominal and retarded timing) was performed by varying the diesel injection timing. For each test mode and timing, two injection pressures were used to simulate normal and "soft" combustion. The purpose of varying injection pressure is to examine the capability of the current sensor configuration and processing method for capturing the SOC with high EGR combustion. Since the current ISB engine is not equipped with an EGR system, we used reduced injection pressure to achieve the lower peak heat release rate and prolonged the combustion duration similar to high EGR combustion.

A second model of Siemens knock sensor (with integrated connector) was also tested on the same engine. It was found that the signal from this sensor model is significantly different from the previous model under identical engine operating conditions. In particular, the high frequency oscillation associated with the ignition observed in the signal from the previous sensor model was not present in this model. As a result, the SOC sensing method developed with the first model could not be applied to the second model, which required a different approach for signal processing.

TABLE 1. Engine Test Modes

ESC Mode	% Load	Torque (Nm)	RPM	Power (BHP)	SOI[1]
5	50	305	1,885	109	a, n, r
6	75	457.5	1,885	164	a, n, r
8	100	610	2,292	266	a, n, r
9	25	152.5	2,292	67	a, n, r
12	75	457.5	2,698	235	a, n, r
13	50	305	2,698	157	a, n, r

[1] Start of Injection: advanced, nominal, retarded

The knock sensor data from the ISB testing are distinct from those of the previous study on the larger ISX engines. In particular, the knock sensor signal shows high frequency oscillations with significant magnitude at the SOC, whereas previous studies with ISX engines showed predominantly low-frequency signals. This is probably due to a lower structural stiffness of the smaller ISB engines when compared with the larger ISX engines. Analysis of the high-frequency signal established the reproducibility of a characteristic frequency between the engines. It was decided that both the high and low frequency signals should be used in the current work as independent measures for determining SOC.

There are three main steps to the processing algorithm:

- pre-process the raw accelerometer data;
- extract SOC information from the accelerometer signals; and
- select the SOC timing with the highest confidence level.

First, the raw accelerometer data is manipulated to increase the combustion signal-to-noise ratio. Standard finite impulse response filters were applied to the raw accelerometer signal to reduce noise. Both the high and low frequency signals were extracted using filters with different bands. The phase shift among different ignition timings was observed in the high-frequency, low-frequency and reconstructed data, so attempts were made to extract the SOC from all of them and examine which one had the best correlation with the actual SOC measured from the in-cylinder pressure. A global method and a local method were used to obtain the phase shift of SOC from the calibration signal. Both methods can provide an independent SOC estimate, and the results were crosschecked with each other to improve the reliability.

A set of data were acquired at a number of engine operating modes to determine how well the accelerometer-based system could measure the SOC. These data include SOC timing swings at advanced, nominal, and slow combustion rates to test SOC detection at the widest expected range of heat release rates. Figure 1 shows a global correlation between the measured and actual SOC from all test points.

Figure 2 shows the total error (standard deviation) for individual modes. It can be seen that the total error was significantly lower than the 0.5 degree target for all modes. The total error averaged over all modes is 0.41 CA°.

The engine-to-engine variability was modeled as the reproducibility of the measurement system. For most modes, the variability is significantly less than 0.5 CA°. The results are also shown graphically in Figure 3. The average sensor-to-sensor variability with 98.9% confidence level is 0.36 degrees, which meets the 0.5 degree target. Thus the conclusion was drawn that the current accelerometer method can meet the performance requirement for SOC detection.

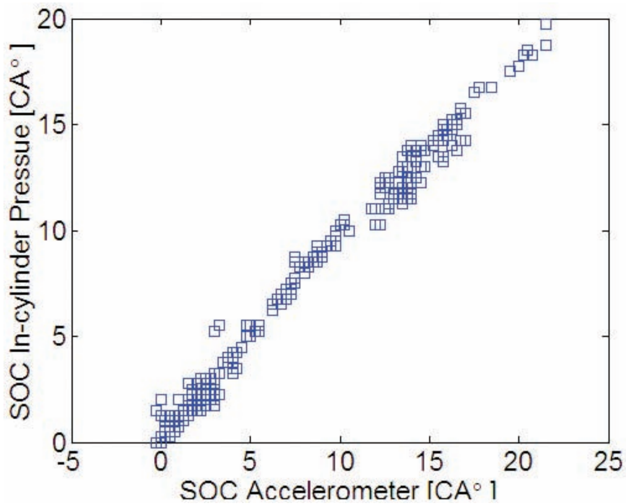

FIGURE 1. Comparison of SOC Determined from Knock Sensor Signal with In-Cylinder Pressure SOC

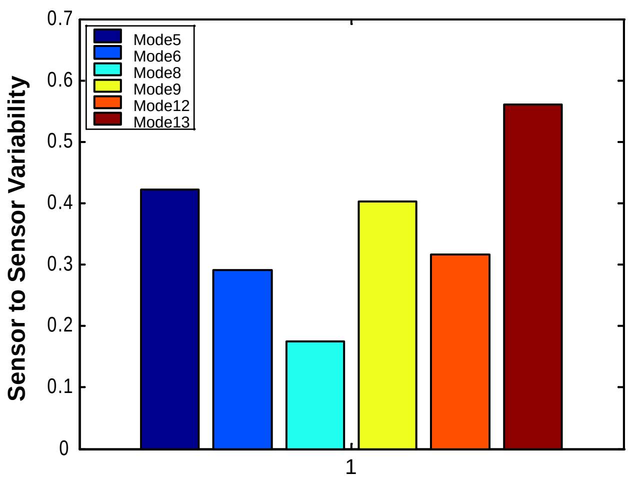

FIGURE 2. Mean Sensor-to-Sensor Variability based on Two Sets of Siemens Knock Sensors (3σ – 0.36 °CA)

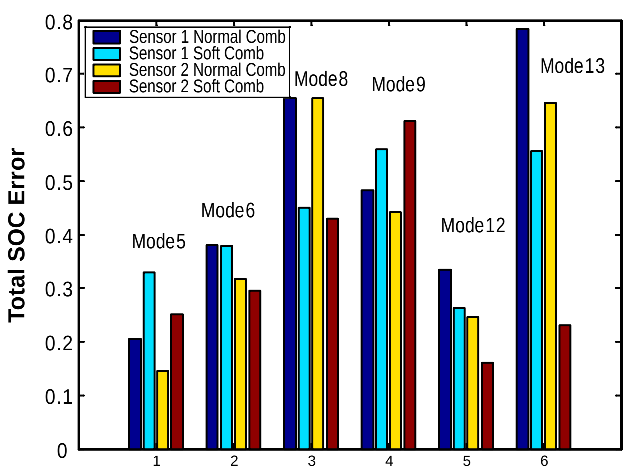

FIGURE 3. Mean SOC Error (1σ – 0.41 °CA)

An algorithm was also developed to reconstruct the in-cylinder pressure and heat release rate from the raw knock sensor signal. The algorithm allows in situ compensation of sensor-to-sensor variation as well as variation of sensitivity over different operating points; the algorithm also compensates for decay in the signal due to the dynamic response of the sensors. Figure 4 shows a comparison of in-cylinder pressure from a research grade in-cylinder pressure sensor and a knock sensor mounted on one of the two adjacent bearing caps. It can be seen that good agreement is achieved between the reconstructed and the actual pressure data.

Summary

- A knock sensor based combustion sensing technology has been developed. Engine test results shows that the system easily meets the initial target of 0.5 degree sensor-to-sensor variation. The average sensor-to-sensor variation over all modes is reduced to 0.36 CA° with 98.9% confidence level.
- The system has exceeded the initial target to achieve total error of measured SOC timing of 0.5 degree. The mode-averaged total error (based on one standard deviation) was reduced to 0.41 degree.

Another algorithm was developed to reconstruct the in-cylinder pressure and heat release rate from the raw knock sensor data. This algorithm allows in situ compensation of sensor-to-sensor variation as well as variation of sensitivity over a wide range of operating conditions; the algorithm also compensates for variations in dynamic response of the sensors. A reasonable agreement has been achieved between the reconstructed in-cylinder pressure and that measured by research-grade in-cylinder sensors for both single and multiple injection modes over a wide range of test conditions.

FY 2008 Publications/Presentations

1. Huang, J., Mumford, D., “Development of a Robust Accelerometer- Based Start of Combustion-Sensing System”, presented in DOE EERE Vehicle Technologies Program 2008 Merit Review.

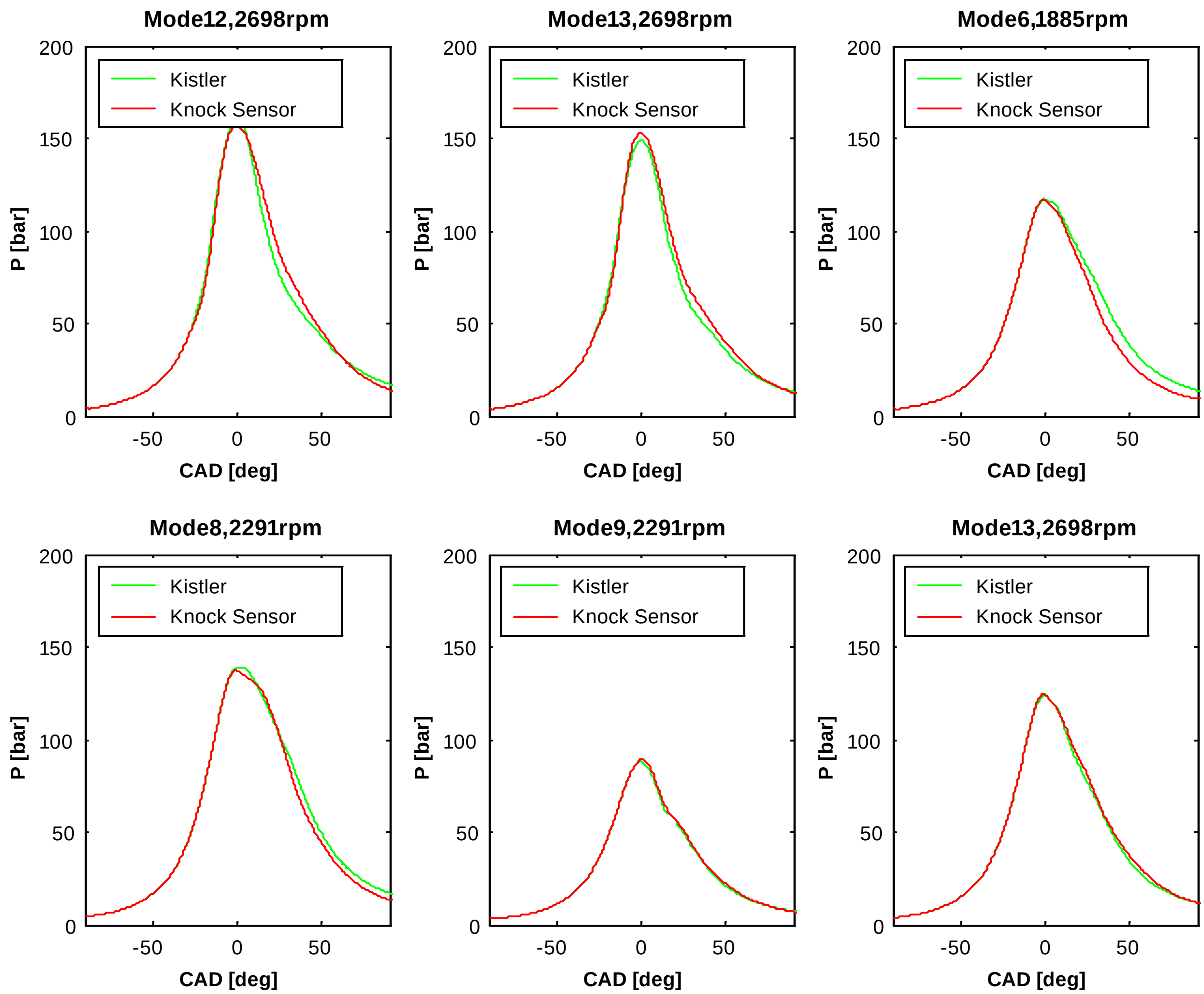

FIGURE 4. Comparison of Actual and Reconstructed In-Cylinder Pressure (data for cylinder #2, knock sensor data from bearing cap #2)

II.C.6 Exhaust Energy Recovery

Christopher R. Nelson
Cummins Inc.
1900 McKinley Ave.
Columbus, IN 47203

DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Carl Maronde

Objectives

- Improve engine fuel efficiency by 10% through the recovery of waste heat energy.
- Reduce the need for additional cooling capacity in Class 8 trucks.
- Provide conditioning (cooling) for combustion charge air.

Accomplishments

- Completed first-generation system hardware design and fabrication of components.
- Completed assembly of first-generation engine system. First generation energy recovery hardware was assembled onto a model year 2007 Cummins ISX engine. This in-production engine was chosen as it offered a stable test platform for the prototype energy recovery system.
- Successfully operated the engine and energy recovery system in a performance test cell. This was the first Cummins on-engine, R245fa-based Organic Rankine Cycle (ORC) energy recovery system. Successfully demonstrated the system's 6% fuel economy benefit from exhaust gas recirculation (EGR)-only energy recovery.
- Developed an effective integrated control system to operate the energy recovery system through practically all engine operating conditions. Stable and repeatable steady-state and transient control of the system was demonstrated. Identified a number of critical system features and control techniques to insure that system operation was stable and robust against system disturbance.
- Successfully demonstrated the predicted 2% additional fuel efficiency benefit through selective exhaust energy recovery. Transient operation of the system while using exhaust energy recovery in addition to EGR energy recovery was successfully performed.

Future Directions

Continued effort is planned in the pursuit of an effective and efficient ORC waste heat recovery (WHR) system. Activities to date have produced a first-generation system which successfully demonstrated that the predicted fuel efficiency benefit of this concept could be achieved. Future work is focused on enhancing system performance and refining system architecture to be integrated into Cummins' future products. During 2009, we expect to:

- Apply our hardware test results to refine system performance models and continue with model-based system development and optimization.
- Create a refined second-generation hardware set which may be integrated into Cummins future engine products. Second-generation hardware is expected to incorporate production-intent design features.
- Refine and develop system subcomponents including feed and boost pumps, integrated controls, and heat exchangers in order to demonstrate long-term durability.
- Proceed to in-vehicle system installation and operation.
- Demonstrate the additional fuel economy benefit from additional exhaust energy recovery and also charge air energy recovery.

The ORC-WHR concept introduces a significant number of new technologies into the engine system architectures which Cummins Inc. has traditionally pursued. Successful system integration for practical implementation will continue to require that subsystem architectures be carefully reviewed for their effect on the overall engine, driveline, and vehicle.

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Introduction

With the advent of low oxides of nitrogen (NOx) combustion techniques using cooled EGR, heat rejection has increased, driving cooling package space claims 'in vehicle' to their limits. A means to mitigate this increased heat rejection is desired to avoid extensive revisions to vehicle cooling packages. A solution which serves this purpose while providing operating efficiency benefits would be ideal. Application of an ORC to an engine's waste heat streams which already require cooling offers this ideal solution. Recovery and conversion of waste heat energy reduces the overall heat rejection load while simultaneously supplementing the engine's output power

The ORC is essentially a steam-turbine thermodynamic cycle wherein a working fluid (akin to water or steam) is heated to boiling and superheated (heated beyond boiling). Thereafter, the fluid is passed to an expansion device (in this case a turbine) where it releases its heating-induced energy and momentum to create mechanical power. When the ORC is applied to an engine's waste heat streams, the additional power it provides is added to and thereby increases the engine's performance for the same amount of fuel burned. Using the Rankine cycle to extract energy from waste heat streams serves to reduce the amount of heat which must be rejected. Reducing heat rejection and minimizing cooling package size serves to provide vehicle manufacturers with continued opportunities to minimize vehicle frontal area, reducing aerodynamic drag, and further improving fuel economy.

In the current work, energy recovery is primarily being performed on the heavy-duty diesel engine's EGR stream (primarily) and main exhaust gas streams (secondarily). Recovery of EGR heat will relieve the engine's cooling system of a significant amount of load. As the EGR energy recovery system must necessarily be designed to capture the peak heat load from this waste energy stream, it is over-designed for off-peak operation. During off-peak operation, this excess capacity is utilized more fully by recovering additional exhaust gas energy. By doing so, the energy recovery system is kept near its full operating capability across a majority of the engine's operating map. This technique maximizes the benefit of the energy recovery system.

Approach

Cummins' approach to the project objectives emphasizes Analysis-Led-Design in nearly all aspects of the research. An emphasis is placed on modeling and simulation results to lead the way into feasible solutions.

With the advent of cooled EGR-based combustion technology, the need to provide an effective cooling system for combustion charge conditioning has become vital. The additional cooling required for EGR and fresh charge air to thereby achieve low intake manifold temperatures (in pursuit of clean combustion) has driven an increase in vehicle cooling system performance.

An ORC extracting heat energy from the engine's EGR stream reduces the heat load on the engine system cooling package and simultaneously provides extra power for the engine system. The cycle's turbine-driven electric generator provides power which may be used for a number of different on-vehicle applications including:

- Traditional alternator load (alternator may be removed)
- Supplemental power to engine output (through the use of a driveline-coupled motor)
- More efficient parasitics in the form of electric coolant pumps, air compressors, etc.

To efficiently accommodate power from the ORC generator and to minimize its size, higher voltage than what is traditionally used on heavy-duty vehicles (12 volts direct current, VDC) is required. A voltage level of approximately 340 VDC creates opportunities to use efficient and cost-effective power electronics developed for use in other industries (rectifiers, power conditioners, motor drives, etc.) and components and techniques common with hybrid electric vehicles. High-speed, permanent-magnet or switched-reluctance generators and motors are also compatible with this higher-voltage environment. This compatibility leads to further applications of these devices with subsequent efficiency benefits to the engine and vehicle.

Results

During the year a first-generation set of hardware was commissioned, fabricated and assembled onto a Cummins engine. The system was successfully tested and demonstrated the performance predicted by model-based analysis.

Hardware Design, Fabrication and Testing

Figures 1 and 2 present the first generation system hardware.

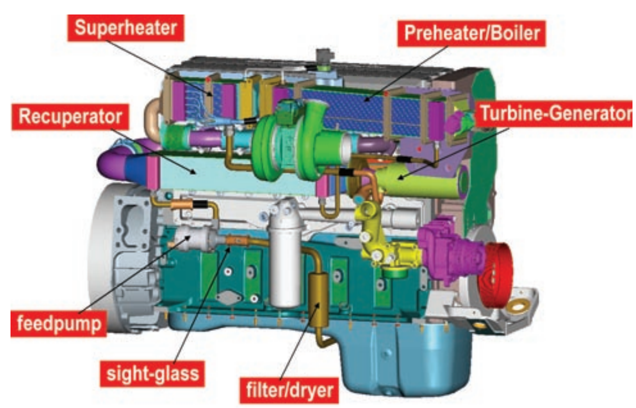

FIGURE 1. Cummins ISX Engine Shown with EGR-Only WHR System Hardware

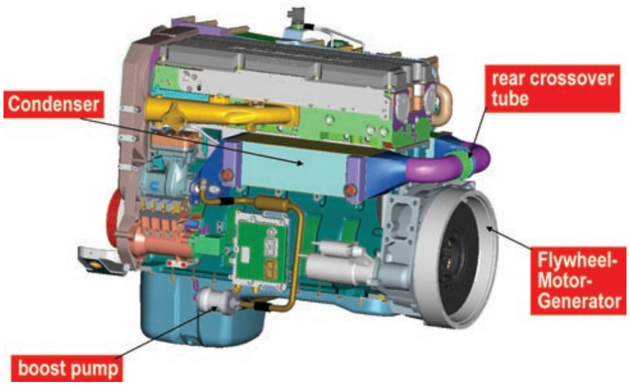

FIGURE 2. Cummins ISX Engine Shown with EGR-Only WHR System Hardware

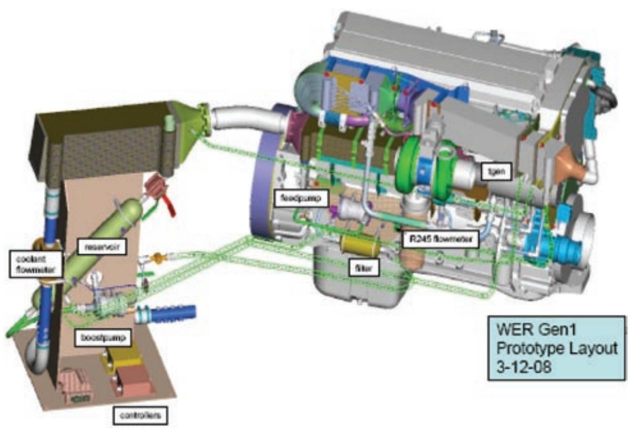

FIGURE 3. Test Cell Hardware Configuration

Figure 3 presents the hardware as installed for testing.

The system condenser was mounted off-engine in order to accommodate the existing fuel system on the model year 2007 ISX which served as the base engine for this initial set of experiments. This production engine was chosen as it would provide a stable base engine upon which to perform energy recovery system experiments.

The calibration of the 2007 ISX engine was modified to increase EGR flowrates to a level equivalent to 2010-intent engines. This level of EGR flowrate was used to design the WHR system components. Testing was conducted at both the 2010 flowrate of EGR and at the 2007 flowrate. Figure 4 summarizes performance testing results.

In Figure 4, operating points are defined by speeds (letters) and numbers (percent of load). 'A' speed was 1,200 rpm. 'B' speed was 1,450 rpm and represented a cruise point condition. 'C' speed was 1,750 rpm.

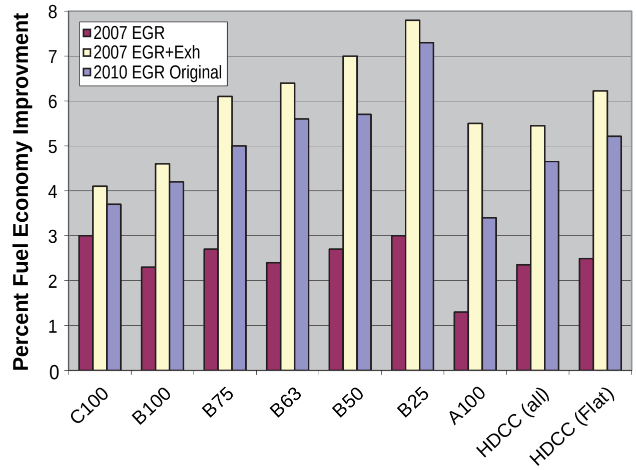

FIGURE 4. Fuel Economy Improvement Through ORC-Based Energy Recovery from an ISX Heavy-Duty Diesel Engine Operating at 2007 and at 2010 Emissions Level Flowrates of EGR

As shown above, ORC-based energy recovery for 2010-based, EGR-only energy recovery provided a 5.2% fuel efficiency improvement across the Heavy-Duty Corporate Composite (HDCC) operating cycle. This benefit was below that initially predicted through model-based analysis. Restrictions within the ORC system plumbing and additional parasitic losses in the system's generator were identified as the cause of these lower results. Removal of plumbing restrictions improved 2010 EGR-only energy recovery results to 5.4%. Greater than expected parasitic losses in the system were accounted to more windage in the system's generator than anticipated. It is expected that an optimized generator design would further improve results to 5.4-5.5%.

Also shown in Figure 4, EGR stream plus exhaust stream energy recovery resulted in a 6.2% fuel efficiency improvement across the drive cycle for an ISX engine running EGR rates necessary to meet 2007 legislated emissions.

The additional benefit offered by selectively recovering exhaust energy would improve the system's performance while meeting 2010 emissions levels by the predicted 2%.

Significantly, during hardware testing, system controls were developed and refined to demonstrate stable transient operation in practically every circumstance. The system was successfully 'driven' through simulated vehicle/engine operations to demonstrate the control system's ability.

Conclusions

A tremendous amount of progress was made this year by this project. The first-generation hardware was designed, fabricated, assembled and successfully tested. Performance predictions for the system were met and our performance models were validated through hardware testing. Critical design features and control functions of the system were identified, created, refined and demonstrated.

The project has demonstrated the feasibility and potential of this method of exhaust energy recovery. The synergistic opportunities offered by the presence of additional electric power with subsequent efficiency gains and improved parasitic load characteristics indicate that this concept has significant potential to improve real, in-use fuel economy.

- The 10% efficiency improvement goal has now been demonstrated. Model-based performance predictions were met and validated.
- Hardware testing has provided a solid foundation to proceed towards next-generation hardware. First-generation hardware demonstrated the practicality of an on-engine EGR energy recovery system and the additional benefits of main exhaust stream energy recovery.
- Robust system controls were developed and demonstrated. These will be further refined in model-based system simulation and applied to the next generation system hardware.
- In-vehicle testing and demonstration in late 2009 will allow further practical enhancements of system performance.

FY 2008 Publications/Presentations

1. 2008 DEER Conference Presentation – "Exhaust Energy Recovery", presented by Christopher R. Nelson, August, 2008

II.C.7 An Engine System Approach to Exhaust Waste Heat Recovery

Rich Kruiswyk
Caterpillar Inc.
PO Box 1875
Mossville, IL 61552-1875

DOE Technology Development Manager:
John Fairbanks

NETL Project Manager: Carl Maronde

Subcontractors:
Alipro, Peoria, IL
ConceptsNREC, Oxon, UK
eServ, Peoria, IL
Turbo Solutions, Norwich, VT
Barber-Nichols Inc., Arvada, CO

Objectives

Overall Objective:

- Develop a new air management and exhaust energy recovery system that will demonstrate a 10% improvement in overall thermal efficiency with no emissions increase.
- Demonstrate the resulting system and the efficiency benefits on a laboratory engine.

Phase III Objective:

- Demonstration of significant progress (+5-10%) in thermal efficiency improvement via testing and analysis of prototype components. This will include an on-engine system demonstration of prototype hardware.

Accomplishments

- Designed and procured a production-viable version of a novel nozzled/divided turbine stage, a technology which demonstrated a 5% turbine efficiency improvement (in a research version) relative to available production hardware.
- Designed a second-generation mixed flow turbine stage, with a predicted improvement of 6-8% in turbine efficiency relative to the first-generation design. Wheel prototypes are on order.
- Performed system analysis of a turbocompound system with aftertreatment backpressures representative of 2010 levels and research-demonstrated turbomachinery efficiencies. Predict a 4% improvement in engine thermal efficiency at the design point.
- Designed a high efficiency bearing system for a mechanical turbocompound power turbine unit. The design incorporates a number of changes that will improve rotor dynamic behavior relative to an earlier design generation.
- Completed a concept design for an electric turbocompound turbogenerator. Design is capable of providing 25 kW of compound power at design point conditions, with acceptable rotor dynamics, structural integrity, and thermal management.
- Completed capability analysis for Brayton and Rankine cycles performing waste heat recovery of a high-pressure loop exhaust gas recirculation (HPL EGR) stream. Benefits range from 1.5 to 6% improvement in thermal efficiency, depending on EGR rates and component efficiencies.

Future Directions

The Phase III objective is to demonstrate significant progress toward the goal of a 10% improvement in thermal efficiency using prototype components. There will be two elements to this demonstration:

- An on-engine demonstration of a 5 to 7% improvement in thermal efficiency using advanced turbocharger technologies, intercooling, insulated exhaust ports, and mechanical turbocompound.
- Parallel developments of technologies for future integration into the system solution, including the mixed flow turbine and electric turbocompound.

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Introduction

On today's heavy-duty diesel engines approximately 25% of the fuel energy leaves the exhaust stack as waste heat. Consequently, recovering energy from the diesel engine exhaust should pay significant dividends in improving diesel engine fuel efficiency. In this project Caterpillar is developing practical and production-viable solutions for improving waste heat recovery from heavy-duty diesel engines, with a goal of demonstrating a 10% improvement in thermal efficiency over today's production engines. Emphasis is placed on developing and incorporating cutting edge technologies that meet demanding cost, packaging, and drivability requirements, and that are compatible with anticipated future aftertreatment needs. Technologies under investigation

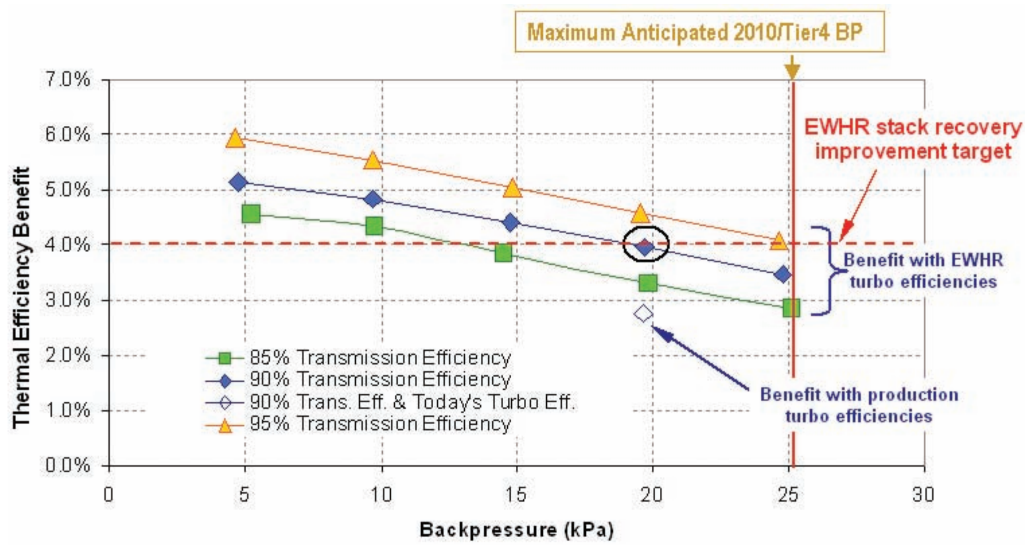

FIGURE 1. Turbocompound Simulation Results

include high-efficiency turbochargers, turbogenerators, advanced bearing systems, and effective engine insulating components.

Approach

Achieving a 10% improvement in engine thermal efficiency via improved waste heat recovery is a very challenging goal. The Caterpillar team determined that achieving this goal with a practical and production-viable solution would require a system approach. This means developing technologies that will reduce all forms of exhaust energy loss, including: blowdown losses, aero machinery losses, fluid frictional losses, losses due to pulsating exhaust flow, heat transfer losses, and losses of energy out the exhaust stack. The team makes use of Caterpillar's advanced engine simulation and test capabilities to determine the performance targets of the individual components in the system. Detailed component design, analysis, and testing are then used to verify that these performance targets can be met. Consultation with outside technical experts is used to help push the envelope of component capabilities.

Results

The Caterpillar recipe for achieving a 10% improvement in engine thermal efficiency breaks down as follows: +4% from implementation of turbocompound to recover stack waste heat, +3.7% from improving turbocharger efficiencies, +1.3% from intercooling the series turbocharging system, +0.5% from insulating the engine exhaust ports, and +0.5% from reducing exhaust piping flow losses. In addition, investigation of methods to recover waste heat from HPL EGR streams is underway. Progress in these areas is reported in the following:

Turbocompound Development: Detailed engine simulations of a C15 on-highway heavy-duty truck engine were conducted, with turbomachinery efficiencies representative of technologies under development in this project. With backpressure levels representative of anticipated 2010 aftertreatment, a 4% improvement in engine thermal efficiency was predicted at the design point as shown in Figure 1.

A high efficiency bearing system has been designed for a mechanical turbocompound power turbine unit. Changes to the bearing design and transmission gearing were incorporated to improve the power turbine rotordynamic behavior and to eliminate failure modes observed on the previous generation design. Testing is planned for the first quarter of 2009.

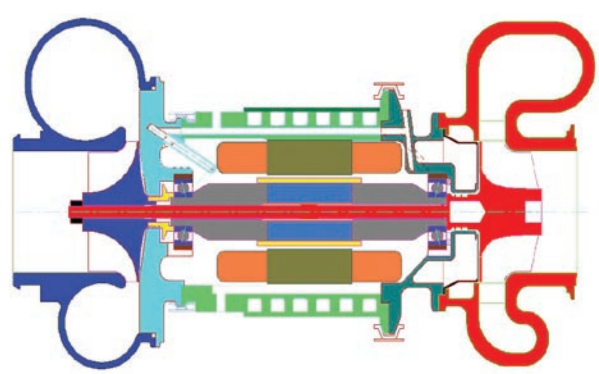

FIGURE 2. Turbogenerator Cross Section

A concept design for an electric turbocompound turbogenerator capable of delivering 25 kW of compounding power to the engine crankshaft was completed, as shown in Figure 2. Thermal, stress, and rotordynamic analysis were conducted, confirming the performance and integrity of the design.

High Efficiency Turbomachinery: As reported previously, a novel high efficiency turbine with a nozzled/divided turbine housing was tested that demonstrated turbine efficiency improvements of 4-6% over today's current production high-pressure (HP) turbine stage. This demonstration utilized a research design not suitable for volume production. The concept has now been converted into a production-viable design, and prototype hardware has been procured. A back-to-back performance test with the earlier research design is planned for the first quarter of 2009.

In Phase II, a novel mixed-flow turbine was designed, procured, and tested on the Caterpillar gas-stand that demonstrated the ability to shape the turbine efficiency characteristic to better match on-engine requirements. Peak turbine efficiencies, however, were short of the design goal. A second-generation mixed flow stage has now been designed with predicted peak efficiencies approximately 6% higher than the first-generation design (Figure 3). Hardware procurement is underway.

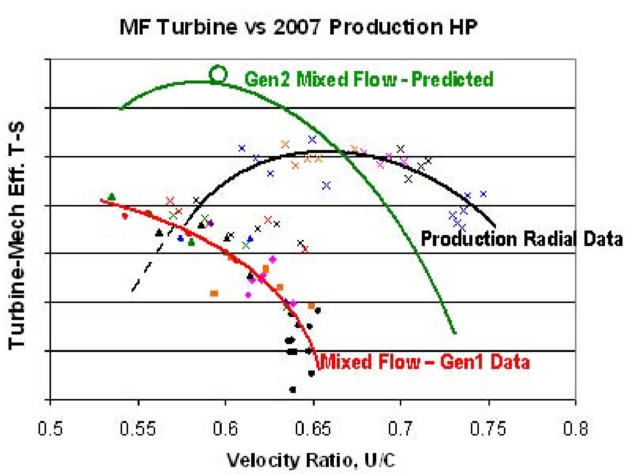

FIGURE 3. Mixed Flow (MF) Turbine Analysis Results

Waste Heat Recovery from HPL EGR Streams: Future low-emissions engine solutions, such as certain high efficiency clean combustion solutions, may benefit from the inclusion of an HPL EGR stream. Depending on the EGR levels, significant amounts of waste heat may be rejected from these streams as the recirculated exhaust is cooled to provide maximum emissions benefits. A capability analysis was completed to evaluate the performance of Rankine and Brayton bottoming cycles for recovering waste heat from the HPL EGR stream. Engine thermal efficiency improvements from 1.5 to 6% are predicted, depending on EGR rates and component efficiencies.

Conclusions

The results of components tests, component design and analysis, and engine simulation has resulted in high confidence that the project goal of a 10% improvement in engine thermal efficiency can be achieved. A predicted system-level benefit of 8.5% is solidly based on a combination of:

1. Components for which performance has been demonstrated via bench tests of prototype hardware.
2. Components for which performance has been predicted from design/analysis tools. In these cases confidence is bolstered by the similarity of these components to prototypes that have been demonstrated in hardware as part of prior research projects.

Additional technologies are under investigation and show promise for further improvements, thus leading to the conclusion that the 10% target can be met.

FY 2008 Publications/Presentations

1. Presented on 27 Feb 08 at the U.S. DOE Merit Review, Washington, D.C.

2. Presented on 6 Aug 08 at the U.S. DOE Diesel Engine-Efficiency and Emissions Research (DEER) conference, Detroit, MI.

II.D.1 Health Effects from Advanced Combustion and Fuel Technologies

Jim Parks (Primary Contact), John Storey,
Sam Lewis, Teresa Barone, Laura Kranendonk
Oak Ridge National Laboratory (ORNL)
P.O. Box 2008, MS 6472
Oak Ridge, TN 37831-6472

DOE Technology Development Manager:
James J. Eberhardt

Objectives

- Understand potential impact of developing fuel, combustion, and aftertreatment technologies on air quality and, thereby, human health.
- Quantify mobile source air toxic emissions from advanced technologies.
- Link emissions measured in laboratory setting to air quality impact, and thereby, health impact.

Accomplishments

- Measured mobile source air toxics (MSATs) from several light-duty vehicles operating on intermediate blends of ethanol (E10, E15 and E20).
  - Higher ethanol blends increase ethanol emissions over a driving cycle but the overall non-methane hydrocarbons (NMHC) and non-methane organic gases (NMOG) emissions are largely unchanged.
  - Higher ethanol blends increase acetaldehyde emissions but formaldehyde emissions were only slightly increased over the driving cycle.
- Characterized mobile source air toxics from High Efficiency Clean Combustion (HECC) on two diesel engines equipped with catalytic aftertreatment. The goal was to determine if higher engine-out levels of carbon monoxide (CO) and hydrocarbons (HCs) affected the destruction of MSATs by the catalyst.
  - Both pre-mixed charge compression ignition (PCCI) and homogeneous charge compression ignition (HCCI) engines were investigated.
  - Despite high levels of CO and HCs, MSATs were efficiently removed except when catalyst temperatures fell below 225ºC.
- Characterized MSATs and particulate emissions from small non-road engines operating on intermediate blends of ethanol and gasoline.
  - E20 dramatically reduced particle emissions for in-use utility engine while increasing acetaldehyde emissions.

Future Directions

- Characterize particulate emissions from PCCI engines for evidence of soot precursors and changes in density and morphology.
- Determine the efficiency of catalytic aftertreatment for reduction of MSATs from HECC diesel operation.
- Resolve differences in thermally-desorbed volatile fraction and solvent-desorbed volatile fraction of diesel particulate matter (PM).

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Introduction

Scientists and engineers at national laboratories, universities, and industrial companies are developing energy efficient technologies for transportation, and the U.S. Department of Energy (DOE) is actively involved in this innovative research. However, care must be taken to insure that any new technology developed for transportation must not adversely directly impact human health or impact the health of the environment, which subsequently may impact human health. To address this need, DOE sponsors research studies on the potential health impacts of advanced technologies for transportation including advanced fuels, combustion techniques, and emissions controls (also known as "aftertreatment" or, more commonly, "catalytic converters"). DOE-sponsored health impact research activities at ORNL are presented in this report.

ORNL conducts research on advanced fuel, combustion and emissions control technologies at the National Transportation Research Center (a joint ORNL and University of Tennessee research center) in Knoxville, TN. As the research is being conducted on engine and chassis dynamometers, specific studies of the potential health impacts of the technologies are conducted by the ORNL team for DOE's health impacts program. Results from three ORNL studies in Fiscal Year 2008 are presented here. Two studies focused on measuring MSATs from future fuels and advanced engine technologies. First, a series of in-use vehicles was operated on intermediate ethanol blends. Second, two different engines, equipped with aftertreatment were operated in the advanced diesel combustion modes of HCCI and PCCI. A third project was concerned with characterizing particulate and aldehyde emissions from small non-road engines operating on intermediate blends.

Approach

MSATs from Vehicles and Small Non-Road Engines Fueled with Intermediate Blends of Ethanol

A series of in-use light-duty vehicles (model years from 1999–2007) and small non-road engines (SNREs) were acquired by ORNL and evaluated as part of a larger study on the use of intermediate blends of ethanol in the existing fleet. The vehicles were driven over the LA92, also known as the Unified Cycle, a driving cycle that is commonly used for inventory and other in-use studies. The LA92 is considered to be more representative of in-use driving than the Federal Test Procedure. The SNREs were all engine-generator sets, operated over a 6-mode test cycle using the generator as the engine brake. Electrical loads were applied to control the engine load and emulate the 6-mode emissions test cycle. In addition to standard emissions, MSAT emissions were collected in canisters and 2,4-dinitorophenylhydorazine (DNPH) cartridges and analyzed with gas and liquid chromatography. Furthermore, additional particle sizing and characterization was performed on the SNREs and the results were presented at a conference [1].

MSATs from HECC Diesel Engines Equipped with Catalytic Converters

A Mercedes 1.7-liter 4-cylinder diesel engine was operated at several modes, representative of light-duty operation, on an engine dynamometer. The modes are shown in Table 1. The engine operated in both production calibration conditions and under PCCI combustion conditions. The engine was equipped with a 2.5 L oxides of nitrogen (NOx) storage and reduction catalyst which is described in detail elsewhere [2]. The MSAT emissions from both engine-out and catalyst-out were measured with Fourier transform infrared and gas and liquid chromatography via collection with DNPH cartridges. Extensive particle characterization was also performed on the exhaust including particle sizing and chemical analysis.

TABLE 1. Multi-Cylinder Engine Modes

Mode	Speed (RPM)	Load (BMEP)	Catalyst T (°C)	Space Velocity(hr-1)
Conv. PCCI Alt. PCCI	1,500	0.8	119	19,000 12,000 12,000
Conv. PCCI Alt. PCCI	1,500	2.6	256	21,000 9,000 9,000
Conv. PCCI Alt. PCCI	2,000	2.2	220	26,000 16,000 16,000

BMEP - brake mean effective pressure

Results

MSATs from Intermediate Blends

Ethanol emissions with all of the e-blends were largely undetectable for the LA92 driving cycle. All emissions essentially occurred in Bag 1 of the driving cycle. Due to the short duration of Bag 1 for the LA92 and the relatively low emissions, ethanol levels were near the detection limit of the analyzer. Acetaldehyde emissions increased with ethanol content in the fuel. The data are covered extensively in a recent report [3].

The SNREs also showed changes in emissions with increasing ethanol content. For four engines ranging from 5 hp to 25 hp, particle mass decreased with increasing ethanol content in the fuel. The in-use engine from 1999 was considered at its full useful life and showed the largest decrease in PM. The addition of ethanol will tend to make open-loop engines operate leaner (closer to stoichiometry) and therefore tend to have lower HC and PM. Figure 1 illustrates the drop in PM mass emissions with increasing ethanol content.

MSATs from HECC Diesel Mode with Catalyst

Diesel operation with the advanced HECC technique leads to a simultaneous reduction in NOx and particulate emissions without sacrificing fuel efficiency. While the operation of engines in advanced combustion modes may be a critical part of meeting future emissions regulations, the impact of HECC on unregulated and toxic emissions needs consideration. Two issues stand out: first, on a mass basis, do the emissions represent a real increase over conventional combustion modes? Second, will the high CO emissions effectively poison the aftertreatment such that it can no longer treat complex organic molecules? At the three operating

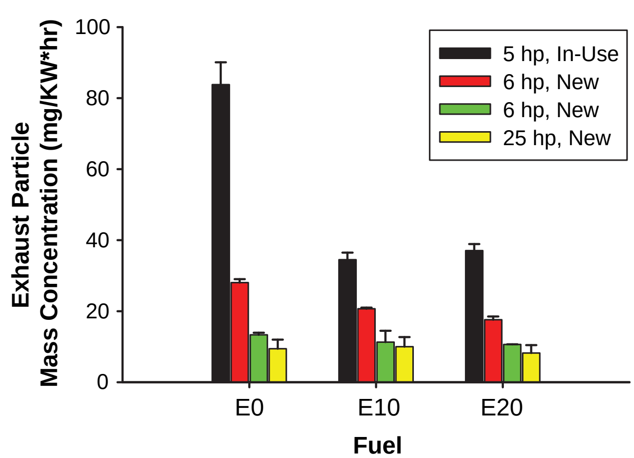

FIGURE 1. Particulate mass emissions for small utility engines operating on intermediate ethanol blends. Note that the older model showed the biggest decrease in emissions.

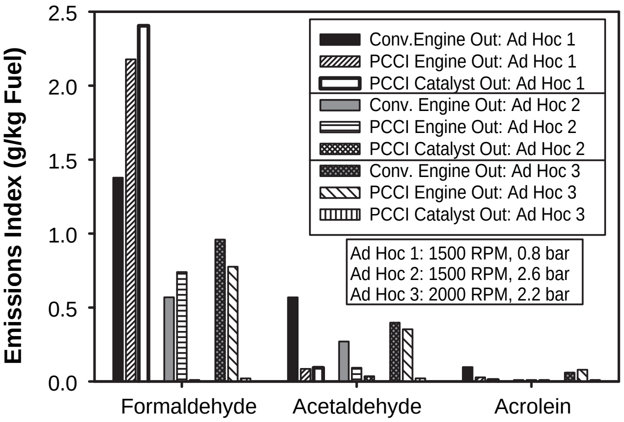

FIGURE 2. Conventional and PCCI emissions indices of aldehydes (collected by DNPH cartridges) for Modes 1-3. The "conventional" point is an original equipment manufacturer-like condition. Light-duty vehicle formaldehyde regulations equate to about 0.25 g/kg emissions index, putting the catalyst-out emissions well below the standard.

modes used in this study, HECC operation resulted in a 70-90% reduction in NOx and a 50-70% reduction in smoke as compared with traditional diesel combustion. However, MSAT emissions for HECC were greater than with traditional diesel combustion.

The catalyst did an effective job at Modes 2 and 3 on MSATs but not at Mode 1, where the catalyst temperature was below 170°C. Figure 2 shows the impact of aftertreatment on formaldehyde, acetaldehyde and acrolein. With the exception of Mode 1, the catalyst-out values for all three MSATs are much lower than both conventional and HECC mode engine-out.

In addition to gas phase measurements, much particulate characterization was performed on the exhaust. Particulate chemistry revealed on the soluble organic fraction and the semivolatile phase found that the catalyst did an excellent job on removing naphthalenes and the multi-ring polycyclic aromatic hydrocarbons (PAHs), which are both important MSATs. Figures 3(a) and 3(b) show the emissions index for Modes 2 and 3, respectively. The alternating PCCI condition refers to alternating between PCCI and conventional combustion. Because the PM filter samples took upwards of 20 minutes to collect, the PCCI setting would result in an upward drift of the HC emissions by as much as 50% due to cooling of the engine cylinder. In contrast, during the alternating PCCI setting (sampling was done only when in PCCI mode), combustion temperatures remained constant, and the HC emissions were steadier. The alternating PCCI setting is a more realistic representation of these advanced combustion modes as it is expected that future engines will switch between multiple modes (known as "mixed-mode" or "multi-mode" operation) to cover all load and speed demands under transient driving

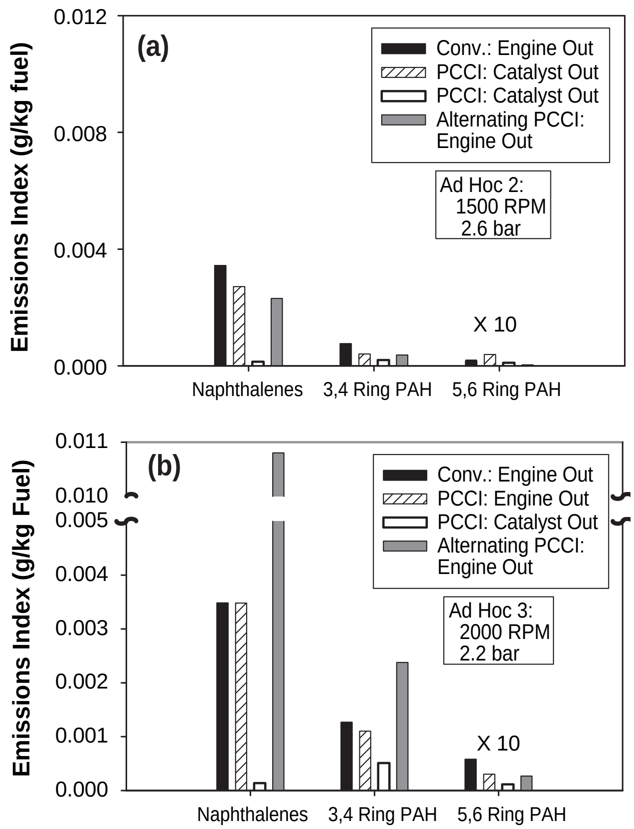

FIGURE 3. Emissions indices of naphthalenes and 3–6 ring PAHs for conventional and PCCI operation at Modes 2 (a) and 3 (b). The catalyst appears to have excellent destruction efficiency for the naphthalenes, which are MSATs.

conditions. Note that the PCCI catalyst-out values are at least 50% lower for these compounds.

Particulate sizing on the exhaust emissions revealed big differences between particulates emitted from conventional combustion and PCCI. The PCCI combustion did not appear to make the largest aggregates, resulting in a dramatic decrease in surface area concentration. This is significant because surface area and the surface species on fine particles is believed to have the most influence on their toxicity in the lung. Although most modern diesels will be equipped with diesel particulate filters (DPFs), it is also important to characterize the engine-out emissions because the changes in morphology will affect the soot packing in the DPF and thus can affect regeneration. Figure 4 shows an example of the differences in surface area concentration for Mode 2. Future studies will examine the relationship of particle density to different combustion modes which has broad implications for DPF operation.

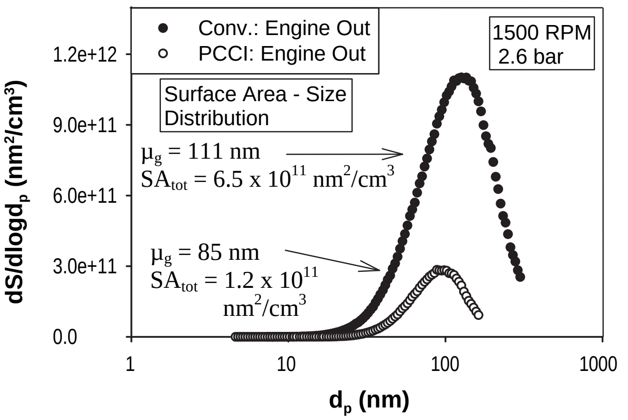

FIGURE 4. Surface area size distributions for engine operating conditions of Mode 2 (1,500 RPM, 2.6 bar). The geometric mean diameter (μ_g) and total number concentration (C_{tot}) or total surface area concentration (SA_{tot}) are given for each distribution.

Conclusions

- Intermediate Blends:
  - Acetaldehyde and ethanol emissions increase with increasing ethanol content.
  - Increasing ethanol content lowers particulate emissions for SNREs.
- High Efficiency Clean Combustion:
  - In comparison to traditional diesel combustion, PCCI operation results in higher MSAT emissions.
    - Likely future precious metal containing catalyst systems treat MSATs effectively when catalyst temperatures are above 225°C
    - Higher CO treatment requirements for the catalyst appear to be offset by lower space velocity during PCCI operation.
    - Particle size and shape are affected by PCCI which has implications for DPF loading and regeneration.

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1. James Parks II, John Storey, Sam Lewis, Robert Wagner, and Teresa Barone," Emissions From Diesel High Efficiency Clean Combustion Operation", *Presentation at the 18th CRC On Road Emissions Workshop* in San Diego, CA on March 31, 2008.

2. John Storey, Samuel Lewis, James Parks II, James Szybist, Teresa Barone, and Vitaly Prikhodko, "Mobile Source Air Toxics (MSATs) from High Efficiency Clean Combustion: Catalytic Exhaust Treatment Effects", *Society of Automotive Engineers Technical Paper Series 2008-01-2431 Society of Automotive Engineers, Warrendale, 2008.*

3. Laura Kranendonk, John Storey, and Teresa Barone, "High Speed Particle Size Distributions Measurements of Diesel Exhaust using a Standard SMPS", *Poster Presentation at the* American Association of Aerosol Research 27th Annual Conference. Orlando, FL. October 2008.

4. John Storey, Teresa Barone, Samuel Lewis, James Parks II, Vitaly Prikhodko, and James Szybist, "Effects of Advanced Combustion Technologies on Particulate Matter Emissions Characteristics" *Diesel Engine-Efficiency and Emissions Research (DEER) Conference* in Dearborn, MI on August 4–7, 2008.

5. John Storey, Samuel Lewis, Scott Sluder, and Andrea Strzelec"Effects of Fuel Chemistry and Combustion Mode on Diesel Particulate Matter," *presented at* 236th American Chemical Society National Meeting, Philadelphia, PA. August 2008.

6. Teresa Barone, John Storey, Brian West, John Thomas, and Tim Theiss," Particle Emissions of Small Non-Road Engines Fueled by Ethanol Blends," presented at the American Association of Aerosol Research 27th Annual Conference. Orlando, FL. October 2008.

II.D.2 Collaborative Lubricating Oil Study on Emissions (CLOSE) Project

Dr. Douglas R. Lawson
National Renewable Energy Laboratory (NREL)
1617 Cole Boulevard
Golden, CO 80401

DOE Technology Development Manager:
Dr. James J. Eberhardt

Subcontractors:
- Southwest Research Institute®, San Antonio, TX
- Desert Research Institute, Reno, NV

Objective

The objective of this project is to quantify the role of engine lubricating oil on particulate matter (PM) and semi-volatile organic compound (SVOC) emissions from in-use motor vehicles fueled with gasoline, 10% ethanol in gasoline (E10), diesel, biodiesel, and compressed natural gas (CNG) while operating on fresh and aged crankcase lubricants.

Accomplishments

- Continued Cooperative Research and Development Agreement between NREL and the South Coast Air Quality Management District and the California Air Resources Board (CARB) for project funding.
- Obtained additional funding from the Coordinating Research Council (sponsored by the automotive and petroleum industries) and Lubrizol for project support.
- The American Chemistry Council Petroleum Additives Product Approval Protocol Task Group provided new and aged engine lubricating oils for all vehicles tested in the project.
- Increased scope of project to include medium-duty vehicles and E10 and biodiesel fuel testing as part of the overall project.
- Completed all light-duty vehicle ("normal" and high-emitter) emissions testing in September 2008. Medium-duty vehicle testing will begin in November 2008.

Future Directions

A variety of light-, medium-, and heavy-duty (LD, MD, HD) vehicles are being tested over different driving test cycles at room (72°F) and cold (20°F) temperatures on chassis dynamometers. The test matrix depicting the vehicles and test conditions is shown as follows. The complete vehicle and emissions testing project will be completed during Fiscal Year 2009.

CLOSE Project Test Matrix

Test Temperature	72°F (nominal)				20°F			
Test Lubricant	Fresh		Aged		Fresh		Aged	
Vehicle \ Sample Number	1	2	1	2	1	2	1	2
LD gasoline ("normal" PM emitter)	√	√	√	√	√	√	√	√
LD gasoline (high PM emitter)	√	√	√	√	√	√	√	√
LD E10 ("normal" PM emitter)	√	√	√	√	√	√	√	√
LD E10 (high PM emitter)	√	√	√	√	√	√	√	√
MD diesel ("normal" PM emitter)	√	√	√	√	√	√	√	√
MD diesel (high PM emitter)	√	√	√	√	√	√	√	√
MD biodiesel ("normal" PM emitter)	√	√	√	√	√	√	√	√
MD biodiesel (high PM emitter)	√	√	√	√	√	√	√	√
HD CNG ("normal" PM emitter)	√	√	√	√				
HD CNG (high PM emitter)	√	√	√	√				
HD diesel ("normal" PM emitter)	√	√	√	√				
HD diesel (high PM emitter)	√	√	√	√				

The engine lubricating oil used in the project is labeled with deuterated hexatriacontane ($C_{36}D_{74}$). This tracer, along with other naturally-occurring compounds found in lubricating oil, such as hopanes and steranes, is used to quantify the relative contributions of PM formed from the fuels and the lubricants in the vehicles in the project.

"Normal" and high-emitting vehicles representing gasoline, diesel, and CNG-powered vehicles are being tested. Lubricants used in each technology are representative of those currently on the market, with both new and aged lubricants being tested in the project. The fuels used in the vehicles will be gasoline containing no ethanol, E10, CARB diesel, biodiesel, and CNG. Room temperature and cold temperature testing will be performed on all of the light- and medium-duty vehicles. Cold temperature testing will not be conducted on the heavy-duty vehicles due to funding limitations.

The data collected throughout the study are being chemically analyzed with detailed speciation to quantify the relative importance of the fuel and lubricant to PM and SVOC emissions from these vehicles under the variety of testing conditions specified in the study design.

Introduction

Air quality studies conducted in Denver, Phoenix, Washington D.C., Pittsburgh, Portland, OR, and the Office of Vehicle Technologies' (OVT's) Gasoline/Diesel PM Split Study in Los Angeles have shown that PM from gasoline engines is a more significant contributor to ambient air quality than PM from diesel engines [1,2]. For example, data collected in Washington, D.C., over a ten-year period suggest that PM from gasoline exhaust is ten times more important to the emission inventory than diesel exhaust, as shown in Figure 1 [3].

OVT's Comparative Toxicity Studies have also shown that the toxicity from gasoline exhaust on a per-unit-mass basis is at least as toxic as that from diesel exhaust, and that high-emitters' toxicity is even greater than that from normal emitters [4].

Because PM and SVOC emissions from both gasoline and diesel exhaust are so important to human health and ambient air quality, it is important to understand their source – whether it derives from the fuel, the lubricant, or both, and to understand the engine operating conditions that are responsible for PM emissions. That is the objective of the CLOSE Project.

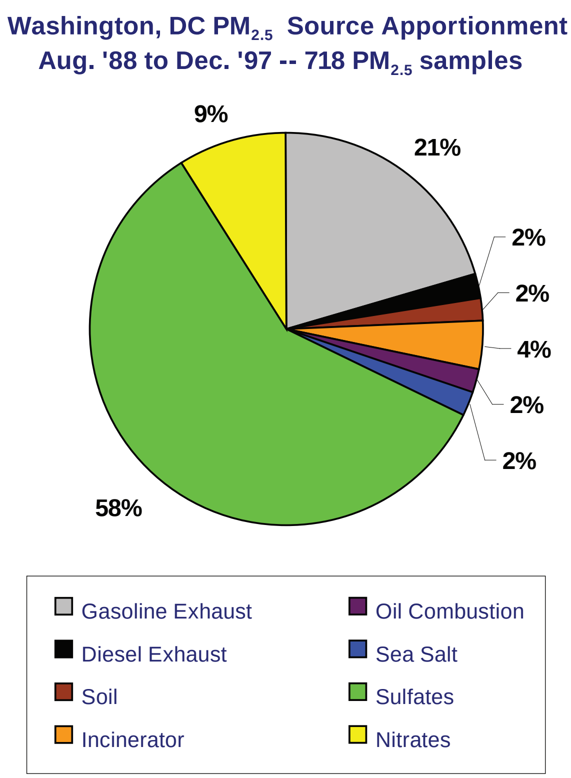

FIGURE 1. Source apportionment of $PM_{2.5}$ in the Washington, D.C., area, samples collected between 1988 and 1997.

Approach

The CLOSE Project is conducting extensive chemical and physical characterizations of PM and SVOC emissions from vehicles fueled with gasoline, E10, diesel, biodiesel, and CNG while operating on fresh and aged crankcase lubricants in an effort to improve our current understanding of the impact of crankcase lubricant formulations on vehicle emissions. In-use light- and heavy-duty vehicles are being recruited, including both "normal" and high-PM emitters, and operated on chassis dynamometers at room temperature (72°F nominal) and cold temperature (20°F). Gaseous (total hydrocarbons [THC], non-methane hydrocarbons [NMHC], carbon monoxide [CO], oxides of nitrogen [NOx]) and real-time particle emissions are being measured, and PM and SVOC samples are being collected for subsequent chemical analyses. Physical PM measurements are being conducted to obtain data on particle size and count, which will be investigated over the various driving test cycles run on the chassis dynamometers.

Results

At the time of this report, vehicle testing has been completed on the light-duty "normal" and high-emitters. Figure 2 shows the "normal" emitter vehicle on the dynamometer, along with the sampling ports and equipment used in the sampling tunnel (Figure 3).

Conclusions

There is much national interest in the results coming from the CLOSE Project. In FY 2008, the Environmental Protection Agency asked for a presentation of the CLOSE Project at its Mobile Source Technical Review Subcommittee meeting in Arlington, VA, in May 2008. Because this project is not completed, there are no conclusions at the time of this report. The CLOSE Project will be completed by September 2009, so results will be available at that time.

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FIGURE 2. Light-duty "normal" emitter tested in the CLOSE Project, a 2006 Chevrolet Impala.

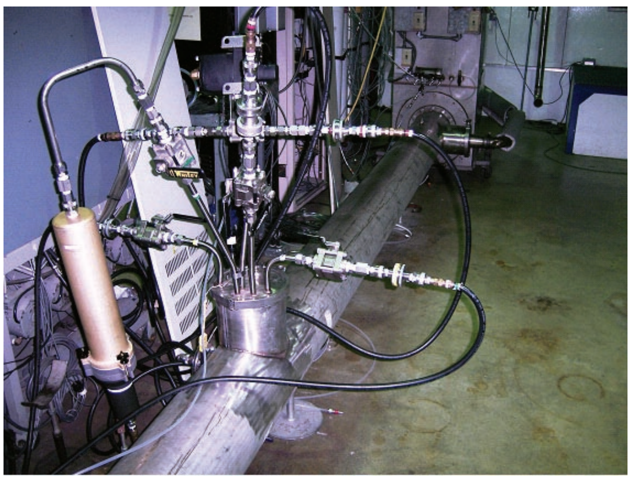

FIGURE 3. Sampling probes used to collect exhaust emissions samples from the dilution tunnel.

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FY 2008 Publications/Presentations

1. "The Collaborative Lubricating Oil Study on Emissions (CLOSE) Project," presented at EPA Mobile Source Technical Review Subcommittee Meeting; May 8, 2008.

2. "The Collaborative Lubricating Oil Study on Emissions (CLOSE) Project," presented at DEER 2008 Conference, Dearborn, MI; August 7, 2008.

II.D.3 The Advanced Collaborative Emissions Study (ACES)

Dan Greenbaum (Primary Contact), Robert O'Keefe, Maria Costantini, Annemoon van Erp
Health Effects Institute (HEI)
101 Federal Street, Suite 500
Boston, MA 02110

DOE Technology Development Manager: James Eberhardt

NETL Project Manager: Ralph Nine

Subcontractor:
Coordinating Research Council (CRC), Alpharetta, GA

Objectives

- **Phase 1:** Extensive emissions characterization at Southwest Research Institute® (SwRI®) of four production-intent heavy-duty diesel engine and control systems designed to meet 2007 standards for particulate matter (PM) and nitrogen oxides (NOx). One engine/aftertreatment system will be selected for health testing.
- **Phase 2:** Extensive emissions characterization of a group of production-intent engine and control systems meeting the 2010 standards (including more advanced NOx controls to meet the more stringent 2010 NOx standards).
- **Phase 3:** One selected 2007-compliant engine will be installed and tested in a specially-designed emissions generation and animal exposure facility at the Lovelace Respiratory Research Institute (LRRI) (Phase 3A) and used in chronic and shorter-term health effects studies to form the basis of the ACES safety assessment (Phases 3B and 3C). This will include periodic emissions characterization during both a core 24-month chronic bioassay of cancer endpoints in rats and biological screening assays in both rats and mice (Phase 3B) as well as emissions characterization during a set of shorter animal exposures and biological screening using accepted toxicological tests after the end of the chronic bioassay (Phase 3C). (NOTE: Only the emissions characterization and biological screening activities during Phase 3 are components of the DOE ACES contract).

Accomplishments

General Oversight

- Held a joint meeting of the HEI ACES Oversight and Advisory Committees to present the results of Phase 1 testing, update the Committees on progress in LRRI facility development, describe the selected studies on biological screening, and discuss the plan for engine selection (April 2008).
- Finalized the plan for engine selection with input from the Engine Selection Process Group (ESPG), a group comprising a subset of members of the CRC ACES Panel and HEI ACES Oversight Committee set up to guide HEI in the process of engine selection (May 2008).
- Conducted a site visit to LRRI to evaluate progress in developing the facility for engine testing and the exposure system (May 2008). A separate visit by members of the CRC ACES Panel was conducted in August 2008.
- Held a meeting of the ESPG at HEI to select the engine for Phase 3 (June 2008).
- Approved selection of engine B (June 2008).

Phase 1

- Completed emissions characterization of the third and fourth engines at SwRI® and conducted in-depth review of the emissions data for the four engines in preparation for engine selection through meetings and conference calls of the members of the CRC ACES Panel (May-June 2008). The results showed that the emission rates of the regulated pollutants were well below the 2007 standards for all four engines and that no engine had higher or lower emissions for all the components than the other engines.
- Completed testing of a 5th engine (back-up engine of the same model and manufacturer as the selected engine) at SwRI® (October 2008). The emission rate of NOx was slightly higher than that of the selected engine while the emissions of carbon monoxide (CO) and PM were lower.

Phase 3

- Completed contract negotiations with LRRI for conducting Phase 3 (October 2008).
- Completed the scientific negotiation of the biological screening studies to be performed by additional investigators funded under request

for application 06-2 and discussed with LRRI allocations of animals for those studies (April 2008).

- Delivered fuel (June 2008) and selected engine to LRRI (August 2008).
- Delivered a mule engine (provided by the manufacturer of the selected engine) to LRRI for initial testing of the engine/dynamometer system (September 2008).
- Approved the protocol for Phase 3A (October 2008).
- Commissioned the engine test facility at LRRI using both the mule and test engines (October 2008).

Future Directions

Phase 1

- Write, review, and publish Phase 1 Final Report (expected publication date June 2009).

Phase 2

- Assess feasibility and timeline for beginning Phase 2 characterization of 2010-compliant engines.

Phase 3

- Complete contract negotiations for the additional biological screening studies.
- Conduct and complete Phase 3A emissions and exposure chamber characterization at LRRI (February 2009).
- Hold a meeting of stakeholders at LRRI to discuss the results of Phase 3A chamber exposure characterization (February 2009).
- Decide on exhaust dilution ratios for animal exposures (February 2009).
- Start chronic bioassay in rats and associated biological screening studies in rats and mice (March 2009).
- Receive a draft final report on Phase 3A (June 2009).
- Expose rats for 24 months and mice for 3 months at three selected diesel exhaust exposure concentrations (high, medium, and low) or clean air and obtain results from biological screening in rats and mice (2009 and 2010).

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Introduction

The ACES is a cooperative, multi-party effort to characterize the emissions and assess the safety of advanced heavy-duty diesel engine and aftertreatment systems and fuels designed to meet the 2007 and 2010 emissions standards for PM and NOx. The ACES project is being carried out by HEI and the CRC. It is utilizing established emissions characterization and toxicological test methods to assess the overall safety of production-intent engine and control technology combinations that will be introduced into the market during the 2007-2010 time period. This is in direct response to calls in the U.S. Environmental Protection Agency (EPA) Health Assessment Document for Diesel Engine Exhaust [1] for assessment and reconsideration of diesel emissions and health risk with the advent of new cleaner technologies.

The characterization of emissions from representative, production-intent advanced compression ignition (CI) engine systems will include comprehensive analyses of the gaseous and particulate material, especially those species that have been identified as having potential health significance. The core toxicological study will include detailed emissions characterization at its inception, and periodically throughout a two-year chronic inhalation bioassay similar to the standard National Toxicology Program bioassay utilizing two rodent species. Other specific shorter-term biological screening studies also will be undertaken, informed by the emissions characterization information, to evaluate these engine systems with respect to carefully selected respiratory, immunologic, and other effects for which there are accepted toxicologic tests. It is anticipated that these emissions characterization and studies will assess the safety of these advanced CI engine systems, will identify and assess any unforeseen changes in the emissions as a result of the technology changes, and will contribute to the development of a data base to inform future assessments of these advanced engine and control systems.

Approach

Experimental work under ACES is being conducted in three phases, as outlined in the Objectives. Detailed emissions characterization (Phases 1 and 2) is performed by an existing engine laboratory (SwRI®) that meets the EPA specifications for 2007 and 2010 engine testing. In Phase 1, emissions from four 2007-compliant engine/control systems have been characterized. One engine has been selected for health testing in Phase 3. In Phase 2, emissions from four 2010-compliant engine/control systems will be characterized. In Phase 3, the selected 2007-compliant engine/control system has been installed in a specially designed emission generation facility connected to a health testing facility at LRRI to conduct a chronic inhalation bioassay and shorter term biological screening in rats and mice. During the 2-year bioassay, emissions will be characterized at regular intervals throughout the testing.

The emissions characterization work is overseen by CRC and its ACES Panel. The health effects assessment is overseen by HEI and its ACES Oversight Committee (a subset of the HEI Research Committee augmented by independent experts from several disciplines), with advice from an Advisory Committee of ACES stakeholder experts. The overall effort is guided by an ACES Steering Committee consisting of representatives of DOE, engine manufacturers, EPA, the petroleum industry, California Air Resources Board, emission control manufacturers, and the Natural Resources Defense Council. Set-up of the emission generation facility at LRRI (for Phase 3) and establishment of periodic emissions characterization throughout Phase 3 will be done with input from the team of investigators who conducted Phase 1 and the CRC ACES Panel.

Results

The results obtained during this reporting period pertain to the Phase 1 characterization of emission rates of regulated and unregulated pollutants from the four engines tested on the heavy-duty Federal Test Procedure (FTP) cycle, selected portions of the California heavy-duty cycle, and a 16-hour cycle specifically developed for generating the exhaust for the animal exposures. Overall, the four engines were very similar in their emissions species and no engine had consistently higher or lower emissions for all the major compounds or classes of compounds than the other engines. Also no engine met the criteria for being defined as an outlier.

The emission of selected compounds and classes of compounds for the 16-hour cycle (see Table 1) were used to rank the engines for engine selection. For the selection, the emission rates were ranked (normalized) using four methods, one parametric and three parametric. Regardless of the methods, the ranks of the individual compounds or classes of compounds (listed in Table 1) were added to obtain an overall score for each engine. There was little or no difference in the total score among the engines, but one of the four engines (D) did happen to rank lowest in all four ranking methods. The ranking of the other three engines changed depending on the ranking method used and no engine was ranked highest with at least three of the four ranking methods. Based on the pre-determined rules, engine D was excluded from the selection and the selection among the other three engines was random; engine B was selected for use in Phase 3.

Engine 5 (back-up engine for the chronic bioassay) was tested at SwRI® to verify that its regulated emissions were similar to those of the selected engine. Tests were conducted using the FTP test cycle and three steady-state tests modes. The emission rate of NOx was slightly higher than that of the selected engine while the emissions of CO and PM were lower. To facilitate the comparison with the emissions characterization that will be done at LRRI using the selected engine, a set of tests was conducted under simulated high altitude conditions (the same as encountered at the LRRI facility). Higher altitude led to a small increase in NOx and CO emissions relative to emissions at sea level under some of the test conditions. Full results will be included in the Phase 1 final report.

TABLE 1. Summary of Emission Rates for Compounds and Classes of Compounds Used for Engine Ranking (6/4/08)

Emissions Components	Engine A	Engine B	Engine C	Engine D	AVG.	St. dev.
NO (g/hp-hr)	0.54	0.48	0.86	0.63	0.63	0.17
NO_2 (g/hp-hr)	0.95	0.91	0.56	0.56	0.74	0.21
Carbon Monoxide (g/hp-hr)	0.09	0.08	0.46	0.15	0.20	0.18
PM Mass (g/hp-hr)	0.0013	0.0012	0.0011	0.0013	0.0012	0.0001
PM Number (Part./hp-hr)	4.13E+13	5.67E+13	1.66E+13	2.38E+13	3.46E+13	1.80E+13
EC (mg/hp-hr)	0.20	0.27	0.26	0.22	0.24	0.03
OC (mg/hp-hr)	1.53	0.24	0.26	0.52	0.64	0.61
Total Metals (by XRF) (μg/hp-hr)	62.37	62.15	28.88	89.91	60.82	24.97
Inorganic Ionic Species (mg/hp-hr)	3.84	3.09	2.86	2.47	3.06	0.57
Carbonyl compounds (mg/hp-hr)	4.99	1.64	4.40	2.44	3.37	1.59
Single ring aromatic compounds (mg/hp-hr)	0.35	1.20	0.81	0.69	0.76	0.35
Total PAHs (mg/hp-hr)	0.55	0.73	0.84	0.80	0.73	0.13
Total Nitro PAHs (μg/hp-hr)	0.44	0.77	0.86	0.58	0.66	0.19
Total oxygenated PAHs (μg/hp-hr)	6.25	5.96	3.76	3.29	4.82	1.51
Nitrosamines (μg/hp-hr)	32.54	28.06	52.89	25.82	34.83	12.36

EC - elemental carbon; OC - organic carbon; XRF - X-ray diffraction; PAHs - polycyclic aromatic hydrocarbons

Conclusions

By completing the emissions characterization of the four heavy-duty 2007-compliant engines and selecting among them the engine that will be used for the chronic bioassay, we have achieved some very important milestones in the project. First, we have obtained detailed characterization of four engines that are employing new technologies to substantially reduce PM and in part NOx. Second, we have provided an engine considered to be representative of the four engines to LRRI that can now be used to generate the test atmosphere for the animal exposures during the chronic inhalation bioassay. In parallel we have tested the back-up engine, thereby completing the experimental work of Phase 1, and developed the protocol for testing the selected engine and characterizing the exposure atmosphere in the inhalation chambers at LRRI. All this work has been conducted with input from the ACES stakeholders. Although there have been some slight delays in implementation to ensure that full quality assurance could be accomplished, we are now ready to start Phase 3 at LRRI.

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1. U.S. Environmental Protection Agency. 2002. Health Assessment Document for Diesel Engine Exhaust. EPA/600/8-90/057F. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Office of Research Development, Washington, D.C.

FY 2008 Publications/Presentations

1. Poster presentation at the CRC On-Road Vehicle Emissions Workshop in San Diego CA, March 2008: "Advanced Collaborative Emissions Study."

2. Platform and poster presentations at the HEI Annual Conference in Philadelphia CA, April 2008: "Advanced Collaborative Emissions Study: Phase 1."

3. Platform presentation at the annual DOE Vehicle Technologies Program Annual Merit Review, Bethesda MD, February 2008: "Advanced Collaborative Emissions Study (ACES)."

4. Platform presentation at the Diesel Engine Emissions Reduction (DEER) meeting in Detroit MI, August 2008: "Status of the Advanced Collaborative Emissions Study (ACES)."

III. SOLID STATE ENERGY CONVERSION

III.1 Develop Thermoelectric Technology for Automotive Waste Heat Recovery

Jihui Yang (Primary Contact), T. Anderson, G. S. Nolas, C. Uher, D. T. Morelli, Q. Li, A. Wereszczak and H. Wang
GM Research and Development Center
30500 Mound Road, MC 480-106-224
Warren, MI 48090

DOE Technology Development Manager: John W. Fairbanks

NETL Project Manager: Carl Maronde

Subcontractors:
- General Electric (GE), Niskayuna, NY
- University of South Florida, Tampa, FL
- University of Michigan, Ann Arbor, MI
- Michigan State University, East Lansing, MI
- Brookhaven National Laboratory, Upton, NY
- Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

Objectives

- Provide initial lab test data for thermoelectric (TE) modules.
- Finalize TE waste heat recovery subsystem design.

Accomplishments

- Developed a novel solid-phase diffusion bonding process to fabricate TE modules.
- Completed a fully transient three-dimensional multi-module finite element model that includes the convective heat transfer physics of the heat sinks.
- Completed the detailed design for the exhaust TE generator, and defined and integrated the generator position and exhaust bypass geometry with the selected General Motors (GM) vehicle.
- Completed a trade-off study to determine the electrical topology of the generator and the direct current (DC)-to-DC converter architecture. Selected the design that maximizes reliability and efficiency over the driving cycles and minimizes system cost.
- Developed vehicle level control algorithms to optimize potential fuel economy gains.
- Measured performance of some initial modules at various temperature gradients.
- Measured the coefficient of thermal expansion and elastic properties of materials selected for module construction.
- Investigated mechanical strengthening methods for PbTe-based materials.
- Completed phonon density of states and high-resolution transmission electron spectroscopy (TEM) for skutterudites and nano-composites, where our findings provide unprecedented insight into the heat transport in these materials.
- Discovered and developed multiple-element-filled skutterudites, which have the best TE figure of merit (ZT) values between room temperature and 500°C amongst n-type skutterudites.
- Analyzed many materials under investigation by scanning electron microscopy (SEM) for mechanical performance and identified strength-limiting flaws, which led to improved materials synthesis processes.
- Initiated the non-equilibrium growth of skutterudites, and characterized their structural and transport properties.
- Optimized the TE properties of antifluorite compounds, which are cost-effective prospective TE materials.
- Established a controllable p-type procedure for producing mechanically robust PbTe.

Future Directions

- Complete prototype TE module construction.
- Start performance tests of prototype TE modules.
- Complete TE exhaust waste heat recovery subsystem prototype construction.
- Complete vehicle modification for TE generator performance testing.

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Introduction

In the past year, the project has been focused on several areas: design of TE waste heat recovery generator; design of electrical power management system for the TE generator; development of vehicle-level algorithms to optimize potential fuel economy gains; and the search for high-performance, mechanically-robust, and cost-effective TE materials and modules.

We have made significant progress in each of these focus areas. As part of the generator design, we have defined geometry and position of various components including heat exchangers, TE modules, interfaces, packing methods, etc; in addition, the generator position and exhaust bypass geometry have been defined and integrated with the selected GM vehicle. A trade-off study was completed to determine the electrical topology of the generator and the DC-to-DC converter architecture. The selected design maximizes reliability and efficiency over the driving cycles and minimizes system cost. Vehicle level control algorithms have been developed for electrical power management and thermal management to achieve optimized fuel economy gains.

The materials discovery part of this project has discovered and developed the best n-type skutterudites via multiple-element-filling. We have also established a controllable p-type procedure for producing mechanically robust PbTe. Many materials under investigation have been analyzed by SEM for mechanical performance, and strength-limiting flaws have been identified, which led to improved materials synthesis processes. Phonon density of states and high-resolution TEM have been completed for skutterudites and nano-composites, where our findings provide unprecedented insight into the heat transport in these materials. The non-equilibrium growth of skutterudites has been initiated and their structural and transport properties have been characterized. We have optimized the thermoelectric properties of antifluorite compounds, which are cost-effective prospective thermoelectric materials.

To support this part of the project, GM has purchased and installed a TE module measurement system. This system measures electrical output of TE modules under various external electrical loads and temperature gradients. This will provide the team with a unique capability as we move forward in the project.

Approach

The overall approach we use to achieve the project goal is to combine science and engineering. Existing and newly developed materials are carefully selected by the materials research partners of the project and supplied to the system engineers at GE. Most of the material properties are also validated at ORNL to avoid potential pitfalls. Mechanical property experts at ORNL have been instrumental in electron microscopy of various materials selected for the project; based on these results and mechanical property measurement results, strength-limiting flaws have been identified that provide critical insight for the materials team in terms of improving the materials processing procedures to achieve better mechanical performance. System engineers at GE work closely with vehicle engineers at GM to ensure that accurate vehicle level information is used for developing subsystem models and designs. Vehicle level electrical and thermal management algorithms have been developed to optimize potential fuel economy gains.

Our project incorporates material, module, subsystem, and integration costs into the material selection criteria. We use this approach not only as a guide for balancing technology options, but also for providing consumer benefits.

Results

1. Thermoelectric Generator Design

Figure 1 shows a Chevy Suburban with an exhaust heat TE generator. The generator is located at the position that the muffler normally occupies. The muffler has been moved to a location after the rear axle. The generator system also consists of a bypass, DC-to-DC converter, radiator coolant loop, and electrical cable. The TE generator assembly is shown in Figure 2(a), and the interior view showing the thermoelectric module mounting is in Figure 2(b).

2. Multiple-Element-Filled Skutterudites

Recently, Yang *et al*. calculated the spring constants and resonance frequencies for various fillers in $CoSb_3$ [1]. We found that a lower thermal conductivity and higher ZT is achieved for Ba and La (or Ce) fillers in double-filled skutterudites due to the large difference in their resonant phonon frequencies. Based on the calculations in Ref. 1, filling Ba and Yb into the voids of skutterudites should be even more effective in scattering phonons, because the spring constants and resonant frequencies for Yb and Ba differ more than other possible filler-pair combinations. Furthermore, the filling fraction limits for Ba and Yb in $CoSb_3$ are well studied experimentally [2-5] and theoretically [6, 7], and both fillers independently yield high ZTs [2, 3, 5]. We have found that double-filling with Ba and Yb is indeed more efficient in scattering lattice phonons than single-filled skutterudites and other double-filler combinations; hence, such an approach leads to an enhancement of ZT.

Figure 3 shows the best experimentally determined ZTs reported so far in *n*-type skutterudites [2, 8, 9], and

FIGURE 1. A Chevy Suburban with an Exhaust TE Generator

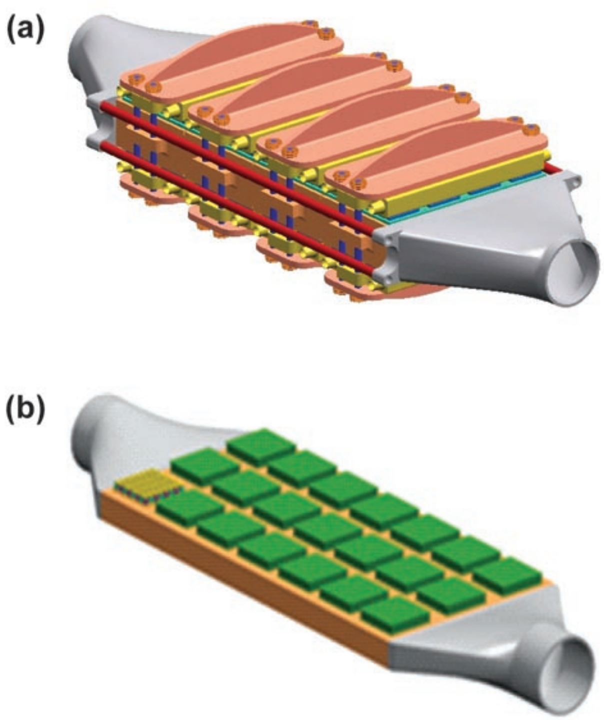

FIGURE 2. (a) Exhaust TE Generator, (b) Interior View Showing the TE Modules

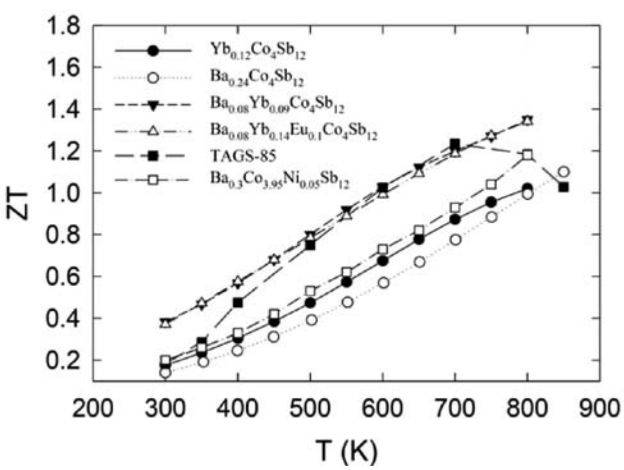

FIGURE 3. Temperature dependence of the *ZT*s for Ba- and Yb-filled skutterudites [2, 8], double- and triple-filled skutterudites [8], $Ba_xNi_{0.05}Co_{3.95}Sb_{12}$ [9], and $(AgSbTe_2)_{0.85}(GeTe)_{0.15}$ [10]. The accuracy of *ZT* is estimated to be 20%.

p-type $(AgSbTe_2)_{1-x}(GeTe)_x$ solid solutions (an exceptional high efficiency TE material in the intermediate temperature range) [10]. The ZTs are obviously improved from single-element-filled skutterudites to double- or triple-filled. The ZT values in our samples are at least 0.2 higher than those of *n*-type skutterudite $Ba_xNi_{0.05}Co_{3.95}Sb_{12}$ [9] and $Yb_{0.12}Co_4Sb_{12}$ [8] over the entire temperature range investigated. In addition, the ZT of $Ba_{0.08}Yb_{0.09}Co_4Sb_{12.12}$ is twice as large as optimized $(AgSbTe_2)_{0.15}(GeTe)_{0.85}$ [10] at room temperature and 0.2 higher near 800 K. Although the ZTs of triple-filled skutterudite in this study do not exceed Ba and Yb double-filled skutterudites, it is still in the class of the best thermoelectric materials.

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1. J. Yang, March 2008, The Annual American Physical Society March Meeting, Opportunities in Energy Research Workshop, New Orleans, LA: "Thermoelectric Energy Conversion" (invited).

2. J. Yang, August 2008, The 27th International Conference on Thermoelectrics, Corvallis, OR: "Thermoelectric Materials for Automotive Applications" (invited).

3. J. Yang, September 2008, Department of Physics, Boston College, Chestnut Hill, MA: "Thermoelectric Materials by Design" (invited).

4. J. Yang, October 2008, 2008 MS&T conference, Pittsburg, PA, "Thermoelectric Materials for Automotive Applications" (invited).

5. J. Yang, December 2008, 2008 MRS Fall Meeting, Symposium W: Computational Materials Design via Multiscale Modeling, Boston, MA: "Thermoelectric Materials by Design" (invited).

6. J. Yang, December 2008, The 2008 IUMRS International Conference in Asia, Nagoya, Japan, “Thermoelectric Materials for Automotive Applications” (invited).

7. X. Shi, August 2008, The 27th International Conference on Thermoelectrics, Corvallis, Oregon, USA: “Thermoelectric Properties of *n*-type Multiple-filled Skutterudites”.

8. X. Shi, October 2008, Materials Science & Technology 2008 Conference and Exhibition, Pittsburgh, Pennsylvania, USA: “Low and High Temperature Thermoelectric Properties of *n*-type Multi-filled Skutterudites”.

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14. de Bock, P. and Novak, V., “EVALUATION OF SYSTEM CONFIGURATIONS FOR THERMOELECTRIC POWER GENERATION,” ITherm 2008, Orlando, Florida, USA May 28–31, 2008.

15. Q. Li, “Thermoelectric Materials with Potential High Power Factors” International Conference on Thermoelectrics, Corvallis, OR, USA, Aug. 3-7, 2008 (organized by International Thermoelectric Society) (invited talk).

16. Qing. Jie (poster presenter), Juan. Zhou, Lijun Wu, Jincheng Zheng, Yimei Zhu, and Qiang Li, “Impact of nanoscale substructures on the thermoelectric properties of AgPbmSbTe2+m”, (MRS Fall meeting (2007).

17. Zhiwei Lin, Xun Shi, Jihui Yang, Qing Jie, Lijun Wu, and Qiang Li , “TEM Investigation of Intermetallic Thermoelectric Materials – Filled Skutterudites” Juan. Zhou (talk presenter), (MS&T08).

18. L. Wu (invited talk), J. Zheng, J. Zhou, Q. Li, J. Yang and Y. Zhu, “Structural analysis of thermoelectric AgPbmSbTe2+m using high resolution transmission electron microscopy” (MS&T08).

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22. G.S. Nolas, ‘Open-framework Inorganic Materials’, Invited, National Institute of Standards and Technology, Gaithersburg, MD, July 22, 2008.

23. G.S. Nolas, J. Martin, S. Stefanoski, L. Wang and L. Chen, ‘Transport Properties of Lead Chalcogenide Nanocomposites’, presented at the American Physical Society March Meeting, New Orleans, LA, March 13, 2008.

Special Recognitions & Awards/Patents Issued

1. J. Yang - National Academy of Engineering U.S. Frontiers of Engineering Symposium.

2. J. Yang – U.S. Department of Energy Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award.

III.2 High-Efficiency Thermoelectric Waste Energy Recovery System for Passenger Vehicle Applications

J. LaGrandeur[1] (Primary Contact), D. Crane[1], Andreas Eder[2], Boris Mazar[2], C. Maranville[3]

[1] BSST LLC
5462 Irwindale Avenue
Irwindale, CA 91706

[2] BMW AG
EG-65
Knorrstrasse 147
80788 Munich, Germany

[3] Ford Motor Company
Scientific Research Lab
Room 2417, MD 3083
201 Village Road
Dearborn, MI 48124

DOE Technology Development Manager: John Fairbanks

NETL Project Manager: Carl Maronde

Subcontractors:
- BMW, Palo Alto, CA and Munich, Germany
- Ford Motor Company, Dearborn, MI
- Visteon, Van Buren Township, MI

Objectives

The primary objective of 2008 was to build and test a thermoelectric generator (TEG) that could be repeatedly operated using 600°C gas and 70°C liquid working fluids. The nominal power output of the TEG was targeted at 150 watts which will be scaled up to meet the planned capacity of 500-750 watts required for Phase 4. The objective was supported by the successful development and testing of lower temperature material systems and interfaces in a full-scale TEG built and tested in 2007.

Objectives for 2008 include:

- Demonstration of thermal cycle fatigue performance of thermoelectric (TE) subassemblies by performing extensive thermal cycling.
- Integration and test of a TEG with the power control system (PCS).
- Build and test of a 150 watt TEG that operates using 600°C gas and 70°C temperature liquid working fluids.
- Updating the system fuel efficiency performance prediction to reflect the change in BMW engine selection to a turbo-charged inline 6-cylinder engine.
- The addition of a Ford Motor Company work package that includes:
  - Development of techniques for characterizing electrical interfaces in TE subassemblies and evaluation of early prototype parts.
  - Assessment of the application of TEG technology for a Ford hybrid vehicle platform.

Accomplishments

- Thermal cycling of TE subassemblies was completed that supported high-temperature TEG build and test at BSST.
- The PCS designed and built in 2007 was successfully tested with a TEG at BSST.
- A high-temperature TEG was built and substantially tested by BSST that provided 125 watts of power using 600°C gas.
- The system performance model was updated to incorporate a transient TEG model and more efficient BMW engine to prepare for 4th phase testing at the National Renewable Energy Laboratory (NREL) by BMW.
- Characterization techniques for TE subassembly electrical interfaces were developed and applied by Ford that provided an important tool and basis for further improving the technology.
- Initial assessment of the application of TEG technology in a hybrid vehicle platform was completed and fuel economy improvement predictions made by Ford.

Future Directions

In the coming year BSST will:

- Test a 150 W high-temperature TEG on a single-cylinder engine dynamometer.
- Complete the build of a full-scale high-temperature TEG and perform testing on an engine dynamometer at NREL.
- Finalize dynamometer performance results and prepare report. Following this evaluation the system will be ready for vehicle installation and test.

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Introduction

BSST began work to develop a high efficiency TE waste energy recovery system for passenger vehicle applications in November 2004.

Phase 3 began in February 2007 and concluded in December 2008. In 2007, BSST built partial-and full-scale low-temperature TEGs, small prototype high-temperature TE subassemblies and a 10% net efficiency TEG. The system model was updated to incorporate a simplified system architecture, refined TEG and vehicle modeling capabilities.

In 2008, Phase 3 continued with modification of the TEG for operation at automotive exhaust gas temperatures (~600°C) and concluded with bench testing of a +100 watt high-temperature TEG at BSST.

Approach

In 2007, BSST successfully built and tested a 530 watt, low-temperature (hot fluid inlet temperature ~200°C) TEG based on the proprietary TE subassembly design shown in Figure 1. The TE subassembly included n and p types Bi_2Te_3 material, hot oil and cold liquid (ethylene glycol/water) heat exchangers. Building on this experience, the design evolved by adding high-temperature TE materials, gas heat exchangers and modified electrical and thermal interfaces to accommodate 600°C exhaust gas.

In order to prove thermal and electrical interface capability to operate at high temperature, thermal cycling of subassemblies was performed in a fixture representative of the full-scale TEG. In addition, finite element modeling was performed to understand and predict thermal induced stresses, and interfaces were characterized using microscopy techniques to understand failure modes in order to improve the design.

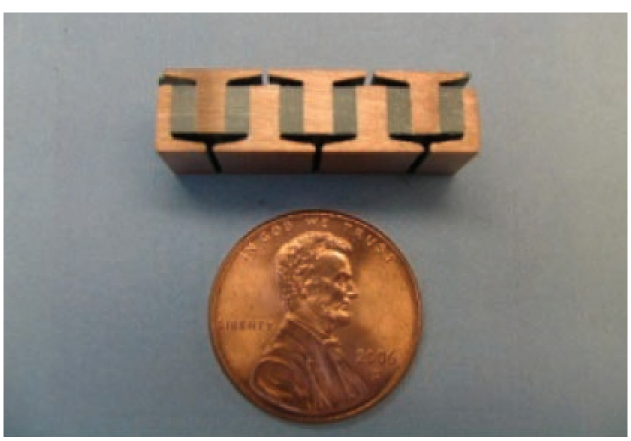

FIGURE 1. TE Subassembly

Results

High-Temperature TEG Design, Build and Test

Thermal cycling of TE subassemblies was performed using small TE subassemblies to evaluate and prove-out thermal and electrical interfaces. The testing was performed in a fixture consisting of electric cartridge heaters, liquid cold plate, separately adjustable thermal and electrical compressive loads, thermocouple and voltage sensor instrumentation. Fluid flowed through the cold plate continuously while electric power was cycled to bring the TE subassembly hot side up to the desired maximum temperature and then back down to the equilibrium temperature for the desired number of cycles.

Compressive forces, interface materials and other factors were varied in the evaluation of low-, medium- and high-temperature TE subassemblies. While the long-term goal is to provide a design that is suitable for the automotive environment, a threshold of 100 cycles with no degradation in performance was established as the Phase 3 prototype minimum requirement. Results for the low-temperature TE subassembly are shown in Figure 2.

Single Layer Results

A high-temperature single-layer TEG was built in Phase 3 (see Figure 3). Performance results as a function of air inlet temperature for the TEG are shown in Figure 4. The device achieved a peak power output of 125 W at 600°C air inlet temperature with an air flow of 45 cfm and a water temperature and flow of 25°C and 10 lpm.

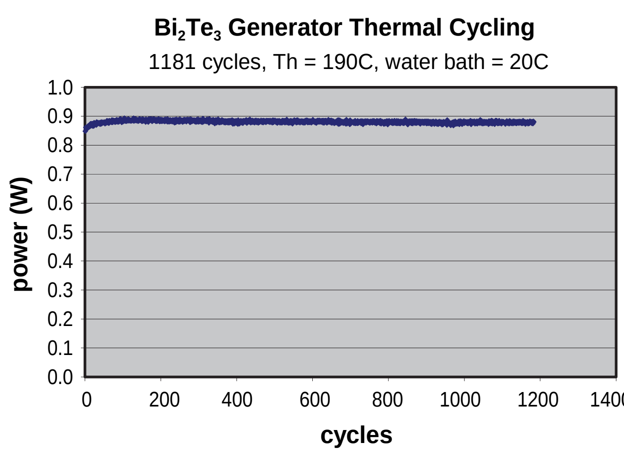

FIGURE 2. Low-Temperature TE Subassembly Thermal Cycling

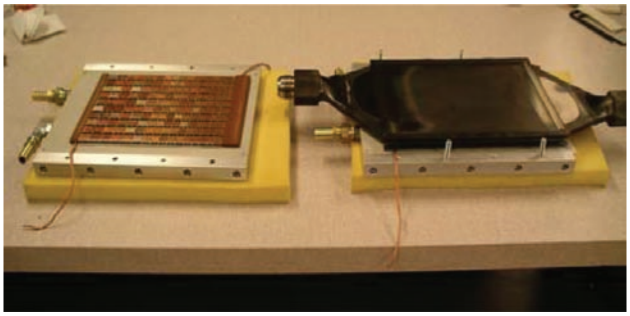

FIGURE 3. Single-Layer High-Temperature TEG

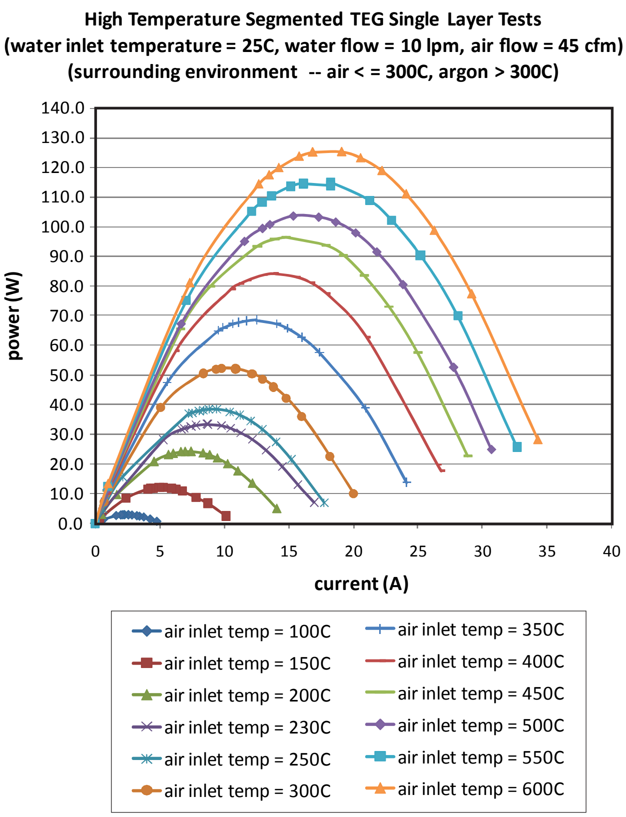

FIGURE 4. TEG Single-Layer Performance as a Function of Air Inlet Temperature.

PCS Test

The 100 W BiTe TEG was tested with a prototype Visteon PCS and resistive load. The prototype PCS includes:

- Boost and buck converters with microprocessor control to provide a maximum voltage of 12.8 volts direct current (resistive load maximum operating voltage).
- Serial data interface to report input and output voltage, current, power and converter efficiency.

The output of the TEG was connected to the PCS which in turn was connected to three 50 W automotive headlamps serving as the electrical load. The efficiency of converting TEG power produced using the PCS was measured. PCS conversion efficiencies ranged from 93% to 99%.

BMW Internal Combustion Engine Performance Results

In order to further improve the fuel efficiencies of automobiles it is essential to reduce first the fuel consumption of the energy conversion process of the internal combustion engine. One means is to downsize the displacement of the engine which results in a shift from naturally aspirated to turbo-charged engines in order to maintain the engine performance. For this type of engine, a part of the exhaust enthalpy is used to increase the charge-air pressure and thus increases the maximum power output per liter displacement. The turbine in the exhaust flow has an influence on the exhaust temperature and consequently on the potential of waste heat recovery measures, e.g. the TEG.

To reflect the growing importance of turbo-charged engines, the validated bumper-to-bumper simulation model that was presented in last year's report has been updated to this very efficient BMW engine. The investigated power train is equipped with an inline 6-cylinder engine with two turbochargers (displacement of 3 L with a maximum power output of 225 kW).

In consequence, several parts of the model had to be updated, e.g. the exhaust temperature map, the exhaust line geometry and the fuel consumption map. In addition to that the updated vehicle model has been coupled to the latest version of the transient TEG model from D. Crane (BSST). This version of the TEG model includes the most realistic simulation method of temperature-dependant TE material properties at higher thermoelectric figure of merit (ZT) values. Two different topologies for the TEG integration in the exhaust line have been analyzed. The after-flange position which is close to the catalytic converter, and the pre-tube position which is located further downstream in front of the middle muffler.

The cooling strategy has been changed from last year's concept using an auxiliary radiator to a new concept integrating the TEG into the low-temperature cooling loop of the powertrain.

Consequently the total fuel efficiency benefits due to the accelerated warm-up of the powertrain are significantly higher by the disadvantage of a higher temperature level at constant speeds compared to the system using an auxiliary coolant loop. Furthermore the influence of thermally insulating the exhaust line after the catalytic converter up to the TEG integration position and the effect of different ZT values on the fuel efficiency results were analyzed in order to evaluate the maximum technical potential of a TEG in an exhaust system.

The results of the fuel efficiency (FE) potential analysis for thermoelectric waste heat recovery in a vehicle equipped with a turbocharged BMW inline 6-cylinder engine are summarized in Table 1.

Table 1 shows the positive influence on the fuel consumption due to the unloading of the alternator and the accelerated powertrain warm-up (for the cold-start transient cycles) as well as the negative effects of an increased vehicle weight. The reduction of engine performance due to increased exhaust backpressure has been minimized by limiting the exhaust mass flow to 40 g/s.

The New European Driving Cycle (NEDC) shows FE improvements between 0.9% and 2.4% depending on the exhaust line integration position and the ZT value. The Federal Test Procedure (FTP) and U.S.-combined driving cycles show higher potentials between 1.5% and 5% as a result of higher engine loads and increased recuperated electrical power.

The constant speed operating points between 50 kph (~30 mph) and 160 kph (~100 mph) show promising results of 0.9% to 5.2% dependent on vehicle speed and the TEG configuration. The TEG has been designed for an operating point which is equivalent to approximately 130 kph on level tangent track. Therefore, a fraction of the exhaust gas has to be bypassed in case of higher engine loads, e.g. 160 kph point in Table 1, which leads to reduced FE benefits.

Ford Modeling Performance of a TEG in a Hybrid Electric Vehicle (HEV) Architecture

HEVs have the large, deep-discharge batteries and the electrical infrastructure to take advantage of electrical power generated in a TEG. To determine the amount of improvement in fuel economy achievable, a transient model was developed for a Ford Escape HEV with an inline 4-cylinder Atkinson-cycle engine using a combination of models: Gamma Technologies – Power for the engine performance, a BSST-developed Matlab-Simulink performance model, and a proprietary Ford systems model. The modeling study incorporates a design-of-experiments to determine the relative effect of different parameters in the TEG on engine exhaust backpressure (engine pumping losses), and cycle-averaged power generation. The FTP City and Highway driving cycles were used for optimization purposes. Results of this modeling are shown in Table 2. The performance of the TEG was limited, due to a requirement that the TEG performance model assume materials and manufacturing practices that are achievable in the near-term (2-5 years). Therefore, the average ZT equaled 0.97 and interfacial resistance was 2 Ω/cm^2 for this study. Table 2 shows the TEG power output for the City and Highway cycles. The results indicate a very small improvement in fuel economy. It is expected that as ZT and interfacial resistance are improved, FE results will also benefit.

TABLE 2. Summary Results of TEG Performance Modeling using Currently Available TE Materials

Cycle	Power (W)	% FE Increase
Highway	348	1.60
City	91	1.24

Future Directions

Single-Cylinder Engine Dynamometer Test of a Single-Layer, High-Temperature TEG

The performance of a high-temperature TEG will be evaluated in a Ford, single-cylinder hydrogen dynamometer development engine. The use of hydrogen as the fuel adds several engineering benefits to the testing: (1) it improves heat transfer properties of the exhaust gas, (2) combustion temperature can be controlled in a wide range for a given speed and load, and (3) no heat-exchanger fouling due to a lack of carbonaceous species in the exhaust gas. The testing is scheduled to begin in the fourth quarter of 2008. The test plan includes evaluating the performance of the TEG at a range of typical engine speeds, under various loading conditions. The temperature of the exhaust gas and cold-side will be varied at each of these test points. In addition, the effect of exhaust gas pulsation on improving heat transfer will be investigated. The

TABLE 1. FE Improvement by a TEG in a BMW 535i for Various Configurations and Driving Conditions

Position	Insulation	ZT	NEDC	FTP	US-Combined	50 kph	80 kph	100 kph	130 kph	160 kph
after Flange	no	0.85	1.5%	2.8%	3.1%	1.4%	1.3%	1.9%	3.4%	3.0%
after Flange	no	1.25	1.9%	3.4%	3.9%	2.1%	1.9%	2.5%	4.1%	3.6%
after Flange	no	2	2.4%	4.2%	5.0%	3.0%	2.7%	3.5%	5.2%	4.7%
Pretube	no	0.85	0.9%	1.5%	1.8%	0.9%	0.9%	1.4%	2.8%	2.5%
Pretube	no	1.25	1.1%	1.9%	2.4%	2.0%	1.9%	2.7%	4.4%	3.7%
Pretube	no	2	1.4%	2.4%	3.0%	1.4%	1.4%	1.9%	3.4%	3.1%
Pretube	yes	0.85	1.2%	2.2%	2.4%	1.1%	1.1%	1.6%	3.0%	2.7%
Pretube	yes	1.25	1.5%	2.7%	3.2%	1.7%	1.6%	2.2%	3.7%	3.3%
Pretube	yes	2	1.9%	3.4%	4.1%	2.4%	2.2%	3.1%	4.7%	4.3%

output of the TEG will be evaluated using a current-control electronic load sweep. Testing will conclude, by retesting key load-speed data using gasoline as the fuel. Results of the TEG output will be compared to BSST model predictions.

High-Temperature TEG Materials Characterization

Analysis of the high-temperature segmented TEG assemblies will follow the same basic methodologies as the earlier low-temperature studies. Initial characterization will be performed via scanning electron microscope and energy dispersive X-ray, followed by Auger, X-ray photoelectron spectroscopy, and X-ray diffraction. The purpose of this analysis will be to determine: (1) the root cause of any thermally-induced cyclic failures in TEG modules, (2) quantitative mapping of material homogeneity, and (3) any interdiffusion of species or intermetallic formation.

Full-Scale Engine Dynamometer Testing

A full-scale high-temperature TEG (500–750 W) will be tested with BMW's inline 6-cylinder engine with two turbo-chargers (displacement 3 L with a maximum power output of 225 kW) on a dynamometer at NREL in Golden, Colorado. This test will provide an independent, federal laboratory confirmation of fuel economy improvement over a range of driving conditions. The testing will also provide a means for final validation of the BMW computer performance model for the waste heat recovery system and is a key step prior to vehicle integration.

Conclusions

Significant progress in developing a waste heat recovery system for vehicle applications was made in 2008. With completion of Phase 3 activities coinciding with the end of calendar 2008, the BSST-led team is in position to start the 4th phase of the project which provides a demonstration of the system operating on a full-scale engine dynamometer at NREL in Golden, Colorado.

The lessons learned in building a 500 W BiTe TEG using the BSST stack design were applied in the design, build and test of a high-temperature TEG at BSST. The high-temperature TEG operated using 600°C exhaust gas and produced 125 W of electric power. TE subassemblies were thermal cycled and demonstrated an adequate degree of robustness to enable thorough testing at subassembly and TEG levels. Micrographic and spectrographic techniques were developed and used to characterize and improve electrical interfaces between TE materials and substrates.

The PCS was tested with a +100 W TEG and showed high efficiency in TEG power conversion. BMW and Ford modeled the performance of the TEG in internal combustion engine and hybrid platforms respectively. BMW's fuel efficiency improvement was predicted to range from 1% to 5% while Ford showed 1% to 2% improvement. Further gains are anticipated as the evaluation progresses and trade studies are performed to evaluate cost/benefit of various architectural options.

FY 2008 Publications/Presentations

1. 2008 ICT Conference.
2. 2008 DEER Conference.
3. 2008 DTEC Conference.
4. 2008 Semi-Annual Mega Merit Review.

III.3 Thermoelectric Conversion of Waste Heat to Electricity in an Internal Combustion Engine-Powered Vehicle

Harold Schock (Primary Contact), Tim Hogan, Eldon Case, Fang Peng, Fei Ren, Jeff Sakamoto, and Edward Timm
Michigan State University
301 Hannah Administration Building
East Lansing, MI 48824

DOE Technology Development Manager: John Fairbanks

NETL Project Manager: Samuel Taylor

Subcontractors:
- Northwestern University, Evanston, IL
- Iowa State University, Ames, IA
- Jet Propulsion Laboratory, Pasadena, CA

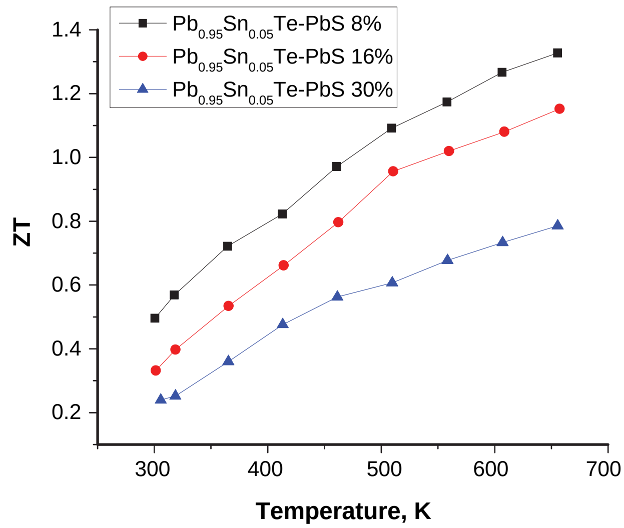

FIGURE 1. Thermodynamic Figure of Merit (ZT) Data Acquired from Individually Prepared Ingots

Phase 2 Objectives

- Evaluate advanced thermoelectric (TE) material properties and down-select a system for a 500 Watt demonstration unit by the end of the Phase 2 effort.
- Quantify material and TE properties of lead, antimony, silver, lead, antimony, silver, and tellurium (LAST)/LAST+tin (LASTT) and skutterudites systems.
- Evaluate other new TE systems with respect to efficiency and mechanical performance.
- Evaluate potential performance improvements possible when utilizing TE generators in a Class 8 truck application.
- Down-select a material based on success in fabricating modules that will be viable for construction of a 500 Watt demonstration generator.
- Select a design and build a 500 Watt demonstration unit from the down-selected material.

Accomplishments

- Bulk mechanical properties and micro-structural analysis of hot pressed LASTT and skutterudites have been evaluated at Michigan State University (MSU).
- The TE system for a number of lead and tellurium (PbTe)-based systems has been evaluated with typical performance shown in Figure 1.
- Performance improvements for an over-the-road truck have been accessed based upon the performance of TE material which has been synthesized and tested at MSU.
- Numerous LAST/T and skutterudite-based modules have been fabricated at MSU.
- Based upon success in fabrication hot pressed modules, we have down-selected skutterudites as the material from which we will construct the 500 Watt demonstration generator.

Future Directions

- Complete the design of a 500 Watt generator to be demonstrated in Phase 2.
- Complete design and fabrication of fixtures required to construct modules which will make up the 500 Watt generator.
- Complete design and fabrication of power electronic systems that will be used in the demonstration of the 500 Watt generator.
- Continue to evaluate advanced systems as Phase 2 resources permit.
- Demonstrate operation of the 500 Watt system by July, 2008.

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Introduction

This project has been an in-depth effort aimed at determining the viability of using advanced TE materials implemented in an electric generator to recover waste heat from an over-the-road (Class 8) truck. Aspects of the project have included evaluation of both the mechanical and TE properties of the new material systems and a study to determine the feasibility of constructing a generator using the advanced material deemed most promising for a demonstration within the time frame of this project. We recognize that segmentation of various systems is a technology which can significantly improve the efficiency of a TE couple. However, the complications associated with mating dissimilar materials such as BiTe with LAST systems at the couple level were beyond the scope allowed for in the Phase 2 effort.

Approach

Evaluating the viability of using TE materials for energy recovery in a transportation-related application requires one to evaluate many topical areas. With respect to TE materials these remarks refer to "bulk" materials, formed in a casting process. The energy conversion efficiency of the bulk thermoelectric material is very important along with it's viability for "mass" production and processing. If a small amount of material or a segment of a cast ingot exhibits a very high efficiency it is of interest from a scientific perspective, but from a commercial perspective it may not be viable. Segmented couples with efficiencies of nearly 15% have been demonstrated by the National Aeronautics and Space Administration-Jet Propulsion Laboratory [1] but the high temperature gradient under which these materials were demonstrated are not available in the exhaust of most transportation systems. High efficiency materials have been reported with other systems such as LAST [2], however the poor mechanical integrity of the cast systems makes it imperative that the materials be ground into powders and pressed into usable ingots with uniform mechanical properties which are superior to the cast material. Developing high efficiency materials, which have been powder processed, is a major challenge. Metallization of the hot-pressed legs and appropriate module construction, which can reduce thermal stresses to an acceptable level, is another important module design issue. In the Phase 2 effort, after carefully evaluating all aspects of generator design, we have decided to construct our 500 Watt demonstration generator using 10-13 Watt skutterudite-based modules.

Development of a heat exchanger system, which can extract the energy from the exhaust and direct it to the hot side of the thermoelectric couple, requires novel engineering designs. Our experience with these problems using extensive simulations has shown that when going from the efficiency of a laboratory-tested couple to a generator it can easily result in a 50% reduction in efficiency of the couple. This of course translates to a 50% reduction in the efficiency of the overall generator.

We have had good success in the design of the power electronics associated with the generator and believe that we will have a 5 volt (V) input, 48 V output systems with efficiencies greater than 90%. Module failure mitigation and compact size for the power electronics has also been addressed.

Results

- We have chosen skutterudite material to be used in the building of a 500 Watt demonstration generator. A 13 Watt sub-assembly (WSA) is shown in Figure 2.
- Potential improvements in fuel economy for a Class 8 over-the-road truck have been evaluated and the results are shown in Figure 3.
- Fuel economy improvements using early 2008 diesel fuel prices could provide $90,909 in savings over the 1 million-mile life of a truck. Deterioration of the generator is an issue which needs to be addressed.
- When evaluating potential TE systems for implementation in energy recovery devices, issues related to generator fabrication and heat exchanger designs are equally critical to the efficiency of the new TE material which is to be developed.

Conclusions

- Systems for material synthesis, powder processing, hot pressing, leg and module fabrication are operational at MSU.

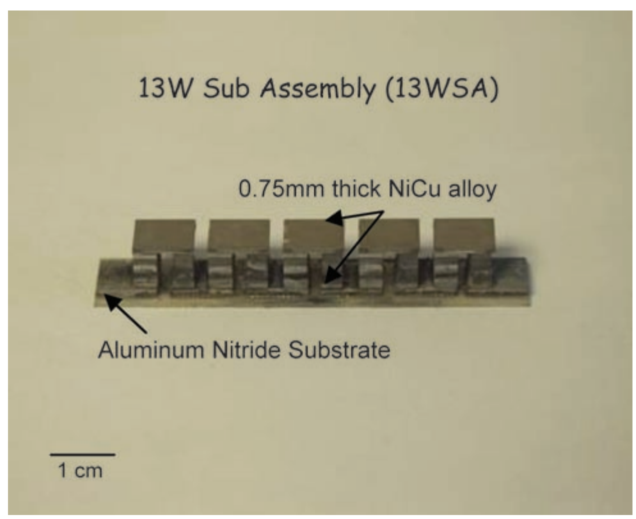

FIGURE 2. 13 WSA Prototype with Metallurgical High-Temperature Bonds on the Hot-Side (discoloration on the sides of the legs from slight sublimation and condensation during bonding)

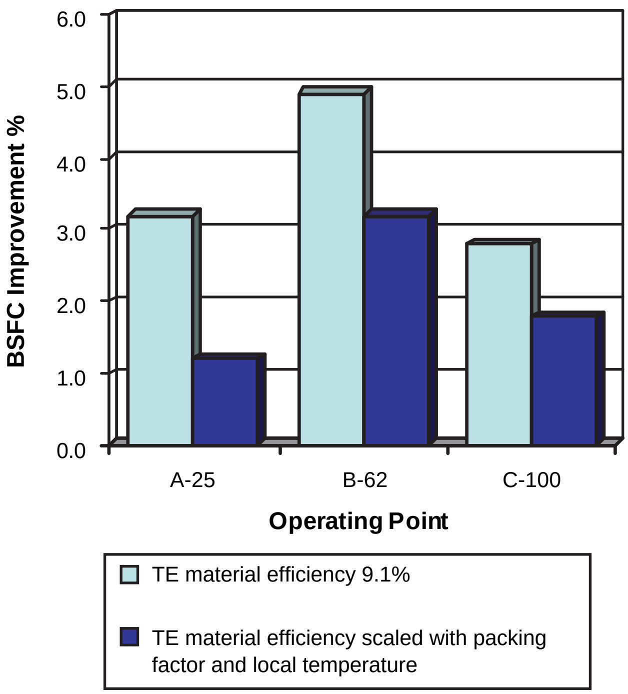

FIGURE 3. Calculated Brake Specific Fuel Consumption (BSFC) Improvement of LAST, LASTT-BiTe Materials

- Performance testing of legs and modules at MSU is in agreement with others doing similar measurements.
- The MSU group has demonstrated the capability to produce materials required for a 500 Watt module in one month.
- Power conditioning electronics are being designed and tested at MSU.
- Improved heat exchanger designs are critical to success of TE effort for waste heat recovery.
- Using TE generator technology, a 5% improvement in BSFC for an over-the-road truck is a reasonable 5-year goal …a 10% improvement possible with new TE materials and advanced heat exchangers.

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IV. UNIVERSITY RESEARCH

IV.1 University Consortium on Low-Temperature Combustion For High-Efficiency, Ultra-Low Emission Engines

Dennis Assanis
University of Michigan (UM)
Mechanical Engineering
2045 W.E.Lay Auto. Lab.
1231 Beal Avenue
Ann Arbor, MI 48109-2133

DOE Technology Development Manager: Gurpreet Singh

NETL Project Manager: Samuel Taylor

Subcontractors:
- Massachusetts Institute of Technology (MIT), Cambridge, MA
- Stanford University (SU), Stanford, CA
- University of California, Berkeley (UCB), Berkeley, CA

Objectives

- Investigate the fundamental processes that determine the practical boundaries of low-temperature combustion (LTC) engines.
- Develop methods to extend LTC boundaries to improve the fuel economy of homogeneous charge compression ignition (HCCI) engines fueled on gasoline and alternative blends, while operating with ultra low emissions.
- Investigate alternate fuels, ignition and after-treatment for LTC and partially premixed compression ignition (PPCI) engines.

Accomplishments

- Last year's experimental high-load limit established by supercharging has been extended by 1 bar net mean effective pressure (NMEP) to near 6 bar in both single- and multi-cylinder tests. Expectations are that this can be extended further by optimizing external exhaust gas recirculation (EGR), pressure level and combustion phasing.
- Fuel injection during negative valve overlap (NVO) was previously demonstrated to extend the low-load limit to near 1 bar NMEP. The recompression reactions believed responsible have been explored in detail using a reduced chemical kinetic model for n-heptane to simulate the reactions and heat release during the NVO period. It was found that ignition on the next cycle can be advanced or retarded depending on the overall oxygen concentration and the NVO temperature.
- The GT-Power® modeling tool with combustion submodel developed in the consortium has been used to generate performance maps for various proposed valve actuation schemes subject to ignition, oxides of nitrogen (NOx) and knock constraints as well as combustion stability considerations. The model has been coupled to a simplified turbocharger model. Results suggest that the high-load limit can be extended without knock provided the mixture is leaned-out or diluted as pressure is increased.
- For direct injection (DI) and PPCI engine applications an improved flamelet combustion model has been developed to describe the interaction between spray and combustion. The proposed spray-interactive reduced dimension model (SIRDM) includes the spray source terms, such that droplet vaporization history can be properly accounted for in the reaction space. The results show good agreement with stratified DI-HCCI experiments reported in the literature.
- A thermodynamic analysis has been carried out to delineate the combustion regimes for spark-assisted (SA)-HCCI. The analysis confirms optical engine experiments reported last year and indicates that the regime for SA exists between normal spark ignition (SI) operation and HCCI. Because robust flame propagation requires somewhat higher burned gas temperatures than HCCI, spark assist is likely to be useful as an ignition helper when not enough sensible heat is available for auto ignition.
- A first generation model of a urea selective catalytic reduction (SCR) catalyst has been assembled using AVL Boost with appropriate chemical equations drawn in part from previous work at UM and from the literature. The model was then used to explore the effect of catalyst size on effectiveness in a typical engine application and validated against second-by-second experimental engine exhaust data from a 6.0 L Navistar V-8 engine over the Federal Test Procedure (FTP) 75 driving cycle.
- Rapid compression ignition delay measurements have been made for a number of isomers of simple five and six carbon esters representative of future bio-derived fuels. The range of ignition delays is significant, and blending with n-heptane shows non-linear effects which may be useful in designing future fuels.

Future Directions

- Carry out experimental work with single- and multi-cylinder engines to further extend upper and lower load limits, with consideration of constraints on knock, NOx and stability. Technologies to be employed include turbo/supercharging, external EGR, fast thermal management and super-critical water injection.
- Complete the validation of the GT-Power®-based LTC engine simulation tool with data from single-cylinder experiments on burn rate, combustion efficiency and stability limits.
- Complete modified KIVA/flamelet model of SA-HCCI and explore potential benefits of the technology from the point of view of control and range extension. Use Hydrodynamics, Chemistry, Thermodynamics (HCT) kinetics code to build up a laminar flame speed database for use in the flamelet model in thermodynamic regimes not currently covered in the literature.
- Refine SCR and diesel oxidation catalyst (DOC) after-treatment models in conjunction with new bench test experiments carried out under simulated LTC conditions.
- Extend ignition delay experiments on alternative fuels to include blends. Establish the nature and extent of interactions of these fuel blends with respect to non-linear behavior and negative temperature coefficient (NTC) effects.

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Introduction

LTC is a new technology for internal combustion engines which promises to provide improved fuel economy with low emissions. With this technology, the engine is operated lean and cool enough to drastically reduce NOx emissions and reduce particulate matter (PM). In addition, operating lean allows high compression ratios for gasoline and reduces particulate emissions in diesels. The overall effect is to increase fuel economy for gasoline applications by up to 20%, and in the case of diesel engines, provide the means of satisfying the new, more stringent emissions regulations.

Because LTC implies operation at temperatures near the limit of flame propagation, reliable combustion is usually initiated by auto-ignition which requires successful control of the thermal history of the gas charge and the engine. In principle this can be achieved with adequate thermal management control; and various methods have been suggested for accomplishing this. However, as seen in Figure 1, full use of LTC has been limited at both high and low loads; this situation threatens to reduce the ultimate fuel economy benefit that can be achieved in a vehicle system. At low load there is not enough heat in the charge to keep combustion healthy, while at high load the combustion is too rapid and may damage the engine structure. The main focus of this consortium is to investigate the limit phenomena and to propose methods of extending the limits. As indicated in Figure 1, consortium experiments (square data points) have demonstrated extended operation at both high and low loads.

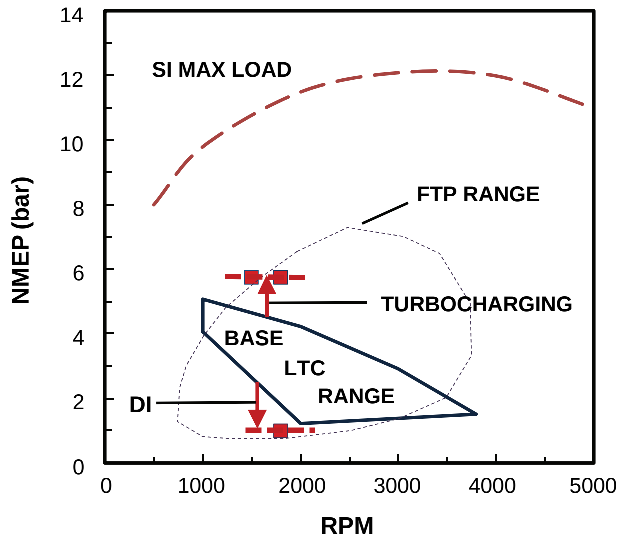

FIGURE 1. Speed-load map for a naturally aspirated automotive engine showing maximum load line, desired region for FTP cycle operation (dashed oval), and base LTC range limited by knock at high load and misfire at low load. Square data points denote consortium engine experiments demonstrating expanded operation by turbocharging and by DI during NVO.

Approach

Our research project, in its third year, combines experiments and modeling at four university research centers in order to acquire the knowledge and technology to extend the load range of LTC engines. To accomplish this, both single-cylinder and multi-cylinder engine experiments are investigating direct fuel injection strategies, turbo/supercharging, and fast thermal management as possible approaches. Other tasks concentrate on spark-assisted LTC, and the ignition characteristics of alternate and bio-fuels. Recognizing the role of emission constraints particularly in the context of transient vehicle operation, studies of after-treatment devices are underway with specific application to the low exhaust temperatures typical of LTC both for HCCI and for PPCI systems.

An array of modeling tools are being developed and refined, and brought to bear on the specific limit problems of importance. These models cover a range of detail from system models for engines and after-treatment devices, through fully coupled computational fluid dynamics (CFD)/kinetic models, to detailed and reduced chemical mechanisms. Our intent is to take advantage of the broad range of capabilities of the university partners and the collaborative relationships among them.

Results

High-Load HCCI

Engine Experiments - At higher loads, combustion in HCCI engines becomes progressively more rapid and eventually results in undesirable rates of pressure rise. One way of decreasing the rate of pressure rise is by dilution either with air or with residual gases. This effectively reduces the temperature rise during combustion and the rate of energy release. Experimental work in the consortium has utilized both turbocharging and cooled external EGR to achieve this effect. The results so far have demonstrated increases in high-load operating range to approximately 6 bar NMEP at 1,500 rpm as shown in Figure 1. Further optimization with respect to combustion phasing and external/internal EGR fraction is underway.

System Modeling - In complementary modeling work focused on high-load limits, we have extended our GT Power©-based model [1] of an HCCI engine to include a simplified turbocharger model which assumes fixed efficiencies for compression and expansion. Three calculated load sweeps are shown in Figure 2 for manifold pressures of 1.1, 1.5 and 2.0 bar. As indicated in the figure, turbocharging to 2.0 bar can potentially raise the load limit to near 8 bar NMEP. The figure also shows that for low loads, higher turbocharging is less efficient. In general our work with the model indicates that the high-load limit is complicated by a number of factors such as the NOx constraint, the knocking constraint, as well as breathing limitations either for fresh charge or for internal EGR. The result is that conclusions are specific to each particular engine valve arrangement and external thermal assumptions. In our future work we will use the model to further identify and quantify the fundamental combustion limitations and link them to the external design parameters to better assess potential implementation schemes.

Low-Load HCCI

DI during NVO - Previously the consortium (Stanford) demonstrated experimentally that injecting fuel during the NVO period, resulted in achieving lower loads as shown in Figure 1. To understand this phenomenon better, a single-zone model was employed using detailed chemical kinetics. The model assumed perfect mixing at various crank angle timings within the overlap period and then tracked the subsequent evaporation and cooling and chemical reactions.

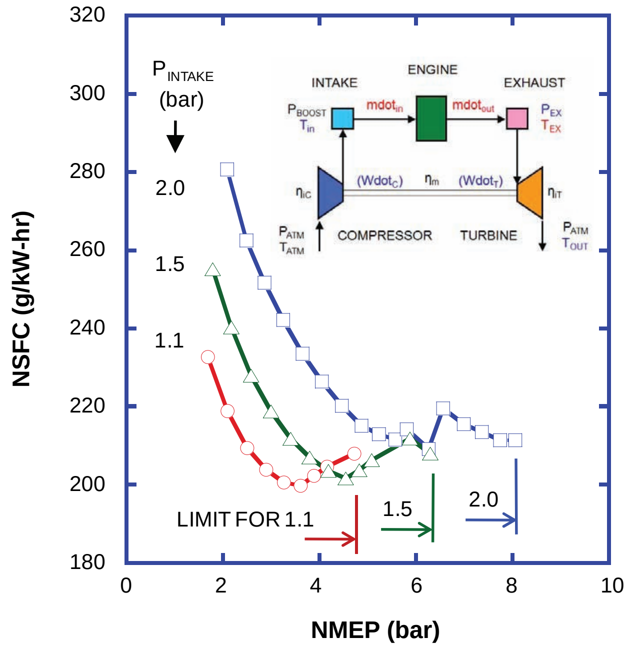

FIGURE 2. Predicted high-load limits and fuel economy using an idealized turbocharger, as computed by the GT-Power® HCCI model with UM-developed combustion model. (NSFC - net specific fuel consumption)

In the simulations [2], detailed kinetic mechanisms of two pure chemicals (n-heptane and iso-octane) were adopted to elucidate both chemical and thermal consequences of recompression reaction. It is noted that the chemical consequence of recompression reactions depends largely on the residual oxygen concentration and sensible state during NVO, while the thermal consequence is affected mainly by the amount of fuel-charge-cooling.

To isolate the chemical effect of recompression reactions on main combustion, the ignition delay of the recompression products after dilution with the fresh charge was evaluated at constant volume. At near-stoichiometric operation, fuel-pyrolysis products exhibit overall shorter ignition delay compared to that of the base fuel (n-heptane). However, the endothermicity of fuel pyrolysis during NVO reduces overall mixture temperature, which counteracts the improved mixture ignitability. At equivalence ratios near 0.8, the transformed fuel mixture combined with modest exothermicity leads to the shortest ignition delays. Finally, near the leanest conditions (equivalence ratio ~0.6), significant oxidation of fuel during NVO results in relatively long ignition delay due to low fuel chemical energy available, while increased temperature from exothermicity partially compensates for the lengthening of ignition delay. Consequently, it is apparent that there are competing effects between thermal and chemical consequences of recompression reactions on mixture ignitability, which leads to an optimum oxygen concentration (here near equivalence ratio 0.8) for the shortest ignition delay.

Spark-Assisted HCCI – In consortium experiments with an optical engine at UM, Zigler, et al. [3] observed the effect of spark assist in extending HCCI operation. These studies, in agreement with others in the literature, have clearly indicated the presence of a wrinkled flame near the spark plug early in the cycle. Later, as the pressure and temperature rise, autoignition of the main charge takes place. Under certain conditions the timing of the autoignition is advanced and the operating range is extended.

In an attempt to better understand spark assist, analytical work was carried out to delineate typical combustion regimes in an SI-HCCI engine in terms of the local thermodynamic conditions. Figure 3 shows the regimes mapped according to unburned (T_U), and adiabatic burned gas temperatures (T_B). Constant equivalence ratio lines progress from lower left to upper right. When EGR is present, equivalence ratio refers to the total diluents ratio, i.e. Φ represents Φ (1-EGR) as a relative measure of energy content of the charge. The rectangular HCCI region to the lower right of the figure is determined by ignition, misfire and NOx constraints. The SI region on the upper left is determined by requirements of good laminar flame propagation, lean or stoichiometric mixture and borderline knock limits.

The region where spark assist is feasible lies between the HCCI and the SI zones. It is interesting

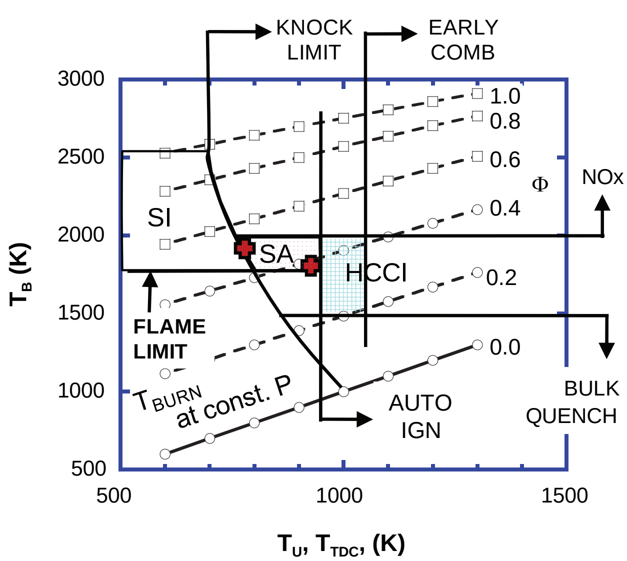

FIGURE 3. Schematic map of combustion regimes for SI, SA, and HCCI determined by constraints on unburned temperature (auto-ignition, combustion phasing and knock); and on burned gas temperature (flame limit, quenching, and NOx limit). Crosses denote conditions of UM optical engine experiments.

that because of the flame speed requirement, SI cannot function at equivalence ratios as low as HCCI. From this it seems likely that spark assist acts primarily as an ignition helper under conditions where insufficient sensible energy is available in the unburned gas. The two data points shown in the SA-HCCI region indicate the conditions under which the spark-initiated flame observations were made in the UM optical engine. Because little or no experimental flame speed data are available in this region we are currently carrying out an analytical study of flame speeds in this regime up to T_U=1,000 K with the one dimensional HCT flame code with the idea of better understanding the flame propagation under near-autoignition conditions, and especially at higher pressures. Ultimately it is planned to use the HCT generated data set as the basis of a KIVA-flamelet model of SA-HCCI.

PPCI and Kinetics

Flamelet Modeling of PPCI Combustion - An improved combustion model based on the flamelet concept has been developed in order to account for the interaction between spray and combustion, for DI and PPCI engine applications. While the representative interactive flamelet model has been successfully applied to DI combustion, the model does not fully incorporate the effects of fuel addition in the reactive space as a result of spray evaporation. In the new SIRDM, the governing equations in the reactive space have been reformulated to include the spray source terms, such that droplet vaporization history can be properly accounted for in the reaction space. The SIRDM is implemented in engine simulations using KIVA-3V to investigate the effect of mixture stratification under PPCI operating conditions utilizing different injection timings. Figure 4 shows numerical results in qualitative agreement with the experimental engine data of Dec and Sjoberg [4] for a sweep of start of injection (SOI) timing in an HCCI engine at a low overall equivalence ratio of $\Phi = 0.1$. The inset images show the KIVA-generated equivalence ratio maps at top-dead center (TDC) for several SOI timings. As injection timing is delayed there is less time for mixing and the mixture becomes progressively more stratified. This leads to less fuel in regions too lean to burn and the combustion efficiency increases while the CO emissions decrease (not shown).

After-Treatment System Modeling - The goal of this task is to develop successful after-treatment models and system models for low-temperature applications in PPCI. For this purpose a systematic methodology was developed to generate heterogeneous global reaction kinetics for hydrocarbons, CO, H_2 and NO under lean conditions and temperature ranges typically observed in oxidation catalysts. The methodology involves bench reactor tests, optimization of kinetic parameters, modifying and re-optimization of the rate expressions

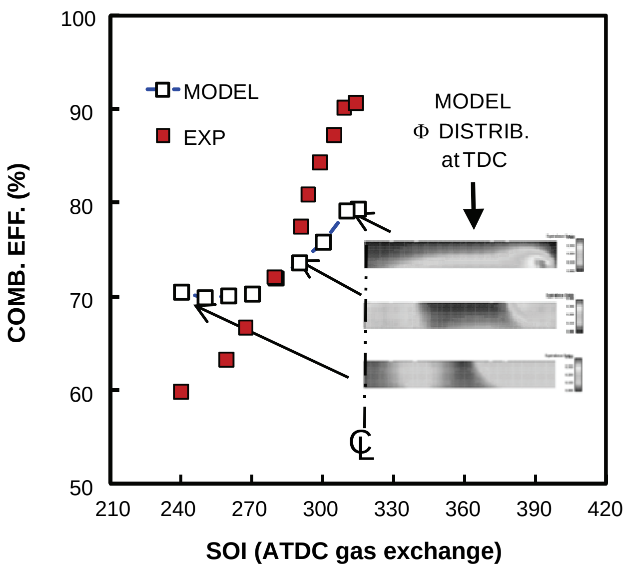

FIGURE 4. Effect of injection timing on HCCI combustion efficiency; SIRDM model compared to experimental results of Dec and Sjoberg [4]. Insets are predicted Φ distributions at TDC showing greater stratification with later injection.

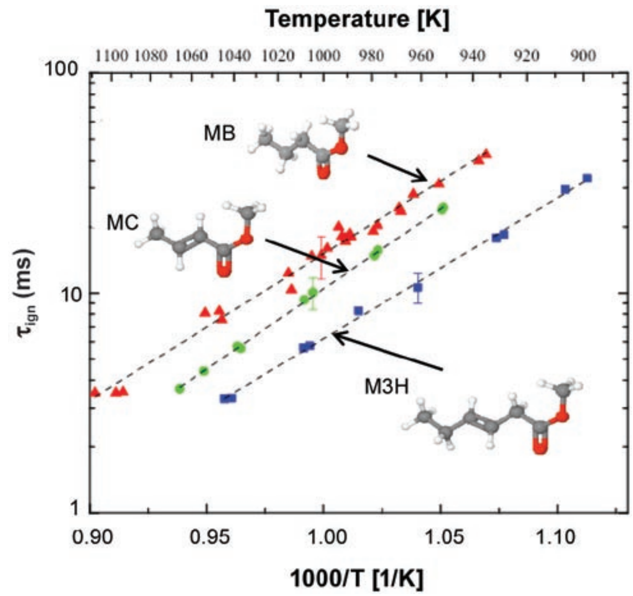

FIGURE 5. Ignition delay times for three biofuel esters measured in the RCF: methyl butanoate (MB) with the longest delay times comparable to isooctane, methyl crotanoate (MC), and methyl trans-3-hexanoate (M3H) the most reactive.

and finally, validation by comparison with actual engine experimental light-off curves. Last year the consortium reported on the development of a successful model for a DOC.

This year a model has been developed for a urea-SCR catalyst. This development extended a model taken from the literature [5] and re-optimized it using new bench test data. The model was tested against second-by-second experimental data from a from a 6.0 L Navistar V-8 engine run over the FTP 75 driving cycle. The new model was compared against the published model of Olsson et al., [5] and showed significant improvement in the integrated error level over the FTP cycle for NH_3, NO, NO_2, and N_2O. Work is underway to set up a new reactor bench at UM to enable further validation of the reaction mechanisms.

Kinetics of Alternative Fuels - During the past year we have conducted UM Rapid Compression Facility (RCF) studies of several classes of oxygenated ester compounds as representatives of bio-derived fuels. We now have a library of ignition data for several prototypical ester structures representing varying degrees of chain length and levels of saturation. By combining our data with the results of shock tube experiments found in the literature, we have developed new reaction mechanisms for two of the ester compounds which yield excellent agreement with the experimental data over a large range of temperatures (900-1,700 K), pressures (1-10 atm) and equivalence ratios ($\phi = 0.3$-1.0). The mechanisms have been developed in collaboration with Dr. Charlie Westbrook, our partner at Lawrence Livermore National Laboratory [6]. These results are shown in Figure 5 and indicate a factor of three difference in ignition delays between the esters at equivalent temperatures.

In addition, we conducted preliminary UM RCF ignition studies of ester/n-heptane blends. Methyl trans-3-hexanoate was used as the reference ester compound due to the larger hydrocarbon chain and because it represents an unsaturated ester (which are typically more prevalent in biodiesels than saturated esters). The results indicate NTC behavior for blends containing larger amounts of n-heptane and non-linear blending behavior as seen in Figure 6. These data are also the first of their kind and provide understanding of the fundamental reaction chemistry important during combustion of oxygenated compounds and blends with hydrocarbon fuels.

Conclusions

- Modeling of the high-load HCCI limit suggests that loads as high as 8 bar NMEP should be possible provided that the mixture is diluted sufficiently by turbo or supercharging with air and external EGR. The results are highly sensitive to the particular valve arrangement for internal EGR.
- Experimentally, the high-load limit has been extended to near 6 bar NMEP in both single- and multi-cylinder tests. Expectations are that this can be extended further by optimizing external EGR, pressure level and combustion phasing.

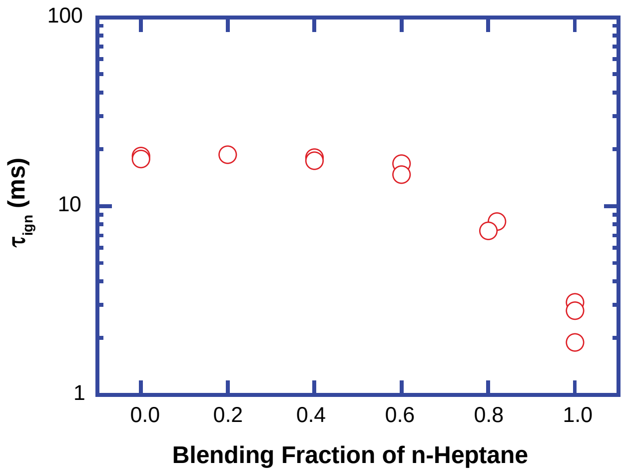

FIGURE 6. Measured ignition delay times of n-heptane/methyl trans-3-hexanoate (M3H) blends at $\Phi = 0.3$, P = 10.5 atm, T = 925 K, inert/$O_2 = 3.76$. Non-linear behavior is seen at higher blending fractions of n-heptane. Blends also exhibit NTC in this region.

- Low-load extension experiments on a single-cylinder engine have shown that varying the timing of NVO injection affects the combustion phasing and shows promise as a control tool.
- The mechanism of low-load extension by fuel injection during NVO has been explored using a reduced chemical kinetic model for n-heptane to simulate the reactions and heat release. It was found that ignition on the next cycle can be advanced or retarded depending on the overall oxygen concentration and the NVO temperature, factors which influence the relative effects of exothermic and endothermic reactions.
- An analysis of the combustion regimes for SA-HCCI indicates that the regime for spark assist exists between normal SI operation and HCCI. Because robust flame propagation requires somewhat higher burned gas temperatures than HCCI, spark assist appears to function as an ignition helper when not enough sensible heat is available for auto-ignition.
- Rapid compression ignition delay measurements have been made for a number of isomers of simple five and six carbon esters that represent future bio-derived fuels. The range of ignition delay times is significant (factor of 3), and blending with n-heptane shows non-linear effects which may be useful in designing future fuels.

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IV.2 Optimization of Low-Temperature Diesel Combustion

Profs. Rolf Reitz (Primary Contact), Pat Farrell, Dave Foster, Jaal Ghandhi, Scott Sanders, Chris Rutland
Engine Research Center (ERC)
University of Wisconsin-Madison
1500 Engineering Drive
Madison, WI 53706

DOE Technology Development Manager:
Gurpreet Singh

Objectives

- Develop methods to optimize and control low-temperature combustion diesel (LTC-D) technologies that offers the potential of nearly eliminating engine oxides of nitrogen (NOx) and particulate emissions at reduced cost over traditional methods by controlling pollutant emissions in-cylinder.
- Use single- and multi-cylinder engine experiments and detailed modeling to study factors that influence combustion phasing, particulate matter (PM), NOx, unburned hydrocarbon (HC) and carbon monoxide (CO) emissions.
- Recommend improved combustion chamber geometries matched to injection sprays.
- Investigate role of fuel-air mixing, fuel characteristics, fuel spray/wall impingement and heat transfer on LTC-D engine control.
- Provide criteria for transition to other engine operation regimes (e.g., standard diesel and low-temperature combustion).

Approach

- Use fully-instrumented engines with prototype fuel injection systems and combustion sensors to map and define homogeneous charge compression ignition (HCCI) combustion regimes, and apply optimization techniques to discover low emissions operation methodologies.
- Develop and apply modeling tools, including multi-dimensional codes (e.g., KIVA with state-of-the-art turbulent combustion and detailed and reduced chemistry models) to reveal combustion mechanisms.
- Use advanced fuel injection strategies, and manipulation of fuel characteristics to explore approaches to achieve optimal low-temperature combustion operation.
- Use fast response diagnostics to formulate transient engine operation strategies during load and speed changes to extend LTC-D engine operating limits.

Accomplishments

- Reduced mechanisms and efficient chemistry solvers have been developed for use in advanced computational fluid dynamics (CFD) and engine system combustion models.
- New high resolution optical diagnostics have been developed for in-cylinder chemical species measurement and for combustion model validation.
- Grid-independent spray models have been developed for improved CFD accuracy.
- Advanced large eddy simulation (LES) turbulence models have been developed.
- Advanced fuel injection concepts, such as variable pressure injection have been proposed and explored, and injector models have been formulated.
- LTC-D engine performance has been characterized in the ERC's light-duty and heavy-duty diesel engine laboratories with a wide variety of fuels, with emphasis on fuel properties such as cetane number (CN), aromatic content and volatility.
- Ultra-low emissions and improved fuel efficiency have been demonstrated when operating a LTC-D engine on gasoline fuel.
- Component heat transfer models have been developed for thermal analysis modeling.
- Advanced optimization tools have been developed and applied to recommend optimal piston bowl geometries.
- Mixed-mode combustion regime transitions have been explored in multi-cylinder engine tests and system models.

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Introduction

This project was initiated in response to a DOE solicitation for research and development on HCCI diesel-fueled engines under the "FreedomCAR and Vehicle Technologies Program Solicitation for University Research and Graduate Automotive Technology Education Centers of Excellence." The program is in response to the fact that the engine industry is currently facing severe emissions mandates. Pollutant emissions from mobile sources are a major source of concern. For example, U.S. Environmental Protection Agency (EPA) mandates require emissions of PM and NOx from heavy-duty diesel engine exhaust to drop at least 90 percent between 1998 and 2010. Effective analysis of the combustion process is required to guide the selection of technologies for future development since exhaust aftertreatment solutions are not currently available that can meet the required emission reduction goals. The goal of this project is to develop methods to optimize and control LTC-D that offers the potential of nearly eliminating engine NOx and PM at reduced cost over traditional methods by controlling pollutant emissions in-cylinder. The work is divided into five tasks, featuring experimental and modeling components:

1. Fundamental understanding of LTC-D and advanced model development,
2. Experimental investigation of LTC-D combustion control concepts,
3. Application of models for optimization of LTC-D combustion and emissions,
4. Impact of heat transfer and spray impingement on LTC-D combustion, and
5. Transient engine control with mixed-mode combustion.

Results

Task 1. Fundamental Understanding of LTC-D and Advanced Model Development

Homogeneous or partially premixed charge compression ignition combustion is considered to be an attractive alternative to traditional internal combustion engine operation because of its extremely low levels of pollutant emissions. However, since the start-of-combustion timing is controlled by chemistry, kinetic models for diesel combustion are needed for engine analysis. The goal is to reduce available detailed chemistry mechanisms to a manageable size (ideally less than 60 species and 100 reactions) for use in multidimensional simulations. A primary reference fuel (PRF) chemistry mechanism has been developed, and validation of the mechanism predictions is being done by comparing measured and simulated in-cylinder gas compositions, under low-temperature combustion conditions. Hyperspectral absorption spectroscopy has been developed for the temperature and species concentration measurements. A water gas thermometer has been developed that allows temperature measurements to be made in the engine at 3.5 kHz (1 crank angle degree [CAD] at 600 rev/min) with an unprecedented 0.1% (2 K at 2,000 K) root-mean-square precision. Comparison of modeled and measured gas temperatures is shown Figure 1. In addition, a methodology based on Fourier transform infrared spectroscopy has been implemented that will allow further comparisons with other species including H_2O, CO_2, CO, C_2H_2, CH_4. Additional information

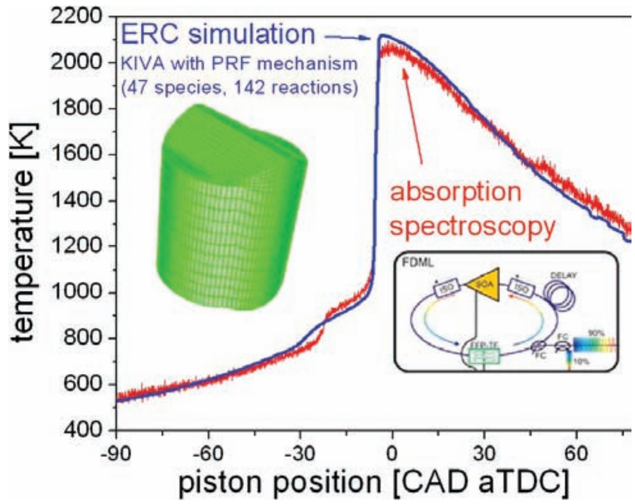

FIGURE 1. Temperature measured by hyperspectral water absorption spectroscopy compared with KIVA PRF fuel model predictions. The temperature measurement has an unprecedented precision of 0.1% (2 K at 2,000 K). (aTDC - after top dead center)

about the diagnostic tools is available at www.erc.wisc.edu (click on "optical diagnostics"), and a patent application has been made [1]. High spatial resolution measurements of scalar fields in an internal combustion engine are also being conducted to help validate the turbulence model development of Task 1. Laser-induced fluorescence measurements have been performed over a wide range of operating conditions to investigate the dependence of the scalar energy and dissipation spectra on the Reynolds numbers for intake jet flows [2].

Task 2. Experimental Investigation of LTC-D Combustion Control Concepts

An advanced two-stage or dual mode combustion strategy for simultaneous reductions of HC, CO, and NOx has been tested on the ERC's Caterpillar 3401 SCOTE heavy-duty diesel engine. In this case, a low-pressure Bosch gasoline direct injector (10 MPa injection pressure) is used together with a high-pressure Bosch common rail injector (150 MPa injection pressure). Two-stage combustion (TSC) was studied as a way to lower emissions from diesel combustion. However, it was found that the PM from the main injection was higher than predicted by the simulation results that were used to guide the development of the TSC approach [3]. To help resolve the discrepancy between the model and experiments, different fuels were used to explore their effects on the PM formation from the main injection. Gasoline and other volatile PRF blends were found to reduce PM compared to diesel. Next, gasoline was used exclusively in both injections. This produced low emissions, approaching EPA 2010 levels, but with high brake specific fuel consumption due to the late timing of the main fuel injection.

Finally, gasoline was again used but with combustion in the partially premixed combustion (PPC) mode and was found to allow low engine-out emissions even at moderately high load ~ 12 bar indicated mean effective pressure (IMEP) (see Figure 2), while maintaining low fuel consumption. Currently PPC is showing great promise to lower engine-out emissions. The results from these tests show significant emissions improvements, with the best results giving NOx 0.41 g/kw-hr, PM 0.0212 g/kw-hr, HC 2.68 g/kw-hr, CO 6.75 g/kw-hr with an indicated specific fuel consumption (ISFC) of 173.5 g/kw-hr, and pressure rise rate of 12.4 bar/deg. Note that it is possible to use production injection hardware and commercially available fuel, while producing low emissions.

The potential of achieving LTC-D operation in a high-speed direct injection (HSDI) automotive diesel engine has also been demonstrated. The work explored fuel volatility and CN effects. The work is a collaborative effort between the ERC, General Motors (GM) Research and Development and BP. Accomplishments and findings over the past year include:

1. Demonstrated the impact fuel characteristics on LTC-D operation.
2. For the engine conditions investigated, fuels with high volatility and high CN gave the lowest fuel consumption, CO, HC, ISFC, and noise.
3. Increasing CN using a nitrate-based cetane improver increased NOx by around 0.35 (g/kg-fuel).
4. Lighter weight/higher volatility fuels reduce soot and HC.
5. Decreasing aromatic content, and increasing cetane number, increases magnitude of low-temperature heat release and advances its location, which in turn controls the start of main combustion.
6. To achieve the <90 dB noise target, with single injection and favorable emissions and ISFC the fuel should have CN between 70 and 80 (ideal CA50 at sweep spot timing), very low aromatic content (reduces noise through phasing/redistribution of heat release), and as few high boiling point components as possible (reduces heavy components of HC and solvent organic fraction of the soot).
7. As shown in Figure 3, running LTC-D at intermediate load (10 bar IMEP) a noise threshold of <90 dB over the target NOx range was met with all fuels tested.

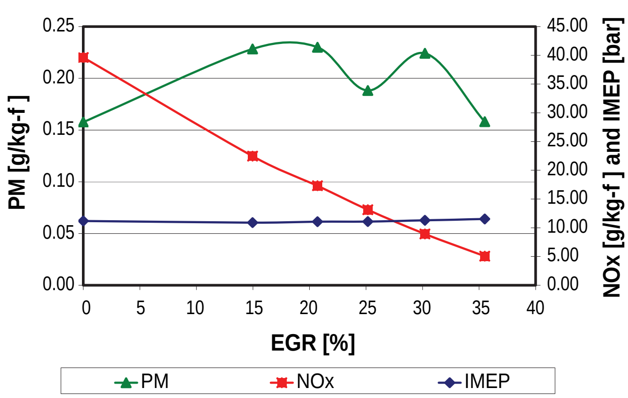

FIGURE 2. Effect of exhaust gas recirculation (EGR) on PM, NOx and IMEP for Compression Ignition Operation with Gasoline

Task 3. Application of Detailed Models for Optimization of LTC-D Combustion and Emissions

Optimization tools have been used to recommend low-emission engine combustion chamber designs. By coupling GA (genetic algorithm) with KIVA-CFD codes, and also utilizing automated grid generation technology, multi-objective optimizations with goals of low emissions and fuel economy have been achieved [4]. This year assessment of different multi-objective genetic algorithms was conduced on a heavy-duty diesel engine operated under high-load. An efficient optimization

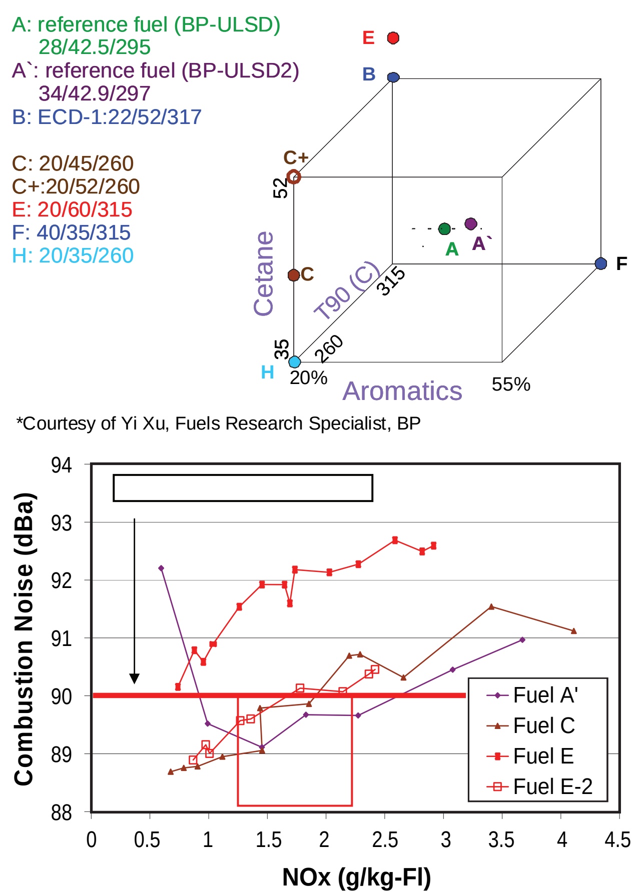

FIGURE 3. Test Fuels Matrix and fuel effect on combustion noise (right) for LTC-D operation with fixed injection timings of -45 and -19 deg aTDC, 46/54 split, 10 bar IMEP.

method, the Non-dominated Sorting Genetic Algorithm II (NSGA II), was found and used to optimize the spray targeting, swirl ratio, injection parameters, as well as piston geometry at low- and high-load. An optimum piston design was found to improve emissions and fuel economy for both low and high loads [4]. In addition, an Adaptive Multi-grid Chemistry model was developed for efficient simulations of HCCI and DI engine combustion. The model is able to reduce computing time by an order of magnitude for HCCI cases, and about a factor of three for DI cases [5].

Models were also developed to describe group-hole injector nozzles. These nozzles are of interest to produce better mixing for HSDI LTC-D combustion. A new spray CFD model that comprises gas-jet, radius-of-influence collision, mean collision time and interpolation method to reduce grid-size, hole-location, and time-step dependencies was used for modeling group-hole nozzle sprays. The spray model has been validated against experimental results in terms of spray penetration and droplet sizes, with much reduction in both grid-size and hole-location dependencies in the spray modeling.

Computations have also been made using advanced turbulence models. Accomplishments include extensive LES-characteristic time combustion (CTC) simulations of high-load engine combustion cases, mesh sensitivity study of the LES-CTC model, and implementation of LES into the KIVA code that includes the advanced spray models. Currently, simulations of a single-cylinder engine with early injection and high EGR are being used to study fuel air mixing in LTC-diesel cases and the impact of LES turbulence models on the results. Single-cylinder engine calculations with early injection and high EGR conditions were simulated to study in-cylinder mixing of fuel and air during ignition delay and prediction of CA10. An analysis was carried out using LES and Reynolds Averaged Navier Stokes (RANS) results on the early mixing and ignition phase using CA10 for various start of injection (SOI) timings. Initial results show that the LES prediction of CA10 is better than RANS, as shown in Figure 4.

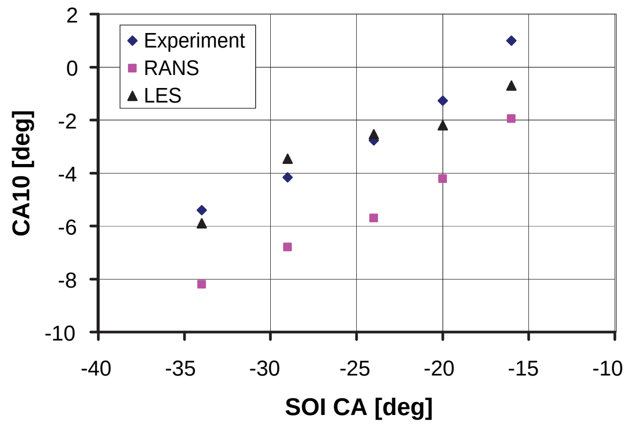

FIGURE 4. Effect of Turbulence Model on CA10 Prediction (LES, RANS and Experiment)

Task 4. Impact of Heat Transfer and Spray Impingement on LTC-D Combustion

Coupled CFD and thermal analysis codes are being applied to consider heat transfer augmentation by fuel films from spray wall impingement and tested against experimental data. A radiation model based on the discrete ordinates method is included in the study. An oil jet cooling model and an oil gallery cooling model has been developed for use with the Heat Conduction in Components (HCC) code which is used in conjunction with the KIVA-CHEMKIN-HCC code to predict the temperature distribution of combustion chamber components. An interpolation kernel for wall film thickness evaluation was developed and applied to reduce the numerical clustering of film particles at grid boundaries previously encountered in particle film models. Heat flux between fuel films and the wall has been added to the communication between KIVA and the HCC finite element solver for the wall temperatures. The oil gallery cooling model considers the oil fill ratio (OFR), and models the motion of the coolant oil in three phases: acceleration, impaction, and dissipation. The model is able to reproduce trends that the heat transfer coefficient increases as the reciprocal frequency of the piston increases. Additionally, the sudden drop of the heat transfer coefficient around OFR=1.0 is reproduced. The model is being applied to compute the operation of the Caterpillar SCOTE engine for validation with experimental data. A linkage system has been developed to allow piston surface temperature and heat flux measurements during LTC-D.

Task 5. Transient Engine Control with Mixed-Mode Combustion

The objective of the research is to incorporate and evaluate LTC-D techniques developed as part of the other tasks into the multi-cylinder engine, operating under transient conditions. In addition to the transient operation we are exploring approaches to transition between normal and LTC operation. The engine experiments use the 4-cylinder GM 1.9L engine, and system level tools have been developed for modeling the engine. Single and multi-zone external cylinder models have been implemented in the most recent version of the commercial cycle simulation code GT-Power, together with incorporation of an improved heat transfer correlation, and application of transient load control strategies and simulation. We have been successful in achieving LTC-D in the multi-cylinder engine and in operating the engine under transient conditions. Transient operation has been investigated for transitions between LTC-D operating points and between LTC-D

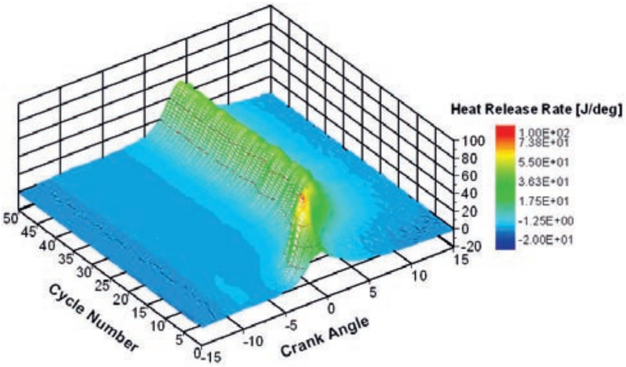

FIGURE 5. Measured Heat Release Rate Progression for a Step Load Change within LTC-D Operation: 1.5 bar to 3.0 bar IMEP

and the stock electronic control unit operating points, such as that shown in Figure 5.

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5. Park, S.W., Abani, N., Reitz, R.D., Suh, H.K., and Lee, C.S., "Modeling of Group-Hole Nozzle Sprays Using Grid-Size, Hole-Location, and Time-step Independent Models," Accepted for publication, Atomization and Sprays, 2008.

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IV.3 Kinetic and Performance Studies of the Regeneration Phase of Model Pt/Ba/Rh NOx Traps for Design and Optimization

Michael P. Harold (Primary Contact) and Vemuri Balakotaiah
University of Houston (UH)
Department of Chemical and Biomolecular Engineering
S222 Engineering Building 1
Houston, TX 77204-4004

DOE Technology Development Manager:
Ken Howden

NETL Project Manager: Aaron Yocum

Objectives

- Carry out studies of regeneration kinetics on lean-oxides of nitrogen (NOx) trap (LNT) catalysts.
- Evaluate and compare the effect of different reductants on LNT performance.
- Incorporate the kinetics findings and develop and analyze a first-principles-based predictive LNT model for design and optimization.
- Test the new LNT designs in a heavy-duty diesel vehicle dynamometer facility.

Accomplishments

- Conducted systematic temporal analysis of products (TAP) studies and are developing a mathematic model framework for elucidating reaction pathways and estimating kinetic parameters.
- Conducted comprehensive steady-state and cyclic studies using H_2 as a reductant on model NOx trap monolithic catalysts comprising Pt, Pt/Ba, and Ba (Task 2).
- Upgraded existing bench-scale reactor system to allow co-feeds of H_2O and CO_2.
- Developed a steady-state LNT model that incorporates our results on the complex regeneration kinetics from the TAP and bench-scale reactor studies, and have applied this model to simulate steady-state bench-scale data.
- Designed and are in the process of constructing a second bench-scale reactor system which will enable the use of synthetic and vehicle exhaust feeds.

Future Directions

During the coming year we will focus our efforts on the following activities:

Experiments

- Conduct bench-scale and TAP experiments on additional catalyst types:
  - Complete study of Pt dispersion for Pt/BaO catalysts
  - Evaluate effects of water and oxygen in feed
  - Evaluate effect of Rh and CeO_2 with H_2 as reductant
- Carry out isotopic TAP studies of storage and reduction using ^{15}NO and $^{18}O_2$.
- Carry out evaluation of stratified monolith configurations:
  - Determine if improved performance with reduced reactor volume, precious metal
- Carry out testing of selected LNTs with engine exhaust in dynamometer facility:
  - Compare synthetic feeds to vehicle feeds

Modeling

- Further upgrade microkinetic model through specific kinetic measurements in bench-scale and TAP reactors:
  - Incorporate upgraded kinetic model into integral transient LNT monolith reactor
  - Converge on simplest regeneration and storage chemistry that predicts data
- Use LNT model to investigate different NOx trap operating strategies and designs:
  - Areas of focus: maximize NH_3 production, maximize N_2 production

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Introduction

During the third year of the four-year grant, we completed an extensive bench-scale reactor study of the Pt/BaO/alumina monolith as a model NOx storage and reduction (NSR) catalyst with H_2 as the reductant, and have carried out experiments with catalysts containing Rh and CeO_2 in addition to Pt and BaO. TAP studies continue to focus on the mechanism and kinetics of interfacial coupling between Pt and Ba. In addition, we are the first to use a monolithic catalyst in a TAP reactor which shows considerable enhancement in the signal needed for quantitative modeling. We have completed a steady-state microkinetic model for the $NO/H_2/O_2$ on

Pt reaction system. Very good agreement was obtained between model and experiments carried out earlier in the project. This kinetic model has been incorporated into an integral transient model of the LNT. Current efforts are focused on the additional chemistry that must be included to capture the detailed chemistry at the Pt/Ba interface. We have also upgraded the kinetic model of the co-oxidation of CO and H_2 on Pt, important reactions occurring in the catalytic converter. In parallel collaborative work with Ford, we have developed low-dimensional models for real-time simulation of 3-way catalysts and NOx traps and are working on the development of global kinetic models for NSR. The project has been productive in terms of publications and presentations.

The fourth year of the project will build on the above progress related to Tasks 1, 2, and 3a. We will continue efforts related to Task 1 (fundamental TAP experiments with monolithic Pt/BaO catalysts), Task 2 (experiments with model catalysts containing Rh and CeO_2), Task 3b (analysis and evaluation of NOx trap designs), and Task 4 (testing of NOx trap with realistic feeds in dynamometer facility). The requested funding will support three full-time graduate students and a half-time technician.

Approach

We utilize a combination of experimental and theoretical tools to advance the LNT technology. Fundamental kinetics studies are carried out of model LNT catalysts containing variable loadings of precious metals (Pt, Rh), and storage components (BaO, CeO_2). A TAP reactor provides transient data under well-characterized conditions of both powder and monolith catalysts, enabling the identification of key reaction pathways and estimation of the corresponding kinetic parameters. The performance of model NSR monolith catalysts are evaluated in a bench-scale NOx trap using synthetic exhaust, with attention placed on the effect of the pulse timing and composition on the instantaneous and cycle-averaged product distributions. From these measurements we formulate a mechanistic-based microkinetic model that incorporates a detailed understanding of the chemistry, and incorporate the kinetic model into a LNT model. The NOx trap model is used to determine its ability to simulate bench-scale data and ultimately to evaluate alternative LNT designs and operating strategies.

Results

During the third year we continued mechanistic studies of NO uptake (storage) and NO reduction by H_2 on Pt/Al_2O_3 and Pt/Ba/Al_2O_3 powder catalysts (provided by BASF Catalysts LLC). We also demonstrated for the first time the use of TAP with a monolith catalyst. The following is a summary of the main accomplishments in this area:

- Carried out study of NO decomposition and NO/H_2 pump/probe on Pt/Al_2O_3 and
- Pt/Ba/Al_2O_3 catalysts; identified conditions leading to N_2, N_2O, and NH_3 formation.
- Developed phenomenological understanding of role of Pt/Ba coupling during storage and reduction.
- Employed TAP using a monolith catalyst (first to do this).
- Carried out NO/O_2 and NO/H_2 pump/probe on Pt/Ba/Al_2O_3 catalysts with varying Pt dispersion.
- Developed TAP model which has parameter estimation capability.

We have made considerable progress in forming a comprehensive database for steady-state and cyclic bench-scale monolith reactor experiments. We utilize a monolith reactor system comprising a simulated exhaust feed system, flow through reactor, and dedicated analytical system (Fourier transform infrared and quadrupole mass spectrometer). Catalysts were provided by BASF Catalysts (Iselin, NJ). We completed the following studies:

- Spatio-temporal features of a LNT using H_2 as reductant on Pt/BaO/Al_2O_3:
  - Measured spatial profiles of main species
  - Established existence of moving fronts of H_2 and NH_3
  - Established role of NH_3 as an intermediate
- Comparison of H_2 and NH_3 as reductants, showing that H_2 is the superior reductant under most conditions.
- Systematic study of effect of Pt dispersion in Pt/BaO/Al_2O_3:
  - Compared three Pt/BaO catalysts with same Pt loading (2.70 wt%) with different dispersion (50%, 10%, 3%)
  - Compared storage, activity, and selectivity effects of dispersion

The performance of a model Pt/BaO/Al_2O_3 monolith catalyst was studied using H_2 as the reductant. The dependence of product selectivities on operating parameters was determined, including the durations of regeneration and storage times, feed composition and temperature, and monolith temperature. The data are explained in terms of a phenomenological model factoring in the transport, kinetic, and spatio-temporal effects. The Pt/BaO catalyst exhibits high cycle-averaged NOx conversion above 100°C, generating a mixture of N_2 and byproducts NH_3 and N_2O. The cycle-averaged NOx conversion exhibits a maximum at about 300°C corresponding to the NOx storage maximum. The N_2

selectivity exhibits a maximum at a somewhat higher temperature, at which point the NH_3 selectivity exhibits a minimum. This trend conveys the intermediate role of NH_3 in reacting with stored NOx. Both N_2 and N_2O are also formed during the storage steps from the oxidation of NH_x species produced during the regeneration.

A study of the spatio-temporal features of the LNT helps to explain the transient selectivities to N_2 and NH_3. The regeneration of a model $Pt/BaO/Al_2O_3$ monolith catalyst was studied with hydrogen as the reductant to elucidate the reaction pathways to molecular nitrogen and ammonia. NSR experiments were conducted with a 2 cm length monolith for a wide range of feed conditions. The NSR experiments were replicated for a series of monoliths of progressively decreasing length, enabling the construction of spatio-temporal profiles of reactant and product concentrations. Typical results are shown in Figure 1. The data indicate that there are two primary competing routes to the desired N_2 product; a direct route from the reduction of stored NOx by H_2 or by a sequential route through NH_3. A comparison between H_2 and NH_3 as reductants revealed H_2 is a more effective reductant in terms of NOx conversion for temperatures below 230°C (Figure 2). At higher temperatures (230 to 380°C), the regeneration of stored NOx is feed-limited and the difference between the reductants H_2 and NH_3 is found to be small with H_2 being a slightly superior reductant. Measurements of the traveling front velocity were compared with a simple feed-limited model that assumes complete consumption of H_2 as stored NOx is depleted. At lower temperatures the regeneration is limited by chemical processes at the Pt/Ba interface.

A detailed study was carried out on the storage and reduction performance of $Pt/BaO/A_2O_3$ monoliths with varied Pt dispersion (3, 10, and 50%) and fixed Pt and BaO loadings. Below 200°C, the differences in storage and reduction activity were the largest between the three catalysts. The amount of NOx stored increased with increased dispersion. The storage and reduction increases with dispersion are attributed to the larger Pt surface area and Pt/BaO interfacial perimeter, which enhances the spillover of surface species between Pt and BaO. The Pt dispersion had a significant effect on the product distribution. The amount of stored NOx that is reduced also increased with increasing Pt dispersion. At high temperature (370°C), the stored NOx was almost completely regenerated for the three catalysts. However, the regeneration of the 3% dispersion catalyst was much slower, suggesting a kinetic limitation such as the reverse spillover of stored NOx and/or of adsorbed hydrogen from Pt to BaO. The results suggest that a transport limitation may exist, such as the diffusion of surface species between the storage sites and Pt particles.

The bench-scale system has been upgraded to allow for co-feed of H_2O and CO_2. We have initiated a comprehensive study of the roles of Rh and CeO_2 during NSR with H_2. We have completed storage and cycling studies of Pt/BaO, Pt/Rh/BaO, and $Pt/Rh/BaO/CeO_2$.

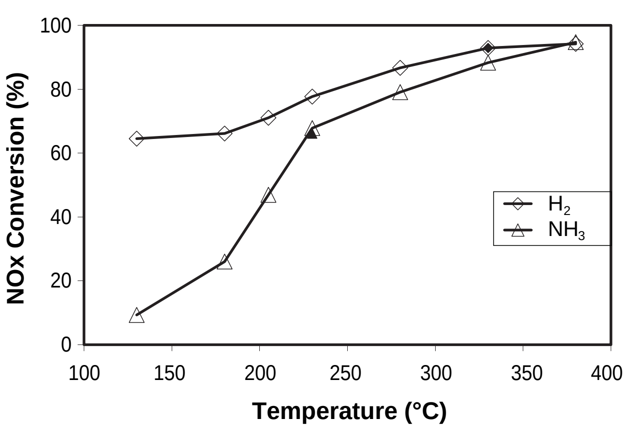

FIGURE 1. Cycle-average results for NOx conversion comparing reductants H_2 and NH_3 as function of feed temperature [Lean: 500 ppm NO and 5% O_2 (60s); Rich: 4% H_2 or 2.67% NH_3 (3s)].

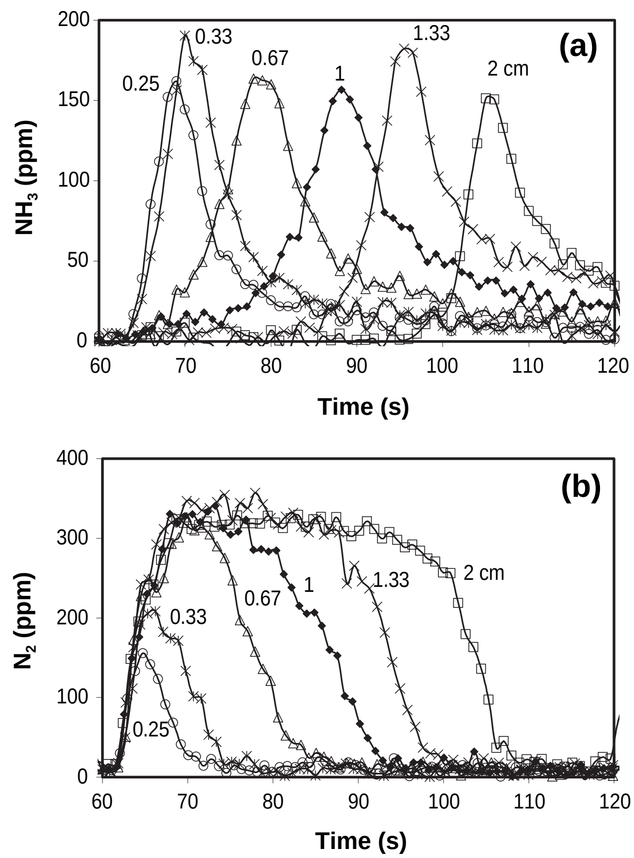

FIGURE 2. Effluent concentrations for varied monolith length at T_f = 275°C (a) NH_3; (b) N_2; [Lean: 500 ppm NO and 5% O_2 (60s); Rich: 0.15% H_2 (60s)].

This past year a steady-state microkinetic model for NO reduction by H_2 and NH_3 in O_2 on alumina supported Pt/BaO was developed based on the measurements from a parallel experimental study. Kinetic parameters not available from the literature were estimated to capture the experimental trends and to meet thermodynamic constraints. The kinetic model was incorporated into a short monolith reactor model to simulate the steady-state NH_3/O_2, NH_3/NO and NO/NH_3/H_2 reaction systems. The predicted conversion/product distribution are in excellent qualitative and good quantitative agreement with the experimental data (paper 8).

Conclusions

During the third year we have made very good progress towards the project objectives 1, 2 and 3. The fourth year efforts will be focused on bench-scale and TAP reactor studies of Pt/Rh/BaO/CeO_2 catalysts, including novel TAP experiments using monolith catalysts and isotopic feeds, completion of a comprehensive microkinetic model and its incorporation into a monolith model to simulate LNT performance, and LNT performance studies on actual diesel vehicle exhaust in the UH chassis dynamometer laboratory.

FY 2008 Publications/Presentations

Refereed Journal Publications:

1. Medhekar, V., V. Balakotaiah, and M.P. Harold, "TAP Study of NOx Storage and Reduction on Pt/Al_2O_3 and Pt/Ba/Al_2O_3," *Catalysis Today*, **121**, 226-236 (2007).

2. Sharma, M., R.D. Clayton, M.P. Harold, and V. Balakotaiah, "Multiplicity in Lean NOx Traps," *Chem. Engng. Science*, **62**, 5176-5181 (2007).

3. Xu, J., R.D. Clayton, V. Balakotaiah and M.P. Harold, "Experimental and Microkinetic Modeling of Steady-State NO Reduction by H_2 on Pt/BaO/Al_2O_3 Monolith Catalysts," *Appl. Catal. B. Environmental*, **77**, 395-408 (2008).

4. Clayton, R.D., M.P. Harold, and V. Balakotaiah, "Selective Catalytic Reduction of NO by H_2 in O_2 on Pt/BaO/Al_2O_3 Monolith NOx Storage Catalysts," *Appl. Catal. B. Environmental*, **81**, 161-181 (2008).

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7. Xu, J., M.P. Harold, and V. Balakotaiah, "Microkinetic Modeling of Steady-State NO/H_2/O_2 on Pt/BaO/Al_2O_3 Monolith Catalysts," *Appl. Catal. B. Environmental*, in press (2008).

8. Bhatia, D., V. Balakotaiah and M.P. Harold, "Bifurcation Analysis of CO and H_2 Oxidation on Pt/Al_2O_3 Monolith Reactors" *Chem. Engng. Sci.*, under review (2008).

9. Kumar, A., V. Medhekar, M.P. Harold, and V. Balakotaiah, "NO Decomposition and Reduction on Pt/Al_2O_3 Powder and Monolith Catalysts Using the TAP Reactor," *Appl. Catal. B. Environmental,* submitted (2008).

Conference and Other Presentations

1. *"Spatio-Temporal Behavior of the Lean NOx Trap,"* Ford Motor Company, Corporate Research, Dearborn, MI 10/07 (M. Harold, speaker).

2. "*Developments in Diesel Emission Control Technology at the University of Houston,*" Baker-Petrolite Inc., Corporate Research, Sugarland, Texas, 10/07 (M. Harold, speaker).

3. *"Modeling of the Lean NOx Trap,"* Ford Motor Company, Corporate Research, Dearborn, MI 10/07 (V. Balakotaiah, speaker).

4. "*Towards Optimal NOx Trap Operation*," presented at the AIChE National Meeting, Salt Lake City, UT, 11/07 (M. Harold, speaker, Robert Clayton, Vemuri Balakotaiah).

5. "*Microkinetic Modeling of Steady-State NO Reduction by H_2 on Pt/Ba/Al_2O_3 Monolith Catalysts*," presented at the AIChE National Meeting, Salt Lake City, UT, 11/07 (poster; Jin Xu, M. Harold, Vemuri Balakotaiah, presenter).

6. "*Optimal Design of Three Way Catalytic Converters to Reduce Cold Start Emissions*," presented at the AIChE National Meeting, Salt Lake City, UT, 11/07 (poster; Divesh Bhatia, presenter, M. Harold, Vemuri Balakotaiah).

7. *"Spatio-Temporal Behavior of the Lean NOx Trap in Diesel Aftertreatment*," Department of Chemical Engineering, University of Florida, 3/08 (M. Harold, speaker).

8. *"Elucidating Catalytic Chemistry and Spatio-Temporal Phenomena in the Lean NOx Trap*," Southwest Section of the North American Catalysis Society, 4/08 (M. Harold, speaker).

9. *"Spatio-Temporal Behavior of NOx Storage and Reduction Monolith Catalysts,"* 2008 CLEERS Meeting, Dearborn, MI, 5/08 (V. Balakotaiah, speaker).

10. "*Bifurcation Analysis of CO and H_2 Oxidation on Pt/Al_2O_3 Monolith Reactors,*" ISCRE 20, Kyoto, Japan, 9/08 (Bhatia, D., presenter, V. Balakotaiah, M.P. Harold).

IV.4 Investigation of Aging Mechanisms in Lean NOx Traps

Mark Crocker (Primary Contact), Yaying Ji, Vence Easterling
University of Kentucky Center for Applied Energy Research
2540 Research Park Drive
Lexington, KY 40511

DOE Technology Development Manager:
Ken Howden

NETL Project Manager: Christopher Johnson

Subcontractor:
Oak Ridge National Laboratory, Oak Ridge, TN

Partners:
- Ford Motor Co., Dearborn, MI
- Umicore Autocat USA, Inc., Auburn Hills, MI

Objectives

- Examine the effect of washcoat composition on lean NOx trap (LNT) catalyst aging characteristics. To this end, prepare model Pt/Rh/CeO_2(-ZrO_2)/BaO/Al_2O_3 catalysts with systematic variation of the main component concentrations.
- Study the physical and chemical properties of the model catalysts in the fresh state and after aging.
- Investigate transient phenomena in the fresh and aged catalysts during lean-rich cycling using spatially-resolved capillary-inlet mass spectrometry (SpaciMS).
- Investigate the kinetics and mechanism of desulfation in fresh and aged catalysts using chemical ionization mass spectrometry for the simultaneous analysis of evolved sulfur species.
- Correlate evolution of catalyst microstructure to NOx storage and reduction characteristics.

Accomplishments

- The effect of ceria addition on the sulfation and desulfation characteristics of a model Ba-based LNT catalyst was studied. According to diffuse reflectance infrared Fourier-transform spectroscopy (DRIFTS) and NOx storage capacity measurements, ceria is able to store sulfur during catalyst exposure to SO_2, thereby helping to limit sulfation of the main (Ba) NOx storage phase and maintain NOx storage capacity.
- Model monolithic catalysts were aged on a bench reactor according to a protocol designed to simulate *ca*. 75,000 miles of road aging.
- The aged catalysts were evaluated on a bench reactor in order to characterize their NOx storage-reduction characteristics and enable a comparison with the fresh (de-greened) catalysts. Spectacular improvement in LNT durability was observed for catalysts incorporating CeO_2 and $CeZrO_2$ (particularly the latter).

Future Directions

- Complete studies pertaining to the dynamics of LNT desulfation. Perform measurements on de-greened and aged catalysts in order to examine possible changes in desulfation behavior with aging.
- Characterize aged catalysts using standard physico-chemical techniques, in tandem with bench reactor tests, in order to correlate catalyst aging characteristics with washcoat composition.
- Apply SpaciMS to probe the transient behavior of aged catalysts (for comparison with results previously obtained on fresh catalysts). This will provide insights into the effect of aging on processes such as intra-catalyst H_2 generation and consumption during rich purging.
- Derive a quantitative model that describes catalyst performance as a function of aging time.

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Introduction

LNTs represent a promising technology for the abatement of NOx under lean conditions. Although LNTs are starting to find commercial application, the issue of catalyst durability remains problematic. LNT susceptibility to sulfur poisoning is the single most important factor determining effective catalyst lifetime. The NOx storage element of the catalyst has a greater affinity for SO_3 than it does for NO_2, and the resulting sulfate is more stable than the stored nitrate. Although this sulfate can be removed from the catalyst by means of high-temperature treatment under rich conditions, the required conditions give rise to deactivation mechanisms such as precious metal sintering, total surface area loss, and solid state reactions between the various oxides present. The principle objective of this project is to improve understanding of the mechanisms of lean NOx trap aging, and to understand the effect of washcoat composition on catalyst aging characteristics.

Approach

The approach utilized makes use of detailed characterization of model catalysts prior to and after aging, in tandem with measurement of catalyst performance in NOx storage and reduction. In this manner, NOx storage and reduction characteristics can be correlated with the evolution of catalyst microstructure upon aging. The effect of washcoat composition on catalyst aging characteristics is studied by systematic variation of the concentration of the four main active components, Pt, Rh, CeO_2 (or CeO_2-ZrO_2) and BaO (supported on alumina). In addition to the use of standard physico-chemical analytical techniques for studying the fresh and aged model catalysts, use is made of advanced analytical tools for characterizing their NOx storage/reduction and sulfation/desulfation characteristics, such as SpaciMS and in situ DRIFTS.

Results

Effect of Catalyst Composition on LNT Sulfation and Desulfation Characteristics

In order to study the influence of ceria on LNT sulfation and desulfation characteristics, two Ba-based model catalysts were used, of which one contained ceria. The composition of the catalysts corresponded to i) 1 wt% Pt/20 wt% BaO/Al_2O_3 (denoted hereafter as "PBA"); and ii) 1 wt% Pt/20 wt% BaO/Al_2O_3 (74 wt%) + 1 wt% Pt/CeO_2 (26 wt%), physical mixture (denoted as "PBAC"). Figure 1 shows a series of DRIFT spectra acquired during exposure of PBA and PBAC to feed gas containing 300 ppm NO, 10% O_2, 5% H_2O and 27 ppm SO_2. In the case of PBA, bands grow in at 1,420 and 1,320 cm^{-1} which can be attributed to monodentate and bidentate Ba nitrate species [1], while an intense band at 1,122 cm^{-1} corresponds to a surface Ba sulfate species. A weaker band at 978 cm^{-1} can be assigned to surface $Al_2(SO_3)_3$. Based on the evolution of the spectra with time, it is apparent that at short reaction times (e.g., 5 min) the nitrates are the dominant surface species, reflecting the higher concentration of NO in the feed relative to SO_2. However, beyond this point the sulfate bands become progressively more intense, while the intensities of the nitrate bands are slightly decreased. This observation is consistent with strong adsorption of SOx on the catalyst, which effectively competes with NOx for storage sites.

In the case of the ceria-containing catalyst, PBAC, rather different behavior is observed. After 5 min of exposure to the feed gas, the spectrum is again dominated by the presence of Ba nitrate bands, while a shoulder at *ca*. 1,510 cm^{-1} is indicative of the formation of a monodentate nitrate species on ceria [2]. At longer reaction times the Ba nitrate bands continue to increase in intensity, while a band due to Ba sulfate grows

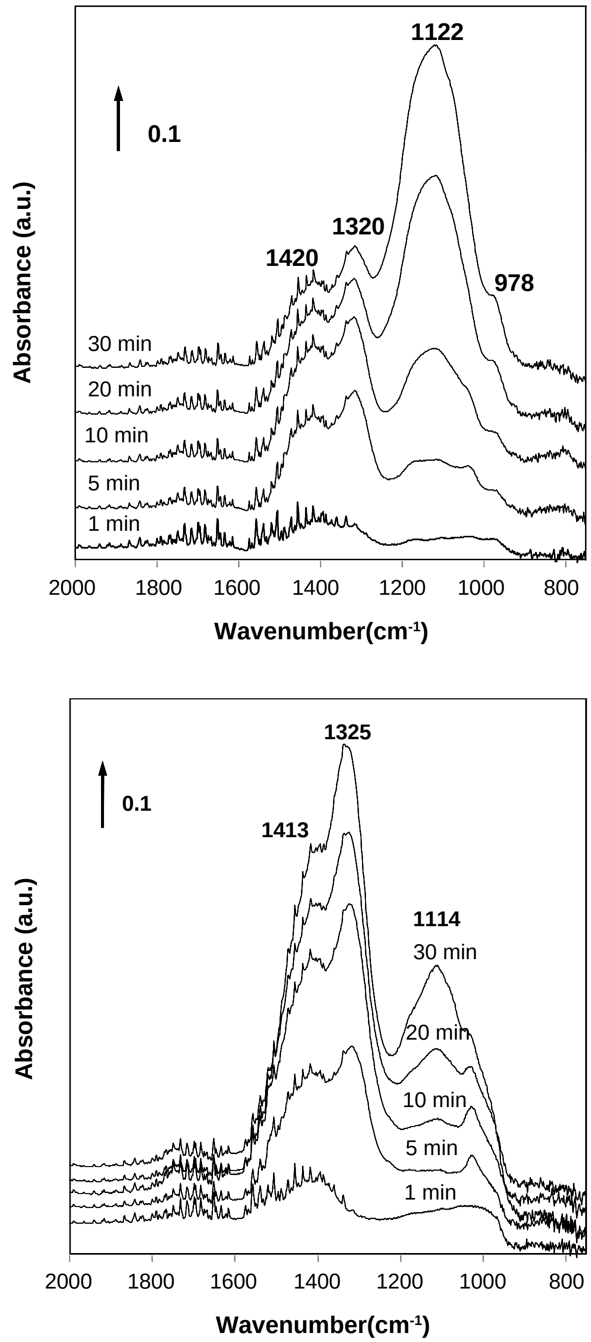

FIGURE 1. DRIFT Spectra Obtained upon Exposure of PBA (top) and PBAC (bottom) to SO_2/NO/O_2/H_2O

in at 1,114 cm^{-1}. Even at the end of the experiment (30 min duration), the sulfate band intensity remains substantially less that of the Ba nitrate bands. These observations suggest that nitrate and sulfate were able to form at different sites on the catalyst.

In order to provide additional insight into their desulfation behavior, temperature-programmed reduction (TPR) experiments were performed on sulfated samples of PBA and PBAC (Figure 2). During

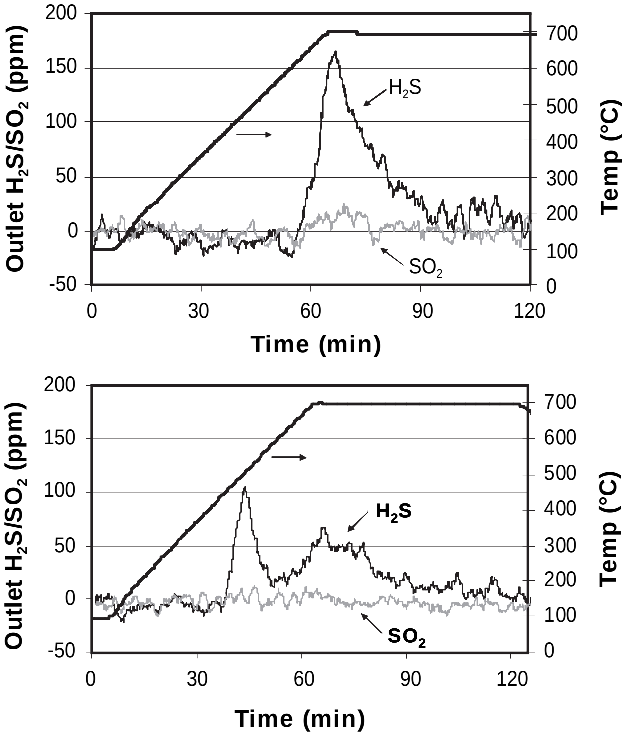

FIGURE 2. Sulfur Release from PBA (top) and PBAC (bottom) during TPR (1% H_2, 5% H_2O, 5% CO_2 in Ar)

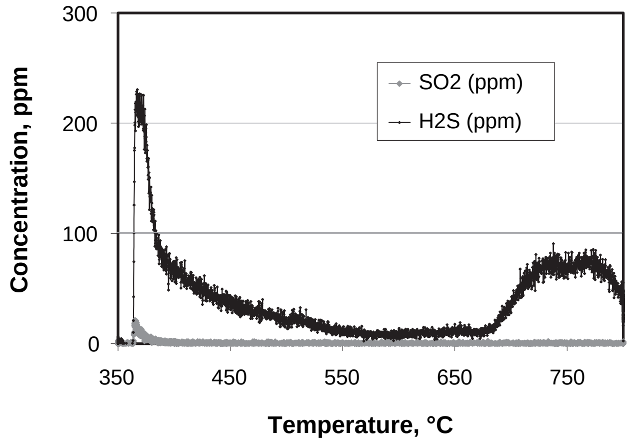

FIGURE 3. Sulfur Release from 20 wt% BaO/Al_2O_3 + 1 wt% Pt/Al_2O_3 (1:1 physical mixture) during TPR (1% H_2, 5% H_2O, 5% CO_2 in Ar)

H_2-TPR sulfur was released from both catalysts mainly as H_2S; release of H_2S occurred at ~650°C from PBA, whereas PBAC showed two discrete H_2S release events at ~450°C and ~650°C. From this it follows that the H_2S release at ~450°C corresponds to desulfation of the ceria phase (confirmed by reference experiments), with Ba desulfation occurring at the higher temperature. Significantly, PBAC displayed relatively lower H_2S evolution from the Ba phase than PBA, confirming that the presence of ceria in PBAC lessened the degree of sulfur accumulation on the Ba phase.

TPR experiments were also performed with the aim of ascertaining the effect of Pt location on the sulfation and desulfation behavior of Ba-based LNT formulations. For this purpose, a simple physical mixture of 1 wt% Pt/Al_2O_3 and 20 wt% BaO/Al_2O_3 (1:1 weight ratio) was used. As shown in Figure 3, two main desorption events are observed. The first corresponds to sulfur release from the alumina phase (370°C, confirmed by reference experiments), while the second maximum is extremely broad and spans the range 725-775°C. Comparing these results with those obtained for PBA at the same sulfur loading, it is apparent that physical separation of the Pt and Ba phases results in increased sulfur storage on the alumina, presumably as a consequence of SO_3 spillover from Pt to the alumina support during sulfation. Additionally, the desulfation temperature of the $BaSO_4$ is shifted by ~65°C towards higher temperature, i.e., towards the position characteristic of bulk $BaSO_4$ [3]. This is in keeping with the idea that decomposition of surface $BaSO_4$ is facilitated by H ad-atoms which spill over from the Pt sites onto the sulfated Ba phase. Physical separation of the Pt and Ba phases appears to inhibit this process, with the consequence that the surface $BaSO_4$ behaves more like bulk $BaSO_4$ with respect to its desulfation properties. We note that somewhat analogous findings have been reported for nitrate decomposition on physical mixtures of Pt/Al_2O_3 and BaO/Al_2O_3 [4]: in the absence of hydrogen spillover from Pt to the Ba phase, considerably higher temperatures are required to achieve nitrate decomposition than is usual for $Pt/BaO/Al_2O_3$ catalysts.

NOx Storage-Reduction Characteristics of LNT Catalysts Subjected to Simulated Road Aging

In order to study the effect of washcoat composition on catalyst aging characteristics, fully formulated monolithic catalysts were prepared containing varying amounts of La-stabilized CeO_2 (5 wt% La_2O_3) and CeO_2-ZrO_2 mixed oxide (Ce:Zr = 70:30), at fixed loadings of Pt (3.5 g/L), Rh (0.7 g/L) and BaO (30 g/L). The BaO phase was supported on alumina. Details of the catalyst preparation have been given previously [5]. Core samples were then aged on a bench reactor using a cycle consisting of (i) sulfating the catalyst at 350°C to an equivalent loading of 1 g S/L, (ii) desulfation at 700°C for 10 min under cycling (5 s lean/15 s rich at λ= 0.90), and (iii) holding at 650°C for 30 min under lean conditions (to simulate diesel particulate filter regeneration). Together, these three conditions constituted one aging cycle. Each catalyst was aged for 50 cycles, which is estimated to be equivalent to *ca.* 75,000 miles of road aging. After aging, the catalysts were exposed to rich conditions at 750°C for 10 min to remove any residual sulfur and then evaluated on a bench reactor.

Representative cycle averaged NOx conversion and N_2 selectivity data for the aged catalysts are shown in Table 1, together with oxygen storage capacity (OSC) data obtained at 350°C. For comparison purposes, data for the fresh (de-greened) catalysts are included. Considering the NOx conversion data, it is apparent that the performance of catalyst 30-0, containing no ceria, was severely degraded after aging. In comparison, catalyst 30-100, containing 100 g/L of ceria, continued to show high levels of NOx conversion at 250-350°C, while catalyst 30-100Z, containing 100 g/L of CeO_2-ZrO_2, retained the highest degree of activity; indeed, NOx conversion levels for the aged catalyst were only slightly lower than for the fresh state. Analysis of data (not shown) pertaining to the lean phase NOx storage efficiency and rich-phase NOx release characteristics of the three catalysts indicates that the decreased NOx conversion after aging mainly results from degradation of the lean-phase NOx storage and rich-phase regeneration efficiency under cycling. Regarding the lean-phase performance, NO_2 slip was consistently observed for all of the catalysts (at all temperatures), indicating that NO oxidation is not the limiting factor; rather, it is the inability of the catalyst to store NO_2 that limits the NOx storage efficiency (NSE). To provide further insights into the origin of the NSE degradation, the NSE measured during the first lean cycle after complete catalyst regeneration was compared with the NSE measured under steady-state cycling (Table 2). Catalyst 30-0 exhibited a large difference between the two NSE values, implying that its NOx storage efficiency was significantly limited by its inability to be completely regenerated during rich purging. However, a small difference between these two NSE values for catalysts 30-100 and 30-100Z indicates that these two catalysts retained their good regeneration characteristics.

TABLE 1. Comparison of OSC, Cycle Averaged NOx Conversion and N_2 Selectivity before and after Catalyst Aging

Catalyst	Temp. (°C)	OSC (mmol/L)		NOx conversion (%)		N_2 selectivity (%)	
		Fresh	Aged	Fresh	Aged	Fresh	Aged
30-0	250	--	--	94.3	39.7	31.7	41.7
	350	10.8	6.2	95.9	40.0	66.4	23.5
30-100	250	--	--	98.7	87.7	76.8	57.8
	350	28.0	18.5	98.7	91.1	95.9	88.3
30-100Z	250	--	--	97.2	92.0	79.5	15.8
	350	36.6	34.1	98.0	93.4	97.0	89.2

Conditions: Lean: 300 ppm NO, 10% O_2, 5% CO_2, 5% H_2O in N_2 (60 s); Rich: 1.575% H_2, 2.625% CO, 5% CO_2, 5% H_2O in N_2 (5 s); GHSV = 30,000 h^{-1}. OSC was measured without lean-phase NO, while using 4.2% H_2 as reductant during the rich phase. (GHSV - gas hourly space velocity)

TABLE 2. Comparison of Cycled Averaged and First Cycle NOx Storage Efficiencies Before and After Catalyst Aging

Catalyst	Temp. (°C)	Cycle ave. NSE (%)		First cycle NSE (%)	
		Fresh	Aged	Fresh	Aged
30-0	250	94.7	38.0	98.8	84.4
	350	96.8	43.2	98.3	74.7
30-100	250	98.8	94.5	99.5	97.0
	350	99.6	92.8	99.4	95.5
30-100Z	250	97.0	93.4	99.2	98.2
	350	97.7	95.5	99.2	98.1

Conditions as for Table 1.

From Table 1 it is apparent that after aging, all of the catalysts showed decreased selectivity to N_2 during NOx reduction, the selectivity to NH_3 being increased. Simultaneously, in each case the catalysts exhibited decreased OSC after aging. This suggests that the decreases in N_2 selectivity and OSC are related, an idea which can be rationalized on the basis that: 1) a decrease in stored oxygen should result in an increased reductant concentration in the gas front, favoring the formation of NH_3 over N_2; and 2) less stored oxygen will be available in the rear of the catalyst to react with initially formed NH_3 to give N_2. SpaciMS measurements currently in progress should help to confirm whether these propositions are correct.

Conclusions

- The addition of ceria to Ba-based LNT catalysts exerts a positive effect on LNT performance in the presence of sulfur. DRIFTS and NOx storage capacity measurements suggest that ceria is able to store sulfur and thereby mitigate sulfation of the main (Ba) NOx storage phase.
- Desulfation of a ceria-containing model catalyst was found to occur in two stages, corresponding to sulfur elimination from the ceria phase at ~450°C, followed by sulfur loss from the Ba phase at ~650°C. Significantly, the ceria-containing catalyst displayed relatively lower sulfur evolution from the Ba phase than its non-ceria analog, confirming that the presence of ceria lessened the degree of sulfur accumulation on the Ba phase.
- Desulfation experiments have revealed the importance of maintaining the Pt and Ba phases in close contact for efficient LNT desulfation
- The spectacular improvement in catalyst durability which can be achieved through the incorporation of CeO_2 and $CeZrO_2$ into LNT formulations has been demonstrated. Insights into the mechanisms by which $CeZrO_2$ improves LNT durability should be useful in aiding the design more robust and cost-efficient LNT systems.

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IV.5 Improved Engine Design Concepts Using the Second Law of Thermodynamics: Reducing Irreversibilities and Increasing Efficiencies

Jerald A. Caton
Texas A&M University
Department of Mechanical Engineering
TAMU 3123
College Station, TX 77843–3123

DOE Technology Development Manager: Gurpreet Singh

NETL Project Manager: Jason Conley

Objectives

- Upgrade the exhaust gas recirculation (EGR) sub-model to reflect combustion termination for high (>20%) levels of EGR for spark ignition engines.
- Complete studies of "reversible" combustion for a reciprocating device using Professor Keenan's concept.
- Extend the cycle simulation to include turbocharging and complete a parametric study of the effects of turbocharging.

Accomplishments

- Work was completed using the improved EGR sub-model which better reflected the actual termination of combustion as EGR levels increase. The improved EGR sub-model was then used in a series of computations to complete a parametric study.
- The examination of hypothetical "reversible" combustion at high temperatures and pressures was completed, documented and presented. As mentioned before, this concept was based on the proposal by Professor Keenan from the 1940s. The results indicate possible scenarios where the availability destruction can be zero by preselecting the reactant composition such that at the end of compression the species are in equilibrium. Although the availability is preserved, most of the availability remains in the exhaust gases and the engine efficiency is typically low.
- Turbocharging capabilities were added to the cycle simulation, and included the use of the first and second laws of thermodynamics. The new components included a compressor, turbine, and intercooler. In addition to adding the new components, an appropriate engine and operating conditions were selected. The enhanced simulation was used in a series of parametric studies.

Future Directions

- Complete the parametric examination of turbocharging from a first law and second law perspective.
- Use the cycle simulation with turbocharging to examine other exhaust gas exergy recovery methods.
- In addition, use the simulation to explore other operating conditions such as low-heat-rejection which would result in higher exhaust energy and exergy which would then need to be recovered.

✧ ✧ ✧ ✧ ✧

Introduction

This project is aimed at using the second law of thermodynamics (in conjunction with the first law) to better understand the thermodynamics of internal combustion engines. In addition to examining engines, some of the work has investigated simple (e.g., constant pressure or volume) systems. The second law of thermodynamics provides a rich and significant insight concerning the proper use of energy and its conversion to mechanical shaft power. The second law allows this feature to be quantified using the thermodynamic property of availability (also known as exergy). A number of fuels have been used in these evaluations. Examples of this work have included detailed examinations of the use of EGR for spark-ignition engines, the use of oxygen enriched inlet gases, comparisons of hydrogen and isooctane for the same engine, and the effects of compression ratio and greater expansion ratios (for the same compression ratio) on performance and second law parameters.

A new capability has been added to the simulation which is turbocharging. Figure 1 is a schematic of the original engine system and Figure 2 is a schematic of the new system which includes the base engine, a compressor, an intercooler, and a turbine. For most conditions, only a portion of the exhaust is needed for the turbine work. The excess exhaust flow is "by-passed" directly to the system discharge piping. New sources of exergy destruction (outside of the original engine system) are due to the compressor and turbine irreversibilities, and to flow past the exhaust valve. The irreversibilities of the flow past the intake valve are included with the original engine system and are already considered. In addition to these new irreversibilities, some exergy is removed with the energy transfer in the intercooler.

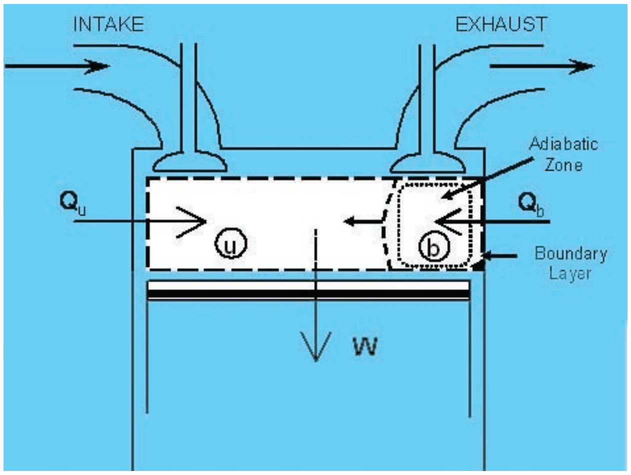

FIGURE 1. Schematic of the Engine Cylinder Depicting the Three Zones During Combustion

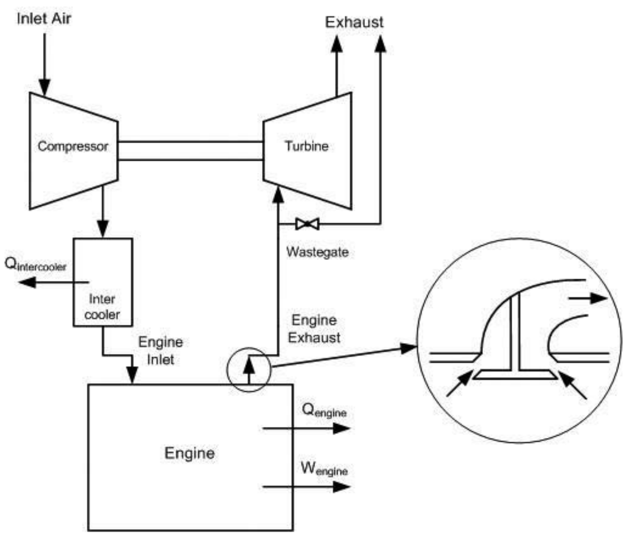

FIGURE 2. Schematic of Engine with Turbocharger Components

The engine selected for this study is an automotive, turbocharged, 3.8 liter, V-6 engine. This engine was selected as representative of this type of application, and some limited information was available on the engine specifications. Table 1 lists the engine specifications and Table 2 lists some of the engine operating conditions and fuel parameters for the base case (2,000 rpm at wide-open-throtte, WOT). Some parameters were selected for simplicity and for comparison to previous studies of naturally aspirated engines, and may not be an exact match for any specific manufacturer. For example, the equivalence ratio was assumed to be stoichiometric ($\phi = 1.0$), and the combustion burn duration was assumed to be 60° crank angle (CA). Start of combustion was determined for maximum brake torque (MBT). The use of these types of consistent conditions provided a less ambiguous comparison as other parameters were varied.

TABLE 1. Engine Specifications for Turbocharger Case

Item	Value
Number of cylinders	6
Bore (mm)	96.5
Stroke (mm)	86.4
Crank Rad/Con Rod	0.305
Compression Ratio	8.0:1
Inlet Valves:	
Diameter (mm)	41.3
Max Lift (mm)	8.75
Opens (°CA aTDC)	344
Closes (°CA aTDC)	-124
Exhaust Valves:	
Diameter (mm)	36.2
Max Lift (mm)	8.75
Opens (°CA aTDC)	110
Closes (°CA aTDC)	396
Valve Overlap (degrees)	52°

aTDC - after top-dead center

TABLE 2. Engine and Fuel Input Parameters for the Base Case: 2,000 rpm, WOT, and "MBT" Timing

Item	Value Used	How Obtained
Engine Speed (rpm)	2,000	Input
Displaced Volume (dm^3)	3.791	Computed
AFstoich	15.13	For isooctane
Fuel LHV (kJ/kg)	44,400	For isooctane
Equivalence Ratio	1.0	Input
Frictional mep (kPa)	88.3	Algorithm
Inlet Pressure (kPa)	137.0	Input
Engine Exit Pressure – Turbine Inlet Pressure (kPa)	148.8	Input
Turbine Exit Pressure – Exhaust System Pressure (kPa)	105.0	Input
Start of Combustion (°bTDC)	23.0	For MBT
Combustion Duration (°CA)	60	Input
Cylinder Wall Temp (K)	450	Input
Compressor Inlet (ambient) Temperature and Pressure	300 K 100 kPa	Input
Compressor Isentropic Efficiency	70.0%	Input
Turbine Isentropic Efficiency	70.0%	Input
Intercooler Effectiveness	80.0%	Input
Coolant Inlet Temperature to Intercooler (K)	300	Input

AF - air/fuel ratio
LHV - lower heating value
bTDC - before top-dead center

Approach

The main feature of this project is the use of a comprehensive engine cycle simulation which is based on consistent and rigorous thermodynamics, and includes the use of the second law of thermodynamics. In summary, this simulation is largely based on thermodynamic formulations, and is a complete representation of the four-stroke cycle including the intake, compression, combustion, expansion and exhaust processes. The simulation uses detailed thermodynamic gas properties including equilibrium composition for the burned gases. The cylinder heat transfer is based on a correlation from the literature, and the combustion process is based on a mass fraction burn relation.

Figure 1 is a schematic of the thermodynamic system for the simulation. For the combustion processes, three zones (each spatially homogeneous) are used. The three zones are: the unburned zone, the adiabatic core burned zone, and the boundary layer burned zone. The adiabatic core and boundary layer zones together comprise the burned zone. The use of an adiabatic core zone is critical for correct nitric oxide rates. The flow rates are determined from quasi-steady, one-dimensional flow equations, and the intake and exhaust manifolds are assumed to be infinite plenums containing gases at constant temperature and pressure.

Results

For consistency and ease of comparison, compressor and turbine isentropic efficiencies were assumed constant at 70%. The intercooler effectiveness was assumed to be 80%. These values will be varied during parametric studies, but otherwise they are constant. Although not exactly true in applications, for purposes of this study these assumptions were useful.

Operating conditions as functions of engine speed and load were specified. In particular, the inlet and exhaust manifold pressures are provided. The inlet manifold (boost) pressure increases from 100 kPa as engine speed increases from 1,000 rpm to 2,500 rpm and then remains constant at 168 kPa. The exhaust manifold pressure increases continually as engine speed increases due to increases in mass flow.

The brake mean effective pressure (BMEP) and the brake specific fuel consumption (BSFC) were determined as functions of engine speed for the wide open throttle (full load) conditions. The BMEP increases from 1,000 rpm to 2.500 rpm, and attains a maximum value of about 1,523 kPa (at 2,500 rpm). This is consistent with the inlet (boost) pressure – the inlet pressure attains its maximum value first at 2,500 rpm. The BMEP then decreases slightly as engine speed continues to increase to 4,500 rpm. This decrease is largely due to the increasing importance of engine friction for the higher speeds. The BSFC decreases from 1,000 rpm to 2,500 rpm, and attains a minimum value of about 235 g/kW-hr (at 2,500 rpm). The BSFC increases as the engine speed increases from 2,500 rpm to 4,500 rpm; again, this is due to the increasing importance of engine friction for the higher speeds. In general, these results are consistent with published experimental results for this type of application.

Results were obtained for the base case (2,000 rpm) based on both the first law and second law. Table 3 lists the percentage of the fuel energy and fuel exergy associated with the various items. The fuel *energy* is divided between indicated work, engine heat transfer, exhaust gas, intercooler heat transfer, and unused fuel. The work associated with the compressor and turbine are not listed since for the complete system these are in balance.

Also listed in Table 3 is the percentage of fuel *exergy* associated with the various items. The exergy percentage associated with the heat transfer (16.24%) is slightly less than the energy percentage (20.42%) since not all the heat transfer energy can produce work. Similarly, the exergy percentage associated with the exhaust flow (22.97%) is less than the energy percentage (41.42%). The major new items are the exergy destruction terms due to the turbocharger components. These terms include exergy destruction due to the compressor, turbine, and exhaust flow. As for the naturally aspirated case, exergy destruction due to combustion and the inlet flow remain.

The most significant of all the exergy destruction terms remains the combustion process. For these conditions, the destruction due to combustion is about 20.5% of the fuel exergy. The other destruction terms are much smaller. In order of decreasing importance, these are: inlet flow (2.48%), exhaust valve flow (1.96%), compressor (0.36%) and turbine (0.15%). In other

TABLE 3. Example Results for the Base Case: 2,000 rpm, WOT, "MBT" Timing

Item	Energy (%)	Exergy (%)
Indicated Work	36.35	34.54
Heat Transfer	20.42	16.24
Net Flow Out	41.42	22.97
Intercooler Heat Transfer	1.12	0.08
Destruction Combustion	n/a	20.51
Destruction Compressor	n/a	0.36
Destruction Turbine	n/a	0.15
Destruction Inlet	n/a	2.48
Destruction Exhaust	n/a	1.96
Unused Fuel	0.68	0.66
Total	**100.0**	**100.0**

n/a - not applicable

words, the use of turbocharging does not significantly add to the overall irreversibilities.

Figures 3 and 4 show the exergy destroyed by combustion as functions of engine load (at 2,000 rpm) and engine speed (at WOT), respectively. In both cases, the percentage of the entering fuel exergy destroyed by combustion decreases as either load or speed increases. The range is rather small: between about 20.2% and 21.0%. These results are consistent with previous results for naturally aspirated engines – exergy destroyed by combustion decreases as the combustion temperatures increase which is the case for both increasing load and increasing speed.

The exergy destruction due to the compressor and turbine as functions of engine speed for the WOT conditions was also determined. The exergy destruction as a percentage of the fuel exergy increases with increases in speed for both components, but for the higher speeds the increase is much less. Again, the exergy destruction due to the turbine is less than for the compressor due to the lower flow rate through the turbine.

The flow exergy from the cylinder past the exhaust valve into the port and the flow exergy entering the port as functions of crank angle for the base case were determined. The exergy destruction is the difference between the cylinder flow exergy and the port flow exergy. This exergy destruction is largely due to the

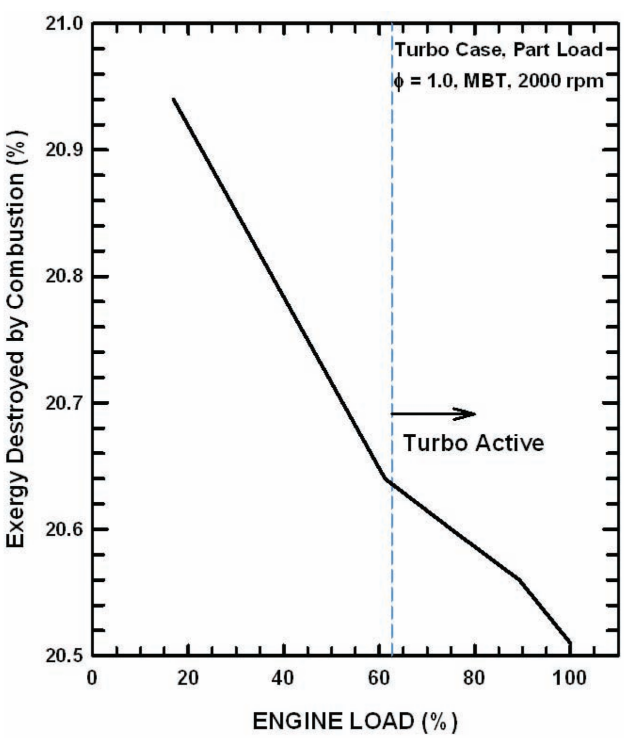

FIGURE 3. Exergy Destroyed by Combustion as a Function of Load for 2,000 rpm

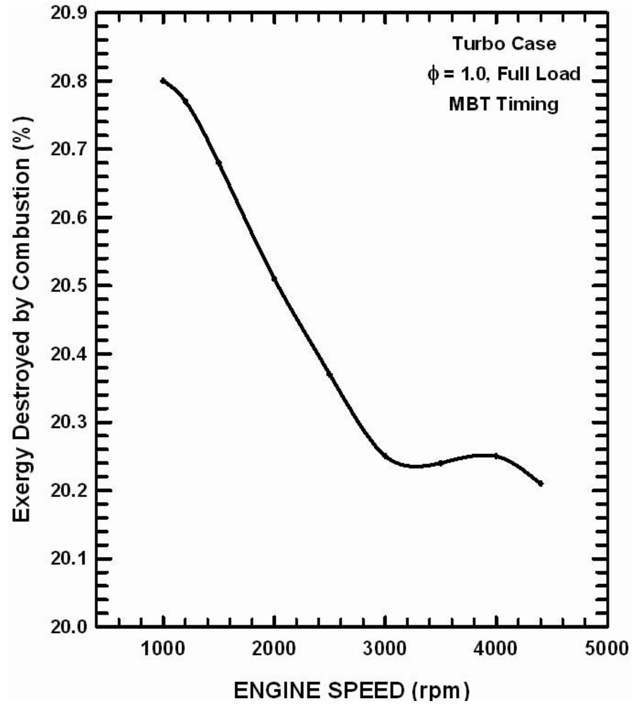

FIGURE 4. Exergy Destroyed by Combustion as a Function of Engine Speed for Full Load

pressure loss and is proportional to the instantaneous mass flow rate. The exergy destruction is largely during the "blow-down" portion of the exhaust event. The integrated value of the exergy destroyed due to the flow past the exhaust valve is listed in Table 3 and accounts for 1.96% of the input fuel exergy.

Due to space limitations, other results can not be presented here. Some of these additional studies included (1) performance as a functions of speed and load, (2) a comparison of the performance of the turbocharged engine with a comparable naturally aspirated engine, (3) performance as a function of compression ratio with and without a maximum cylinder pressure limitation, and (4) performance as functions of the boost pressure ratio.

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IV.6 High-Compression-Ratio Atkinson-Cycle Engine Using Low-Pressure Direct Injection and Pneumatic-Electronic Valve Actuation Enabled by Ionization Current and Forward-Backward Mass Air Flow Sensor Feedback

Harold J. Schock (Primary Contact), Farhad Jaberi, Ahmed Naguib, and Guoming Zhu
Michigan State University
301 Hannah Administration Building
East Lansing, MI 48824

DOE Technology Development Manager: Roland Gravel

NETL Project Manager: Samuel Taylor

Subcontractor:
Visteon Corporation, Van Buren Township, MI

Objectives

1. Develop and demonstrate a low-pressure direct injection system.
2. Develop and demonstrate a mass air flow sensor that would measure the net air flow into the engine on a per cycle basis.
3. Develop and demonstrate a feedback control system enabled by measuring ionization current signals from the spark plug gap.
4. Develop and demonstrate an infinitely variable cam actuation system based on a pneumatic-hydraulic valve actuation.

Accomplishments

Below are the highlights that were accomplished during this effort:

1. A forward-backward mass air flow sensor has been developed and a patent application for the device has been submitted. We are optimistic that this technology will have a particular application in variable valve timing direct injection systems for internal combustion engines.
2. The biggest effort on this project has involved the development of the pneumatic-hydraulic valve actuation system. This system was originally purchased from Cargine, a Swedish supplier and is in the development stage. To date we have not been able to use the actuators to control the exhaust valves, although the actuators have been successfully employed to control the intake valves. Single cycle lift and timing control was demonstrated with this system.
3. Large eddy simulations and KIVA-based simulations were used in conjunction with flow visualizations in an optical engine to study fuel air mixing. During this effort we have devised a metric for quantifying fuel distribution and it is described in several of our papers.
4. A low-pressure direct injection was developed and successfully tested during this effort.
5. A control system has been developed to enable us to test the benefits of the various technologies. This system used is based on Opal-RT hardware and is being used in a current DOE-sponsored project.

Future Directions

The project was completed but additional work is required for the infinitely variable valve actuation system.

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Introduction

This report describes the work completed over a two and one-half year effort sponsored by the U.S. Department of Energy. The goal was to demonstrate the technology needed to produce a highly efficient engine enabled by several technologies which were to be developed in the course of the work.

Approach

The approach used was through a number of technical developments to demonstrate an engine with superior fuel consumption to conventional premixed engines. This was to be accomplished through the use of infinitely variable valves, low-pressure direct injection, and advanced control systems.

Results

Forward-Backward Mass Air Flow Sensor

Three different forward-backward mass air flow sensor (FBMAFS) concepts were evaluated based on the use of hot-wire velocity sensors. The first concept is based on the use of a Michigan State University (MSU) patented idea [1] where an oscillating hotwire is employed to detect the flow velocity magnitude and direction. The second concept, referred to as the dual-sensor concept, was conceived during the investigation and it employs two hot-wire sensors that are mounted behind one another with very small spacing along the flow direction. The final idea, which was also created during the course of this study, employs a variable-area insert as a 'fluidic rectifier' to detect the flow direction. A patent application on this idea [2] (abbreviated as VI-FBMAFS) is currently pending. All sensor concepts were realized and evaluated in the laboratory at MSU under steady and unsteady flow conditions.

Injector Spray, In-Cylinder Fuel Mixture and Flame Combustion Visualization

The effect of spray pattern on fuel mixture preparation in a single-cylinder optical gasoline direct injection (GDI) engine under realistic speed and load conditions was documented and shown in Figure 1. Four injector spray patterns were evaluated. Crank angle (CA) resolved images were taken using a newly acquired high-speed imaging system. Based on extensive image analysis, an optimal spray pattern was identified, which provided a good overall fuel distribution with minimal fuel impinged on the cylinder wall. A technical paper, based on the aforementioned research results, was written and submitted to the 2007 Society of Automotive Engineers World Congress [3].

In this work, three test cases were simulated with our newly developed high order large eddy simulation (LES) model. Validation of the developed LES solver in complex geometries with moving grids was done in the first two test cases, and comparison of LES results for the last test case with experimental data will be presented in future papers. The Eulerian velocity field is calculated by generalized multi-block fourth order compact differencing for spatial derivatives and third order Runge-Kutta for the temporal derivatives. The predicted subgrid-scale turbulent viscosity in LES, which is smaller than the value estimated by RANS, can be highly affected by numerical viscosity. Numerical viscosity can become a serious issue in low order and especially in upwind schemes. For this work, we have only used high order schemes. The first test case considered is the flow around a poppet valve in axisymmetric sudden expansion geometry. This case helps in understanding the complex flow around and behind an intake valve during the intake stroke of real internal combustion (IC) engines and is considered here for validation of the LES model. Thobois et al. [4] used a second order Lax-Wendroff central differencing LES solver to simulate this problem. The second test case considered is the one simulated by Haworth et al. [5] and described briefly above. The geometry is somewhat closer to the first test case, but because of having a moving piston, it may be considered to be closer to realistic IC engines. The last test case considered is the flow in a 3-valve laboratory direct-injection spark-ignition engine, built at the MSU, Automotive Research Experiment Station. This type of engine has been considered for the potential of generating low emissions. Work is in progress to develop experimental data with the controlled and well-defined flow conditions for model validation.

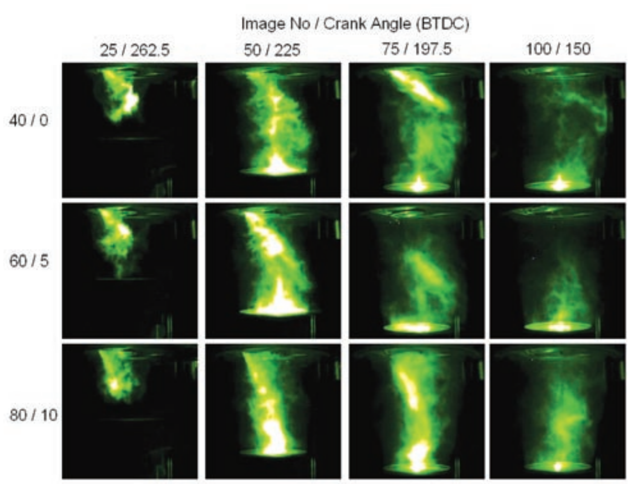

FIGURE 1. In-Cylinder Fuel Mixture Formation at 2,500 RPM/wide-open throttle/30 Bar Fuel Pressure/start of injection at 300° CA Before Top-Dead Center (BTDC)

Electro-Pneumatic Valve Actuator (EPVA) Control System Development for Intake Valves

EPVAs are used to eliminate the camshaft of a traditional internal combustion engine. They are used to control the opening timing, duration, and lift of both intake and exhaust valves. A control-oriented model was developed to reduce computational throughput for real-time implementation. The developed control-oriented model was validated by experimental data. An adaptive valve lift control strategy was developed to improve lift repeatability. A model reference adaptive system identification technique was employed to calculate system parameters needed for generating closed-loop control signals. The convergence of the derived adaptive parameter identification algorithm was verified using the valve test bench data. The bench test data covers engine speed from 1,200 RPM to 5,000 RPM. Parameter identification convergence was achieved within 40 cycles. The closed-loop lift control algorithm was developed and implemented in a prototype controller, and validated on a valve test bench with multiple reference valve lift set points at both 1,200 RPM and 5,000 RPM engine speeds. The experiment results showed that the actual valve lift reached the reference lift within 0.5 mm of lift error in one cycle at 1,200 RPM and in two cycles at 5,000 RPM. The maximum steady-state lift errors are less than 0.4 mm at high valve lift and less than 1.3 mm at low valve lift.

Furthermore, the closed-loop valve lift control improved valve lift repeatability with more than 30% reduction of standard deviation over the open-loop control.

EPVA Control System Development for Exhaust Valves

Variable valve actuation of IC engines is capable of significantly improving their performance. It can be divided into two main categories: variable valve timing with camshaft(s) and camless valve actuation. For camless valve actuation, research has been centered in electro-magnetic, electro-hydraulic, and electro-pneumatic valve actuators. This research studies the control of the electro-pneumatic valve actuator. The modeling and control of intake valves for EPVAs was shown in early publications and this paper extends the EPVA modeling and control development to exhaust valves for lift control, which is the key to the exhaust valve control, since an accurate and repeatable lift control guarantees a satisfactory valve closing timing control. Note that exhaust valve closing timing is a key parameter for controlling engine residual gas recirculation. The exhaust valve lift control challenge is the disturbance from the randomly varying in-cylinder pressure against which the exhaust valve opens. The developed strategy utilizes model-based predictive techniques to overcome this disturbance. This exhaust valve lift control algorithm was validated on a 5.4 liter 3-valve V8 engine head with a pressurized chamber to imitate the in-cylinder pressure. The experimental results demonstrated that the exhaust valve lift tracked the step reference in one cycle with the lift error under 1 mm and the steady-state lift error was kept below 1 mm.

Engine Control Development for High Efficiency Controlled Combustion Engine - Baseline Engine Controller Development

The development of our Opal-RT-based prototype engine controller has been completed. It has been validated in both our engine simulation and on the engine dynamometer. The baseline engine controller contains the following control features:

- Dual fuel control system for both port fuel injection and direct injection fuel systems.
- Ionization detection ignition control and feedback.
- Crank synchronized EPVA control reference generation.

Decentralized Engine and EPVA Control Development

Communication between the Opal-RT engine and EPVA controllers has been established and validated.

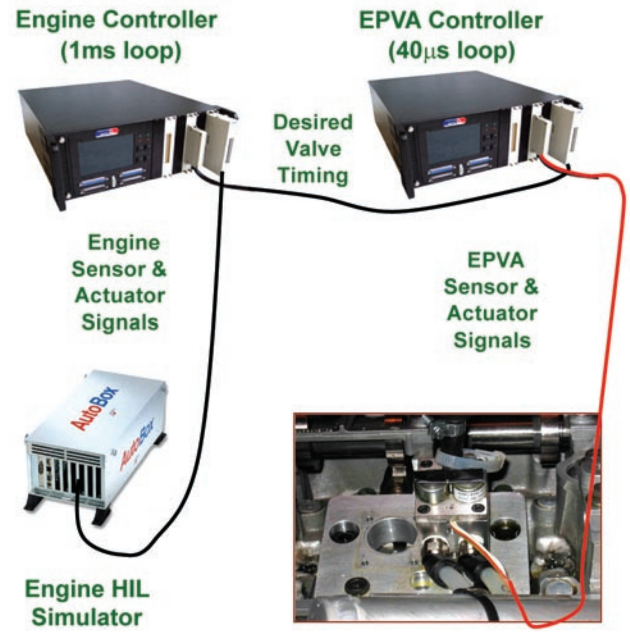

FIGURE 2. Decentralized Engine and EPVA Control Architecture

The basic control principle is that the Opal-RT engine controller sends the crank-synchronized desired valve lift, opening and closing signals to the EPVA Opal-RT controller; and the EPVA controller conducts the valve lift, opening and closing timing control, based upon the reference signals from the engine controller, in a closed-loop.

Both engine and EPVA controllers have been validated using our engine simulation station and EPVA test bench, see diagram in Figure 2. EPVA valve control strategy is under development using this setup. Dynamometer validation tests of both engine and EPVA control strategies are the last task to be completed.

Conclusions

Several new concepts were demonstrated during the course of this investigation and they are described in the above sections. A major impediment to conducting the engine tests of interest was the development of an exhaust valve actuator which could reliably open the exhaust valve. This is due to the variable force required to open the valve under conditions of variable back pressure at different loads. Additional work will be required specifically to develop a sensor to measure the position of the exhaust valve. Also, a redesign of the exhaust valve actuator will be necessary to provide the needed opening force against the high back pressures seen at the end of the expansion stroke.

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3. Hung, D.L.S., Zhu, G., Winkelman, J., Stuecken, T., Schock, H., and Fedewa, A., (2007) "A High Speed Flow Visualization Study of Fuel Spray Pattern Effect on a Low Pressure Direct Injection Gasoline Engine," SAE Technical Paper No. 2007-01-1411, 2007.

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1. Jia Ma, George Zhu, Harold Schock and Tom Stuecken, "Method and Apparatus for Enhancing the Performance of a Camless Valve Actuator," Application made November 1, 2007. US Patent pending.

2. A.M. Naguib, A. Aditjandra, B. Trosin, H.J. Schock, T.R. Stuecken, and E. Timm, "Mass Air Flow Sensor," US Patent pending 2007 (MSU ID#07-019F).

IV.7 On-Board Engine Exhaust Particulate Matter Sensor for HCCI and Conventional Diesel Engines

Matthew Hall (Primary Contact) and Ronald Matthews
University of Texas at Austin (UT)
1 University Station, C2200
Austin, TX 78712-0292

DOE Technology Development Manager: Roland Gravel

NETL Program Manager: Ralph Nine

Subcontractor:
Cummins Engine Co., Columbus, IN

Objectives

- The primary goal of the research is to refine and complete development of an on-board particulate matter (PM) sensor, bringing it to a point where it can be commercialized and marketed. The work is performed through a joint effort between the University of Texas at Austin and the Cummins Engine Company. The research is to be completed in two phases.
- The objective of Phase 1 is to refine the current PM sensor system, adapting it to account for the velocity dependence of the PM sensor signal response, and to further improve and verify the accuracy, durability, and sensitivity of the sensor.
- The objectives of Phase 2 are to determine whether the sensor can be successfully used for diesel engines, including the diesel particulate filter (DPF) and determine if the sensor has the potential to provide useful sensing for individual cylinder control of homogeneous charge compression ignition (HCCI) engines. The sensor will also be tested upstream and downstream of a DPF to determine whether it would be useful as a diagnostic of the need for DPF regeneration and DPF failure.

Accomplishments

We have just completed the second year of this three-year and three-month project. During the second year, the progress we made understanding the fundamental operation of the sensor led to breakthroughs in sensor design and performance that were responsible for our progress toward commercialization of the PM sensor.

- Through studies of PM sensor behavior in steady-state (non-engine) PM-laden flows we discovered that the sensor detects not only the natural charge that is present on diesel PM in engine exhaust, but more importantly, the sensor induces charge on neutral particles that are then detected. The recognition of this effect was very important because we also discovered that the magnitude of the natural charge on the particles diminishes rapidly downstream in the exhaust and can be rather unpredictable in both its sign (whether positively or negatively charge) and its magnitude from cycle-to cycle. Further downstream the induced charge is dominant and quite consistent in its response.
- Through the fundamental investigations we discovered that the velocity dependence of the PM sensor signal is more complex that we originally thought. We found that if the PM sensor signal is dominated by the natural charge on the particles the sensitivity of the sensor increases with increasing exhaust gas velocity. If the signal is dominated by the induced charge the sensitivity of the sensor decreases with increasing exhaust gas velocity. Overall, the velocity effect appears to be relatively small, however.
- New sensor designs were developed, tested, and calibrated. The new designs make use of new manufacturing technologies that bond electrodes directly to ceramic support posts which are electrically isolated in metal bases. By eliminating small diameter metal wire electrodes, vibration noise was significantly reduced. The new foil-type electrodes were found to enhance electric field strength, as well, resulting in higher sensitivity for the same size sensor. Measurements of sensor sensitivity found resolutions as low as approximately 3 mg/m^3 of dry PM, and improvements beyond this level are expected.
- The durability of the sensors has been greatly improved though the application of active heating of the electrode supports. We have sensors with several hours of operating time on them that are still working without changes in signal baseline values or sensitivity.
- The response of the sensor to PM emissions created during engine transients has been assessed. The response time of the sensor was found to be less than 20 ms.
- In addition to the single-cylinder diesel engine testing we initiated vehicle testing. PM sensors were installed and tested at two locations in the exhaust of a diesel-powered sport utility vehicle (SUV) that

was without a DPF. The sensors showed good response and durability for city and highway driving.

- A licensing agreement to commercialize the PM sensor technology was signed in February 2008 with Emisense, Inc. a division of Ceramatec, Inc., which is a division of Coorstek, Inc. We are currently pursuing joint development of the technology and are in the process of finding a large sensor original equipment manufacturer (OEM) to partner with. So far two trips to OEM sensor manufacturers have been made; further discussions are pending.

Future Directions

- Evaluate new sensor designs to further evaluate and, if necessary, improve sensor durability and sensitivity.
- Complete our analysis of the effects of exhaust gas velocity on sensor output.
- Begin testing the sensor in a model-year 2007 6.7 liter Cummins diesel engine that we plan to install in the UT Combustion Laboratory.
- Evaluate suitability for HCCI applications.
- Begin evaluations of the PM sensor applied to local Austin area school busses planned through a cooperative agreement with the Austin Independent School District.
- Commercialization efforts are to continue.

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Introduction

In view of the tightening restrictions on engine emissions of particulate matter there has been increased interest in developing a fast, inexpensive sensor for measuring PM concentrations in engine exhaust flows. Numerous applications can be envisioned for diesel, HCCI, and direct-injection gasoline engines. These include: feedback for control of engine operating parameters, failure detection of DPFs, and as an indicator of the need for DPF regeneration.

Approach

The first 15 months of the project comprised Phase 1. The next 12 months comprised the first part of Phase 2. A major focus of Phase 2 was the design and construction of new sensor types, and testing them using our single-cylinder diesel engine test rig to gain a better understanding of the sensor characteristics. Of particular interest was the sensitivity of the sensor, its response time, its accuracy, and durability. A procedure to calibrate the sensors for quantitative measurements based on filter measurements was established. We built a steady-state flow rig for sensor testing that led to new understanding of sensor fundamentals. Because there was a delay of approximately eight months in the delivery of our 6.7 liter engine from Cummins we initiated vehicle testing of the sensor to further its development.

Results

Five tasks comprise the second year budget period as outlined in the original proposal. The original work plan had to be revised somewhat because Cummins was not able to provide us with the 6.7 liter engine within the time-frame originally specified. This impacted Task 2.2, 2.3, and 2.4, as listed below. We did finally receive the engine in October 2008 and are now working toward these tasks. Fortunately, the delay in receiving the Cummins engine did not substantially slow our PM sensor development efforts as mentioned above under *Accomplishments*. We created new important tasks including the fundamental studies in the steady-flow rig, and we leap-frogged to on-board vehicle testing of the sensor.

Task 2.1. Identify qualified sensor commercialization partner.

Task 2.2. Complete set up of the 6.7 L Cummins light-duty engine on a dynamometer test stand.

Task 2.3. Measure and document sensitivity, time response, and durability of the best PM sensor in the exhaust of the 6.7 L Cummins engine.

Task 2.4. Measure and document sensitivity, time response, and durability of the best PM sensor in the exhaust of the heavy-duty Cummins engine operating as diesel and make preliminary measurements in HCCI mode.

Task 2.5. Optimize sensor design for high durability and sensitivity.

Sensor Design

The sensor design has evolved greatly over the last year. Figure 1 shows this evolution with an older design at the top and a newer design at the bottom. The sensor evolved to improve durability, reduce vibration noise, and improve manufacturability.

Sensor Sensitivity

We wanted to establish an estimate of the resolution of our current PM sensors and the lower limits of PM concentration they could resolve. Figure 2 shows the sensor signal for a 450 s period prior to shutdown of our single-cylinder test engine. The engine was run at 1,500 rpm at a very low load of 1.5 Nm torque. A foil-electrode-type sensor similar to the bottom sensor shown in Figure 1 was used. One may notice the voltage scale of these measurements; instead of being in the volts range, these measurements are in the 10s of mV range.

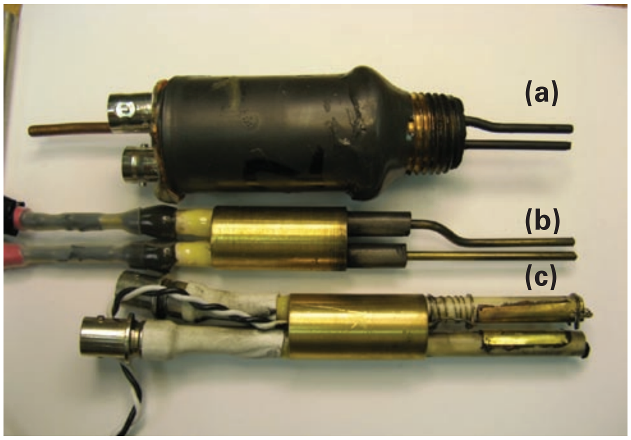

FIGURE 1. Three PM Sensor Designs–From top to bottom: (a) air purged sensor, (b) brass housing sensor with ceramic tube electrode shields, (c) brass housing foil-electrode sensor with active heater coil.

These measurements were acquired simultaneously with a filter measurement which showed an average dry PM emissions mass of 17 mg/m^3. The offset voltage is approximately a factor of four or five time greater than the bandwidth of the noise. This suggests that even in its current configuration considerably lower PM concentration levels can be resolved, perhaps to a level as low as about 3-4 mg/m^3. We feel this can be improved upon further with enhanced designs.

Vehicle Measurements

The PM emissions from a light-duty SUV were measured using the PM sensors. The purpose of the vehicle testing was two-fold: to evaluate the sensor behavior on an actual vehicle and to characterize the PM emissions behavior of the vehicle. For the sensor, we were primarily interested in its time-response, its sensitivity to PM, its noise characteristics, particularly with respect to vibration, and its durability.

The testing was performed on the Chevrolet Equinox SUV used by the UT Student Society of Automotive Engineers (SAE) Team for the U.S. Department of Energy/General Motors-sponsored Challenge X Competition. Originally equipped with a gasoline engine, the student SAE team removed the original drive-train and installed a manual transmission along with a new 1.9 liter Fiat/Opel turbo-diesel. The engine had a compression ratio of 17.5 and a rated peak power of 106.8 kW. All of the measurements were made without the DPF installed. The sensor was installed at two locations in the exhaust. One location was approximately mid-way between the engine and muffler; the other location was in a metal housing attached to the tailpipe of the vehicle. This housing also contained an opacity meter for comparison with the PM sensor. For the testing, we made use of the extensive data recording capabilities provided by the student SAE team. Data were recorded with 40 ms time resolution. The parameters recorded include:

- PM sensor output voltage
- Opacity meter output voltage
- Vehicle speed (km/hr)
- Engine speed (rpm)
- Pedal position (% of maximum)
- Engine Torque (Nm)

The vehicle was driven on city streets around the university for the testing.

Figure 3 shows a one minute period from a 27 minute long drive-cycle presenting only PM sensor output and opacity meter output. There is good qualitative agreement between the two; the short duration peaks are well correlated. For two engine transients near the 2 s time mark, the PM concentrations were great enough to saturate the PM sensor, sending its output off-scale (beyond 5 V). The time-response of the sensor is evident through its rapid recovery time from the transient puffs. The PM sensor response time was limited by a low-pass filter set to approximately 0.9 Hz. This was considered adequate to resolve the transients since its signal durations were comparable to those of

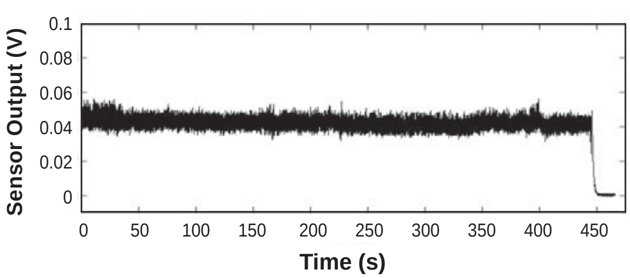

FIGURE 2. PM sensor signal at a steady-state 1,500 rpm condition and subsequent shutdown.

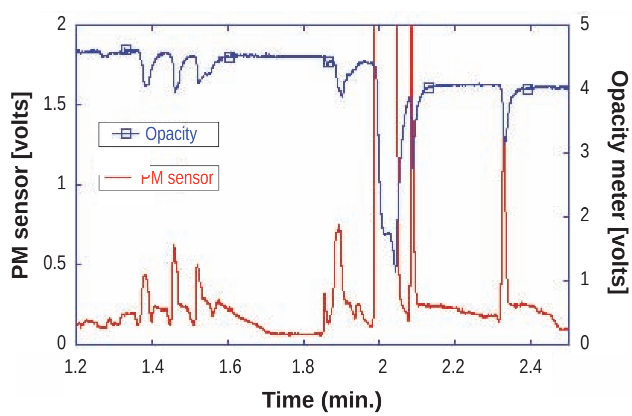

FIGURE 3. Approximately one minute portion of drive-cycle from Equinox showing PM sensor output and opacity meter output.

the opacity meter which had a detector time-response in the sub-millisecond range.

Conclusions

Development of the UT electronic PM sensor is proceeding well. New, more durable sensors having a longer life have been designed, built, calibrated, and tested. Development was aided by new studies that provided insights into the fundamental operation of the sensors. The sensor has a response time of less then 20 ms. Long-duration testing in both a stationary engine and onboard a vehicle demonstrated stable baselines and sensitivities. Sensitivities of at least 3-4 mg/m^3 dry PM have been demonstrated. Tasks 2.2-2.4 were delayed due to the delay in receiving the 6.7 liter test engine from Cummins. Commercialization efforts are proceeding through our industrial partner.

In summary, the UT PM sensor is fast, portable, inexpensive to build, and shows promise for use in closed-loop control of particulate emissions from diesel and HCCI engines. Future work will refine its design and test its operation in a modern, heavy-duty diesel engine of an order of magnitude larger displacement.

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3. Hall, M.J., Diller, T.T., and Matthew, R.D. "Fast-response electronic particulate matter sensor for diesel engine control and DPF failure detection," 8th International Symposium on Combustion Diagnostics, ISBN 978-3-00-022057-9, Editor Peter Ziegler, AVL Europe, Baden-Baden, Germany, June 10–11, 2008.

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V. Acronyms and Abbreviations

Φ	Fuel air equivalence ratio
γ	Ratio of specific heats (c_p/c_v)
τ_{id}	Ignition delay time
η	Effectiveness
°C	Degrees Celsius
°CA	Degrees crank angle, 0° = TDC intake
°F	Degrees Fahrenheit
0-D	Zero-dimensional
$1C_6H_{12}$	1-hexene
1-D	One-dimensional
3-D	Three-dimensional
3P	3-pentanone
4Q	Fourth quarter
A_2	Strain rate based on air side of stagnation plane [s^{-1}]
AC	Alternating current
ACE	Advanced Combustion in Engines
ACEC	Advanced Combustion & Emissions Control
ACES	Advanced Collaborative Emissions Study
AEC	Advanced Emission Controls Working Group
AEC	Advanced Engine Combustion
AEI	After end of injection
A/F	Air to fuel ratio
AFR	Air/fuel ratio
AHRR	Apparent heat release rate
AIChE	American Institute of Chemical Engineers
Al	Aluminum
Al_2O_3	Aluminum oxide
AMDC	Advanced mode diesel combustion
ANL	Argonne National Laboratory
APU	Auxiliary power unit
ARES	Automotive Research Experiment Station
ASC	Ammonia slip catalyst
ASI	Time after the start of injection
ASME	American Society of Mechanical Engineers
atdc, ATDC	After top dead center
a.u.	Arbitrary units
B100	Mid-speed & 100% engine load point of ESC Test Procedure
B25	Mid-speed & 25% engine load point of ESC Test Procedure
B75	Mid-speed & 75% engine load point of ESC Test Procedure
Ba	Barium
$BaAl_2O_4$	Barium aluminate
$Ba(NO_3)_2$	Barium nitrate
BaO	Barium oxide
BDC	Bottom dead center
BES	Basic Energy Sciences
BET	Named after Brunauer, Emmett and Teller, this method for determining the surface area of a solid involves monitoring the adsorption of nitrogen gas onto the solid at low temperature and, from the isotherm generated, deriving the volume of gas required to form one monolayer adsorbed on the surface. This volume, which corresponds to a known number of moles of gas, is converted into a surface area though knowledge of area occupied by each molecule of adsorbate.
bhp-hr	Brake horsepower hour
BiTe	Bismuth telluride thermoelectric material
Bi_2Te_3	Bismuth Telluride
bmep, BMEP	Brake mean effective pressure
BOI	Beginning of injection
BP	formerly British Petroleum
bsfc, BSFC	Brake specific fuel consumption
bsNOx	Brake specific NOx emissions
btdc	Before top dead center
BTE	Brake thermal efficiency
C_1	Carbon content in the exhaust or reformer in terms of carbon atoms
C_2H_4	Ethene
C_2H_6	Ethane
C_3H_6	Propylene
C8	A fuel molecule with 8 carbon atoms
C16	A fuel molecule with 16 carbon atoms
ca.	about, approximately
CA	Crank angle
CA50	Crank angle at which 50% of the combustion heat release has occurred
CAC	Charge air cooler
CAD	Computer-aided design
CAD	Crank angle degrees
CARB	California Air Resources Board
cc	Cubic centimeter

CCD	Charge coupled device
CDI	Compression direct injection
CDPF	Catalytic diesel particulate filter
CeO_2	Cerium oxide
CFD	Computational fluid dynamics
CFR	Waukesha Cooperative Fuel Research Engine
CFR	Coordinating Fuel Research
CFR	Critical functional response
CH_4	Methane
CHEMKIN	Sandia chemical kinetics code
CI	Compression ignition
CIDI	Compression ignition direct injection
CLEERS	Cross-Cut Lean Exhaust Emissions Reduction Simulations
CLOSE	Collaborative Lubricating Oil Study on Emissions
cm	Centimeter
cm^3	Cubic centimeters
CN	Cetane number
CNC	Computer numerically controlled
CNG	Compressed natural gas
CO	Carbon monoxide
CO_2	Carbon dioxide
COV	Coefficient of variation
CP	Chevron Phillips
CPER	Counterflow preheating with near-equilibrium reaction
CPF	Catalyzed particulate filter
cpsi	Cells per square inch
CPU	Central processing unit
CR	Compression ratio
CRADA	Cooperative Research and Development Agreement
CRC	Coordinating Research Council
CR-DPF	Continuously regenerating diesel particle filter
CRF	Combustion Research Facility
CT	Computed tomography
CTC	Characteristic time combustion
CVT	Continuously variable transmission
CVVD	Continuously variable valve duration
CVVL	Continuously variable valve lift
d	Nozzle diameter
DC	Direct current
DDC	Detroit Diesel Corporation
DEER	Diesel Engine Emissions Reduction
deg	Degrees
$DeNO_x$	Oxides of nitrogen reduction
De-S	Desulfation
DI	Direct injection, direct injected
DIP8	Dual in-line package, 8-pins, an integrated circuit type
DISI	Direct-injection spark-ignition engine
DME	Dimethyl ether
DNS	Direct Numerical Simulation
DNPH	2,4-dinitorophenylhydorazine
DOC	Diesel oxidation catalyst
DOE	U.S. Department of Energy
DOHC	Double overhead camshaft
DOM	Discrete ordinates method
DP	Pressure differential
DPF	Diesel particulate filter
DPNR	Diesel Particulate NOx Reduction
DRF	Directed relational graph method for mechanism reduction
DRIFTS	Diffuse reflectance infrared Fourier-transform spectroscopy
dt_{inject}	Injection duration
E10	10% ethanol, 90% gasoline fuel blend
E85	85% ethanol, 15% gasoline fuel blend
EC	Elemental carbon
ECM	Electronic control module
ECN	Engine Combustion Network
ECU	Electronic control unit, engine control unit
EERE	Energy Efficiency and Renewable Energy
EEVO	Early exhaust valve opening
EDS	Energy dispersive spectroscopy
EDX	Energy dispersive X-ray
EGR	Exhaust gas recirculation
EOI	End of injection
EPA	U.S. Environmental Protection Agency
EPMA	Electron probe microanalysis
EPVA	Electro-pneumatic valve actuator
ER	Expansion ratio
ERC	Engine Research Center
ESC	European Steady State Cycle
ES&H	Environment, safety, and health
ESPG	Engine selection process group
ETC	Electric turbocompound
EtOH	Ethanol
EVC	Exhaust valve closing
EVO	Exhaust valve opening
EWHR	Exhaust waste heat recovery

FBMAFS	Forward-backward mass air flow sensor
FCVT	FreedomCAR and Vehicle Technologies
FEA	Finite-element analysis
FEERC	Fuels, Engines and Emissions Research Center
FFVA	Fully flexible valve actuation
FiO	Fuel in oil
FMEA	Failure mode and effects analysis
fmep	Friction mean effective pressure
F/PAH	Combined formaldehyde and polyaromatic hydrocarbons
FSN	Filter smoke number
FTIR	Fourier transform infrared
ft-lb	Foot-pound
FTP	Federal Test Procedure
FTP-75	Federal Test Procedure for LD vehicles
FVVA	Full variable valve actuation
FY	Fiscal year
g, G	Gram
GA	Genetic algorithm
GATE	Graduate Automotive Technology Education
g/bhp-hr	Grams per brake horsepower-hour
GC	Gas Chromatography
GC-FID	Gas chromatograph combined with a flame ionization detector
GC-MS	Gas chromatography – mass spectrometry
GDC	Gadolinium-doped Cerium Oxide
GDI	Gasoline direct injection
Ge	Germanium
g/hphr	Grams per horsepower-hour
GHSV	Gas hourly space velocity
gIMEP	Gross indicated mean effective pressure
GISFC	Gross indicated specific fuel consumption
g/kWh	Grams/kilowatt-hour
GM	General Motors
g/mi	Grams per mile
GT-Power	Gamma Technologies engine modeling software
GUI	Graphical user interface
GVWR	Gross vehicle weight rating
H_2	Diatomic (molecular) hydrogen
H2-ICE	Hydrogen-fueled internal combustion engine
H_2O	Water
H2-SpaciMS	Hydrogen-calibrated spatially resolved capillary inlet mass spectrometry
HC	Hydrocarbons
HCC	Heat conduction in components
HCCI	Homogeneous charge compression ignition
HC-SCR	Hydrocarbon selective catalytic reduction
HCT	Hydrodynamics, Chemistry, Thermodynamics code
HD	Heavy-duty
HEA	Hydraulic Element Assembly
HECC	High-efficiency clean combustion
HEI	Health Effects Institute
HEV	Hybrid electric vehicle
HFPE	Hydrogen free-piston engine
HHV	Higher heating value
HIL	Hardware-in-loop
hp	Horsepower
HPL	High-pressure loop
HPLC	High-performance liquid chromatography
HR	Heat release
hr	Hour
HRR	Heat release rate
HSDI	High-speed direct-injection
HTML	High Temperature Materials Laboratory
HWFET	Highway Fuel Economy Test
Hz	Hertz
IC	Internal combustion
I/C	Intercooler
ICCD	Intensified charged-coupled device
ICE	Internal combustion engine
ID	Internal diameter
IMEP	Indicated mean effective pressure
$IMEP_g$	Indicated mean effective pressure, gross
INCITE	Innovative and novel computational impact on theory and experiment
I/O	Input-output
IR	Infrared
ISB	Cummins Inc. 6.7 liter displacement inline 6-cylinder diesel engine
ISFC	Indicated specific fuel consumption
ISX	Cummins Inc. 15-liter displacement, inline, 6-cylinder heavy duty diesel engine
ITEC	International Truck and Engine Corporation
IVA	Intake valve actuation
IVC	Intake valve closing

IVO	Intake valve opening
J	Joule
k	Mass transfer coefficient
k	Thousand
K	Kelvin
K	Potassium
kg	Kilogram
kHz	Kilohertz
KIVA	Combustion analysis software developed by Los Alamos National Laboratory
kJ	Kilojoules
kJ/L	Kilojoules per liter
kPa	Kilopascal
KS	Converging hydroground nozzle
kW	Kilowatt
L	Liter
LA92	Drive cycle for vehicle tests
LANL	Los Alamos National Laboratory
LAST	Lead, antimony, silver, and tellurium, an n-type TE material
LAST/T	LAST/Tin, a p-type TE material
L/D	Length-to-diameter ratio
LB	Lattice-Boltzmann
lb ft	Pound foot
lb/min	Pounds per minute
lbs	Pounds
lbs/sec	Pounds per second
LD	Light-duty
LDA	Laser doppler anemometry
LDD	Light-duty diesel
LDT	Light-duty truck
LED	Light emitting diode
LEM	Linear eddy model
LES	Large eddy simulation
LHV	Lower heating value
LIBS	Laser-induced breakdown spectroscopy
LIDAR	Light detection and ranging
LIDELS	Laser-induced desorption with elastic light scattering
LIF	Laser-induced fluorescence
LII	Laser-induced incandescence of soot
LIVC	Late intake valve closing
LLNL	Lawrence Livermore National Laboratory
LM	Lost motion
LNT	Lean-NOx trap
LP	Low pressure
LPEGR	Low pressure exhaust gas recirculation
LPL	Low pressure loop
LRRI	Lovelace Respiratory Research Institute
LSC	Lanthanum strontium chromite
LTC	Low-temperature combustion
LTC-D	Low-temperature combustion-diesel
LTHR	Low temperature heat release
m^2	Square meters
m^2/gm	Square meters per gram
m^3	Cubic meters
mA	Milliamps
MB	Mercedes-Benz
mbar	Millibar
MBC	Model-based control
MBT	Minimum (spark advance) for best torque; Maximum brake torque
MD	Medium-duty
MDO	Mechanism Design Option, Parametric Technologies software
MECA	Manufacturers of Emission Controls Association
mg/cm^2	Milligrams per square centimeter
mg/mi	Milligram per mile
mg/mm^2	Micrograms per square millimeter
mg/scf	Milligrams per standard cubic foot
mi	Mile
min	Minute
MIT	Massachusetts Institute of Technology
MK	Modulated Kinetics
μm	Micrometer
mm	Millimeter
mmols	Micro-moles
Mn	Manganese
Mo	Molybdenum
mol	Mole
mol/s	Moles per second
MOU	Memorandum of Understanding
MPa	Megapascals
mph	Miles per hour
ms	Millisecond
MSATs	Mobile source air toxics
MSU	Michigan State University
MTU	Michigan Technological University
MY	Model year
N_2	Diatomic nitrogen
N_2O	Nitrous oxide
N_2O_3	Nitrogen trioxide

Na	Sodium
NAHRR	Normalized apparient heat release rate
NEDC	New European Drive Cycle
NETL	National Energy Technology Laboratory
NH_3	Ammonia
nm	Nanometer
Nm	Newton meter
NMEP	Net mean effective pressure
NMHC	Non-methane hydrocarbon
NMOG	Non-methane organic gases
NMR	Nuclear magnetic resonance
NO	Nitric oxide
NO_2	Nitrogen dioxide
NOx	Oxides of nitrogen (NO and NO_2)
NRDC	National Resources Defense Council
NRE	NOx reduction efficiency
NRT	NOx reduction technology
NSE	NOx storage efficiency
NSFC	Net Specific Fuel Consumption (g fuel/kW-hr)
NSGA	Non-dominated sorting genetic algorithm
NSLS	National Synchrotron Light Source
NSR	NOx storage and reduction
NTC	Negative temperature coefficient
NTE	Negative temperature effect
NTRC	National Transportation Research Center
NVO	Negative valve overlap
NZ-50	Near-zero emissions at 50% thermal efficiency
O_2	Diatomic (molecular) oxygen
O_3	Ozone
OBD	On-board diagnostics
OC	Organic carbon
OEM	Original Equipment Manufacturer
OHC	Oxygenated hydrocarbons
OFCVT	Office of FreedomCAR and Vehicle Technologies
OFR	Oil fill ratio
OH	Hydroxyl
OH*	Hydroxyl radical that emits ultraviolet photons
OH PLIF	Planar laser-induced fluorescence of OH
OHW	Oscillating hotwire
ORC	Organic Rankine Cycle
ORNL	Oak Ridge National Laboratory
OS	Office of Science
OSC	Oxygen storage capacity
OSR	Oxygen storage and reduction
OTR	Over-the-road
OVT	Office of Vehicle Technologies
P	Pressure
PAH	Polycyclic aromatic hydrocarbon
PBA	1 wt% Pt/20 wt% BaO/Al_2O_3
PBAC	1 wt% Pt/20 wt% BaO/Al_2O_3 (74 wt%) + 1 wt% Pt/CeO_2 (26 wt%)
PbTe	Lead telluride thermoelectric material
PCI	Partially premixed compression ignition
PCCI	Premixed charge compression ignition
PCM	Power control module, powertrain control module
PCP	Peak cylinder pressure
PCS	Power control subsystem
PFI	Port fuel injection, port fuel injected
PFI-DI	Port fuel injection/direct injection
PIV	Particle image velocimetry
PLII	Planar laser-induced incandescence
PLIF	Planar laser induced fluorescence
PM	Particulate matter
PNNL	Pacific Northwest National Laboratory
ppb	Parts per billion
PPC	Partially premixed combustion
PPCI	Partially premixed compression ignition
ppi	Pores per square inch
ppm	Parts per million
ProE	ProEngineer CAD software
PRF	Primary Reference Fuels (iso-octane and n-heptane),
PRF60	Primary reference fuel blend, 60% iso-octane and 40% n-heptane
PRF80	Primary reference fuel blend, 80% iso-octane and 20% n-heptane
PRR	Pressure rise rate
PSAT	Powertrain Systems Analysis Toolkit
psi	Pounds per square inch
psig	Pounds per square inch gauge
Pt	Platinum
PV, P-V	Pressure-volume
Q1, Q2, Q3, Q4	First, second, third and fourth quarters
QW	Quantum well
R&D	Research and development
RANS	Reynolds Averaged Navier Stokes
RAPTR	Regenerative air preheating with thermochemical recuperation
RCF	Rapid compression facility

REV	Representative equivalent volume
RGF	Residual gas fraction
Rh	Rhodium
RMS	Root mean square
ROI	Rate of injection
rpm	Revolutions per minute
RT	Room temperature
S	Entropy
S	Sulfur
SA	Spark assist
SAE	Society of Automotive Engineers
SCAQMD	South Coast Air Quality Management District
sccm	Standard cubic centimeters
SCE	Single-cylinder engine
SCF/min	Standard cubic feet per minute
SCORE	Sandia Compression-ignition Optical Research Engine
SCOTE	Single-cylinder oil test
SCR	Selective catalytic reduction
SCTE	Single-cylinder test engine
sec	Second
SEM	Scanning electron microscopy
SGS	Subgrid-scale
Si	Silicon
SI	Spark ignition
SiC	Silicon carbide
SIDI	Spark ignition direct injection
SIRDM	Spray-interactive reduced dimension model
SFC	Specific fuel consumption
SFTP	Supplemental Federal Test Procedure
SLPM	Standard liters per minute
SMR	Steam methane reformation
SMSI	Strong metal support interaction
SNL	Sandia National Laboratories
SNR, S/N	Signal-to-noise ratio
SO_2	Sulfur dioxide
SOC	Start of combustion
SOI	Start of injection
SOF	Soluble organic fraction
SOx	Oxides of sulfur
SpaciMS	Spatially resolved capillary inlet mass spectrometer
Sr	Strontium
SR	Steam reforming
Star-CD	A three dimensional numerical simulation of engine flows and combustion
SU	Stanford University
SUV	Sports utility vehicle
SV	Space velocity
SVOC	Semivoltaic organic compound
SwRI	Southwest Research Institute®
T	Temperature
T_2	Temperature of air at autoignition [K]
TAGS	Tellurium, antimony, germanium and silicon thermoelectric material
TAP	Temporal Analysis of Products
T_B	Temperature burned gas
TC	Turbocompund
TCR	Thermo-chemical recuperation
TDC	Top dead center
TDI	Turbocharged direct injection
TDL	Tunable diode laser
TE	Thermoelectric
TEG	Thermoelectric generator
TEM	Transmission electron spectroscopy
TER	Thermal energy recovery
TGA	Thermal gravimetric analysis
TGM	Thermoelectric generator module
THC	Total hydrocarbon
TP	Tailpipe
TPD	Temperature-programmed desorption
TPGME	Tri-propylene glycol monomethyl ether
TPR	Temperature-programmed reduction or reaction
TPRX	Temperature-programmed reaction
TP-XRD	Temperature-programmed X-ray diffraction
TR-XRD	Time-resolved X-ray diffraction
t_{ss}	Time to achieve a steady-state liquid length
TSC	Two-stage combustion
T_U	Temperature unburned gas
UEGO	Universal exhaust gas oxygen
UHC	Unburned hydrocarbons
ULSA	Ultra-low solidity airfoil
ULSD	Ultra-low sulfur diesel
UM	University of Michigan
USCAR	U.S. Cooperative Automotive Research
US06	Supplemental Federal Test Procedure (SFTP)
UV	Ultraviolet

UW	University of Wisconsin
UW-ERC	University of Wisconsin Engine Research Center
V	Volt
VAC	Volts, alternating current
VAT	Variable admission turbine
VCR	Variable compression ratio
VCT	Variable cam timing
VDC	Volts, direct current
VGC	Variable geometry compressor
VGT	Variable geometry turbocharger
VI-FBMAFS	Variable-area insert, forward-backward mass air flow sensor
VIGV	Variable inlet guiding vane
VNT	Variable nozzle turbine
VOCs	Volatile organic compounds
VPTNA	Volvo Powertrain North America
VTG	Variable turbine geometry
VVA	Variable valve actuation
VVT	Variable valve timing
W	Watt
W	Work
WAVE	Ricardo engine and one-dimensional gas dynamics simulation software
WGS	Water-gas shift
WGSR	Water-gas shift reaction
WHR	Waste heat recovery
WOT	Wide-open throttle
WSA	Watt sub assembly
wt%	Weight percent
XAFS	X-ray aborption fine structure
XANES	X-ray absorption near-edge spectroscopy
XPS	X-ray photoelectron spectroscopy
XRD	X-ray diffraction
Y	Yttrium
yr	Year
YTZP	Yttrium oxide (Y_2O_3) partially stabilized zirconia (Zr)
Zn	Zinc
YSZ	Ytrria-stabilized zirconia
ZT	Dimensionless thermoelectric figure of merit; equal to: (electrical conductivity)(Seebeck coefficient)^2(temperature)/(thermal conductivity)

VI. Index of Primary Contacts

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

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