U.S. Department of Energy
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ADVANCED COMBUSTION ENGINE TECHNOLOGIES

Less dependence on foreign oil, and eventual transition to an emissions-free, petroleum-free vehicle

FreedomCAR and Vehicle Technologies Program

2006 ANNUAL PROGRESS REPORT

21st Century Truck Partnership

FreedomCAR & Fuel Partnership

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FY 2006 PROGRESS REPORT FOR ADVANCED COMBUSTION ENGINE TECHNOLOGIES

Energy Efficiency and Renewable Energy
Office of FreedomCAR and 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 FreedomCAR and Vehicle Technologies, we are pleased to introduce the Fiscal Year (FY) 2006 Annual Progress Report for the Advanced Combustion Engine R&D Sub-Program. The mission of the FreedomCAR and Vehicle Technologies (FCVT) Program is to develop more energy-efficient and environmentally friendly highway transportation technologies that enable America to use less petroleum. The Advanced Combustion Engine R&D Sub-Program supports this mission and the President's initiatives by removing the critical technical barriers to commercialization of advanced internal combustion engines for light-, medium-, and heavy-duty highway vehicles that meet future Federal and state emissions regulations. The primary goal of the Advanced Combustion Engine R&D Sub-Program is to improve the brake thermal efficiency of internal combustion engines:

- for passenger vehicles, from 30% (2002 baseline) to 45% by 2010, and
- for commercial vehicle applications, 40% (2002 baseline) to 55% by 2013,

while meeting cost, durability, and emissions constraints. R&D activities include work on combustion technologies that increase efficiency and minimize in-cylinder formation of emissions, as well as aftertreatment technologies that further reduce exhaust emissions. Research is also being conducted on approaches to produce useful work from waste engine heat through the development and application of thermoelectrics, electricity generation from exhaust-driven turbines, and incorporation of energy-extracting bottoming cycles.

Advanced internal combustion engines are a key element in the pathway to achieving the goals of the President's FreedomCAR and Fuel Partnership for transportation. Advanced engine technologies being researched will allow 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 and are carried out in collaboration with industry, national laboratories, and universities. Because of the importance of clean fuels in achieving low emissions, R&D activities are closely coordinated with the relevant activities of the Fuel Technologies Sub-Program, also within the Office of FreedomCAR and Vehicle Technologies.

Background

The compression ignition direct injection (CIDI) engine, an advanced version of the commonly known diesel engine, is a promising advanced combustion engine technology for achieving dramatic energy efficiency improvements in light-duty vehicle applications, where it is suited to both conventional and hybrid-electric powertrain configurations. Light-duty vehicles with CIDI engines can compete directly with gasoline engine hybrid vehicles in terms of fuel economy and consumer-friendly driving characteristics; also, they are projected to have energy efficiencies that are competitive with hydrogen fuel cell vehicles. The primary hurdles that must be overcome to realize increased use of CIDI 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 CIDI 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 fuel sulfur. Even the recent reduction of diesel fuel sulfur content to below 15 ppm does not assure that CIDI engine catalytic emission control devices will be durable and cost-effective. The CIDI engine offers a propulsion platform with the potential for further significant efficiency improvements beyond its current capabilities. Although the Advanced Combustion Engine R&D Sub-Program initially sought a wide range of combustion technologies applicable to the CIDI engine, work has since transitioned to focus on advanced low-temperature combustion (LTC) regimes that offer substantial improvements in efficiency and near-zero emissions.

The heavy-duty diesel engine is already 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 are to be 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 oxides of nitrogen (NOx) and particulate matter (PM).

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 CIDI engines with inherently lower emissions, and eventually advanced engines operating in low-temperature 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.
- Increase overall engine efficiency through fundamental improvements such as advanced combustion processes, reduction of parasitic losses, and recovery of waste heat.
- Improve the effectiveness, efficiency, and durability of CIDI 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 air pollution and greenhouse gas emissions.

Technology Status

Recent advances in fuel injection systems have made the CIDI engine very attractive for light-duty vehicle use by reducing the combustion noise associated with diesel engines, and consumers are discovering that diesel engines offer outstanding driveability and fuel economy. The change-over to ultra-low-sulfur diesel fuel will enable 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. Mercedes-Benz has started selling a CIDI passenger car that is certified to Tier 2 Bin 8 in the U.S. using a NOx adsorber and diesel particulate filter (DPF) and has added diesel engine options for its SUVs. Mercedes-Benz has announced that it plans to offer CIDI vehicles in 2008 that meet the Tier 2 Bin 5 standard through the use of selective catalytic reduction (SCR) employing urea for regeneration (urea-SCR). Volkswagen, Audi, and BMW also plan to incorporate urea-SCR technology into their CIDI vehicles in 2008. In 2009, Honda plans to introduce a CIDI passenger car to the U.S. 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.

Current heavy-duty diesel engines have efficiencies in the range of 43–45%. These engines have significantly improved efficiency over engines produced just a few years ago. Improvements are being made in a wide variety of engine components such that engines a few years from now may have efficiencies between 47 and 48% without employing waste heat recovery.

Starting in 2007, heavy-duty diesel engines for on-highway commercial trucks will be equipped with DPFs to meet particulate emissions standards. This will be the first very broad application of aftertreatment devices in the trucking industry. In some cases, DPFs are paired with oxidation catalysts to facilitate passive or active regeneration. DPFs are typically capable of reducing PM emissions by

90% or more. For NOx control, aftertreatment devices are not likely to be needed in the heavy-duty sector until 2010 emissions regulations take effect.

Among the options for NOx aftertreatment for diesel engines, urea-SCR is the clear leader because of its performance and superior fuel sulfur tolerance. The U.S. EPA is in the process of establishing vehicle design guidelines to assure that urea is widely available and that the proper inducements are in place to assure that users of urea-SCR vehicles don't operate them without replenishing the urea. 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 will be 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.

The other technology being considered for NOx control from CIDI engines is lean-NOx traps (LNTs), also known as NOx adsorbers. LNTs appear to be favored by light-duty manufacturers (as witnessed by Honda's announcement of their intent to use them with their CIDI engines in 2009) since overall fuel efficiency is less of a concern than for heavy-duty manufacturers, and because urea replenishment represents a larger concern for light-duty customers than for heavy-duty vehicle users. LNTs appear to be able to achieve the Tier 2 Bin 5 light-duty vehicle emission levels when new using ultra-low-sulfur fuel, although full-useful-vehicle-life emissions have not yet been demonstrated. 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 to ten 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 (PGM), and the cost of these materials has been rising at a concerning rate.

An optimum solution to CIDI 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 new combustion regimes such as homogeneous charge compression ignition (HCCI), pre-mixed charge compression ignition (PCCI) and modes of low-temperature combustion (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, and Ford has announced that it intends to release a light-duty CIDI engine employing HECC before 2012 which may not include any NOx aftertreatment devices.[1]

Complex and precise engine and emission controls will require sophisticated feedback systems employing new types of sensors. NOx and PM sensors are in the early stages of development and require additional advances to be cost-effective and reliable, but are essential to control systems for these advanced engine/aftertreatment systems. Much progress has been made, but durability and cost

[1] "Ford, PSA Developing HCCI Diesel" by William Diem, WardsAuto.com, Oct. 11, 2006.

remain as the primary issues with these sensors. Start-of-combustion sensors have been identified as a need, and several development projects have been started.

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 recent expansion of the Renewable Fuel Standard, which calls for 7.5 billion gallons of renewable fuel (mostly ethanol) to be used in transportation fuels by 2012.

Waste heat recovery represents an area of significant potential for efficiency improvements. 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%.

Future Directions

Internal combustion engines have a maximum theoretical fuel conversion efficiency that is similar to that of fuel cells; it approaches 100%. 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 "new combustion regimes" might impact the irreversibility 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 internal combustion engine 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.

Fuels can also play an important role in reducing combustion irreversibility losses. Preliminary analyses show that combustion irreversibility losses per mole of fuel are considerably less for hydrogen than for hydrocarbon fuels. This finding is consistent with the understanding that combustion irreversibility losses are reduced when combustion is occurring nearer equilibrium (high temperature), since hydrogen has the highest adiabatic flame temperature of the fuels studied to date. This bodes well for the development of highly efficient hydrogen-fueled internal combustion engines.

Emission control devices for CIDI engines to reduce PM and NOx will become widespread over the next few years. Much work still needs to be done to make these devices more durable 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 with increased attention to CO and HC control.

Goals and Challenges

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

- Combustion and Emission Control R&D
- Heavy Truck Engine R&D
- Waste Heat Recovery
- Health Impacts

Combustion and Emission Control R&D

The Combustion and Emission Control R&D activity focuses on enabling technologies for energy-efficient, clean vehicles powered by advanced internal combustion engines (ICEs) using clean hydrocarbon-based and non-petroleum-based fuels and hydrogen. R&D has been focused on developing technologies for light-, medium-, and heavy-duty CIDI engines and is being transitioned to developing technologies for advanced engines operating in combustion regimes that will further increase efficiency and reduce emissions to near-zero levels.

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 CIDI engines into the light-duty truck market would reduce fuel use by 30-40% per gasoline vehicle replaced.) The major challenges facing CIDI 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.

The FreedomCAR and Fuel Partnership technical targets for ICEs are shown in Table 1. The following goals are energy-efficiency improvement targets for advanced combustion engines suitable for passenger cars and light trucks; they also address technology barriers and R&D needs that are common between light- and heavy-duty vehicle applications of advanced combustion engines.

- By 2007, achieve peak engine efficiency of at least 42% and, combined with some emission control devices, meet EPA Tier 2, Bin 5 requirements in a light-duty vehicle using diesel fuel (specified by the Fuels Technology Sub-Program) with a fuel efficiency penalty of not more than 2%.
- By 2010, develop the understanding of novel low-temperature combustion regimes needed to simultaneously enable engine efficiency of 45% with a fuel penalty of less than 1%.
- By 2015, lower the cost of hydrogen ICEs to $30/kW.

Heavy Truck Engine R&D

The long-term (2013) goal of this activity is to develop the technologies that will increase the thermal efficiency of heavy-duty diesel engines to at least 55% while reducing emissions to near-zero levels. More specifically,

- By 2006, increase the peak thermal efficiency of heavy-duty engines to 50% while meeting EPA 2010 emission standards.
- By 2013, increase the peak thermal efficiency of heavy truck engines to 55% while meeting prevailing EPA emission standards.

The interim goal for FY 2006 of achieving 50% efficiency while demonstrating 2010 emission standards was successfully achieved. This activity also supports the goal of the 21st Century Truck Partnership to develop and validate a commercially viable, 50%-efficient, emissions-compliant engine system for Class 7 and 8 highway trucks by 2010.

TABLE 1. Technical Targets for the Combustion and Emission Control Activity

Characteristics	Units	Fiscal Year			
		2007	2009	2010	2015
FreedomCAR Goals, ICE Powertrain					
Peak brake thermal efficiency (HC fuel) (H_2 fuel)	%			 45 45	 45
Cost (HC fuel) (H_2 fuel)	$/kW			30 45	 30
Reference peak brake thermal efficiency[a]	%	32	34	35	
Target peak brake thermal efficiency/part-load brake thermal efficiency (2 bar BMEP[b] @1500 rpm)	%	42/29	44/30	45/31	
Powertrain cost[c,d]	$/kW	30	30	30	
Emissions[e]	(g/mile)	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] Brake mean effective pressure
[c] High-volume production: 500,000 units per year
[d] Constant out-year cost targets reflect the objective of maintaining powertrain (engine, transmission, and emission control system) system cost while increasing complexity.
[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.

As seen in Table 2, researchers will need to increase thermal efficiency of heavy-duty truck engines significantly while maintaining low emissions by the end of 2013. To date, all the 2006 targets have been achieved. Further increases in engine efficiency will be needed to achieve the interim efficiency objectives for 2009 and 2013.

TABLE 2. Technical Targets for Heavy Truck Diesel Engine R&D

Characteristics	Fiscal Year			
	2006 Status	2006	2009	2013
Engine thermal efficiency, %	50	50	51	55
NOx emissions, g/bhp-hr	<0.20	<0.20	<0.20	<0.20
PM emissions, g/bhp-hr	<0.01	<0.01	<0.01	<0.01
Stage of Development	prototype	prototype	prototype	prototype

Waste Heat Recovery

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. Turbocompounding 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 8% 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 used in one of the heavy truck engine efficiency projects.

The longer-term goal of this activity is to develop the technologies for recovering engine waste heat and converting it to useful energy that will improve overall diesel engine thermal efficiency to 55% while reducing emissions to near-zero levels. More specifically,

- By 2012, enable commercially viable turbocompound units that can produce up to 40 kW of additional power from heavy-duty engine waste heat recovery.
- By 2012, achieve at least 21% efficiency in quantum well thermoelectric devices for waste heat recovery.

This activity also supports the overall engine efficiency goals of the FreedomCAR and Fuel Partnership and the 21st Century Truck Partnership.

The technical targets for the waste heat recovery R&D activities are listed in Table 3. Significant progress will be needed to meet the 2008 targets. Ongoing and newly awarded projects are focused on achieving this progress.

TABLE 3. Technical Targets for Waste Heat Recovery

Characteristics	Units	Fiscal Year		
		2006 Status	2008	2010
Turbocompound system				
Class 7-8 trucks				
Fuel economy improvement Power Projected component life	% kW Hrs.	<5 >10 <10	>5 >20 >5,000	>10 >40 >10,000
Thermoelectric Devices				
Efficiency bulk semiconductor quantum well	%	6-8 --	-- >15	-- >20
Projected cost/output (250,000 production volume)	$/kW	TBD	500	180

Health Impacts

The FCVT Program and its industry partners are on the leading edge in the technology development of future technologies to improve fuel economy and enable the use of non-petroleum-based fuels in passenger and commercial vehicles. The Health Impacts Research activity performs the critical role of elevating potential health issues related to these future technologies to the attention of industry partners and DOE/FCVT management. This 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.

The goals of the Health Impacts Research activity are as follows:

- 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.
- Ensure that vehicle technologies being developed by FCVT for commercialization by industry will not have adverse impacts on human health through exposure to toxic particles, gases, and other compounds generated by these technologies.

Project Highlights

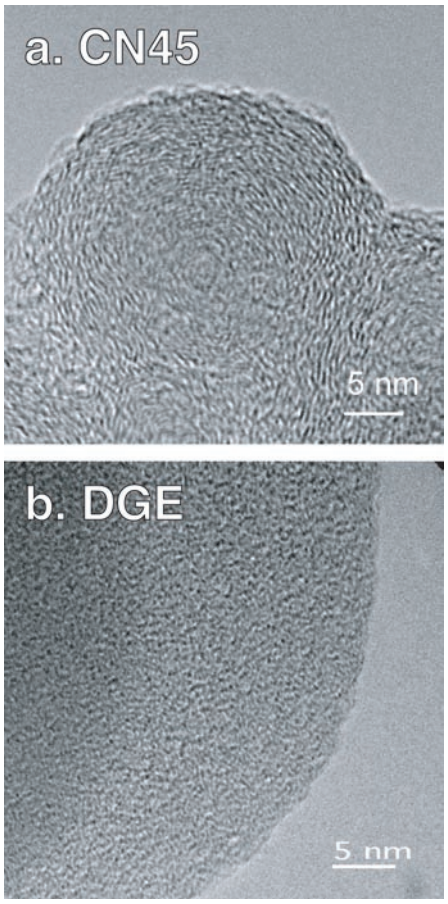
The following projects highlight progress made in the Advanced Combustion Engine R&D Sub-Program during FY 2006.

Advanced Combustion and Emission Control Research for High-Efficiency Engines

A. Combustion and Related In-Cylinder Processes

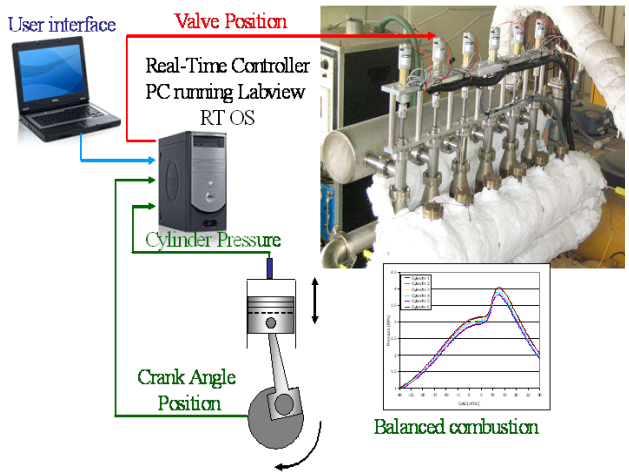
The objective of these projects is to identify how to achieve more efficient combustion with reduced emissions from advanced technology engines.

- Argonne National Laboratory (ANL) made the first-ever X-ray measurements of CIDI fuel injector sprays at an ambient pressure of 30 bar which is representative of the ambient density inside a turbocharged light-duty diesel engine at the start of injection.
- Sandia National Laboratories (SNL) identified the existence of a toroidal vortex at the exit of re-entrant bowl CIDI combustion chambers, and the role of this vortex in trapping soot and unburned hydrocarbons. The vortex also prevents mixing of combustion products exiting the bowl with additional squish volume oxidizer.
- SNL studied spray, combustion, and pollutant formation for two conventional and three low-temperature combustion conditions and developed an optical diagnostic technique to identify sources of unburned fuel emissions.
- SNL demonstrated that fuel changes (e.g., oxygenation) can lead to the production of soot with a disordered nanostructure that could oxidize up to five times faster than highly ordered soot from conventional diesel fuel. They also showed that while neat biodiesel can lower smoke emissions by ~50% relative to conventional diesel fuel when high levels of cooled exhaust gas recirculation (EGR) are used, further reductions of at least an order of magnitude are required to meet the 2010 PM emission target without using aftertreatment.
- SNL generated unique datasets for *in situ* soot volume fraction in reacting sprays as a function of EGR level, ambient temperature, ambient density, injection pressure, and fuel type. They also found that reduced soot formation using extensive EGR is caused by soot kinetics rather than mixture equivalence ratio.
- Oak Ridge National Laboratory (ORNL) expanded the speed-load range of operation under high-efficiency clean-combustion (HECC) using combinations of high- and low-pressure EGR methods. They also characterized the potential emissions reduction of using fuel injectors with reduced orifice diameters for improved atomization and mixing.
- ORNL achieved and demonstrated the 2007 FreedomCAR goal of 41% peak brake thermal efficiency in an automotive-size diesel engine and validated the part-load efficiency target.



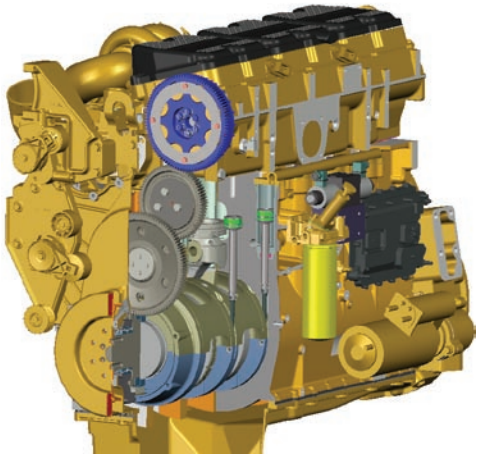
High resolution transmission electron micrographs of soot from a) a hydrocarbon reference fuel and b) a fuel blend with the oxygenate diethylene glycol diethyl ether. SNL found that the highly disordered nanostructure of soot from the oxygenated fuel is correlated with oxidation rates up to five times greater than those for soot with a more-orderly nanostructure.

- SNL conducted a suite of validation studies aimed at simultaneous treatment of turbulence and combustion phenomena in internal combustion engine environments. They also established the "Computational Combustion and Chemistry Laboratory" specifically dedicated to internal combustion engine calculations.
- Lawrence Livermore National Laboratory (LLNL) developed a very fast methodology for analysis of HCCI combustion - only ~10% longer computational time than a motored (non-firing) case. They also demonstrated innovative control strategies and applied them to the Caterpillar 3406 experimental HCCI engine, demonstrating accurate cylinder balancing and fast load and ignition timing adjustment.

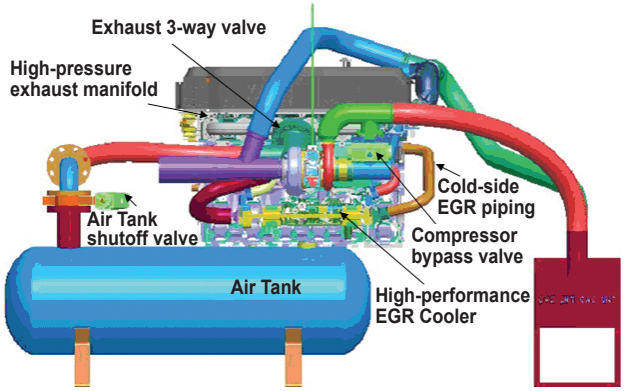


HCCI Control System Developed by LLNL for Experimental Caterpillar 3406 HCCI Engine

- SNL found that the HCCI combustion process consists of a series of distinct phases, each with its own unique chemiluminescence spectral and spatial signature, indicating different key reactions. They also determined that chemiluminescence intensity tracks the heat-release rate well during the main high-temperature combustion for higher fueling rates, but it is not a reliable marker of the heat-release rate at low loads.
- SNL uncovered correlation between laser-induced fluorescence based probability density function statistics of fuel-air mixing and measured engine-out NOx emissions during low-load, late-injection HCCI operation. Taken together with earlier data for carbon-based emissions, these results indicate that the developed probability density function method could be a useful tool for formulating and assessing advanced mixture-preparation strategies.
- Los Alamos National Laboratory (LANL) completed the parallelization of KIVA-4, which reduces computational time by a factor of 3.2 using a moving square bowl grid. KIVA-4 was tested against several analytical solutions, and the results, along with KIVA-4's numerical algorithms, are to appear in the Journal of Computational Physics.
- LLNL completed models for chemical kinetics of combustion of three major fuel components, plus methyl cyclohexane, and di-isobutylene. They continued development of surrogate mixtures to describe HCCI ignition.
- SNL established collaborative modeling research with the University of Michigan and General Motors to simulate a full hybrid vehicle platform powered by a free-piston engine.
- ANL obtained endoscope images at over 2,000 RPM and over 6 bar indicated mean effective pressure (IMEP) for port fuel injection, single injection direct injection, and double injection direct injection of hydrogen. OH* chemiluminescence images were obtained using ultraviolet imaging, showing the progression of the combustion event. A correlation between heat release and OH* intensity was obtained.
- SNL measured flame front propagation speeds for hydrogen injection prior to intake valve closure at various equivalence ratios. They also found an empirical correlation between OH* chemiluminescence emission intensity and equivalence ratio that is used to obtain a semi-quantitative measure of the maximum in-cylinder equivalence ratio.
- Cummins has demonstrated 6% improvement in fuel economy relative to the baseline value with preliminary steady-state multi-cylinder engine testing optimized for premixed charge compression ignition (PCCI) combustion.



Cross-Section of Caterpillar Variable Compression Ratio Engine



Compressed Air Hybrid System Developed by Mack Trucks

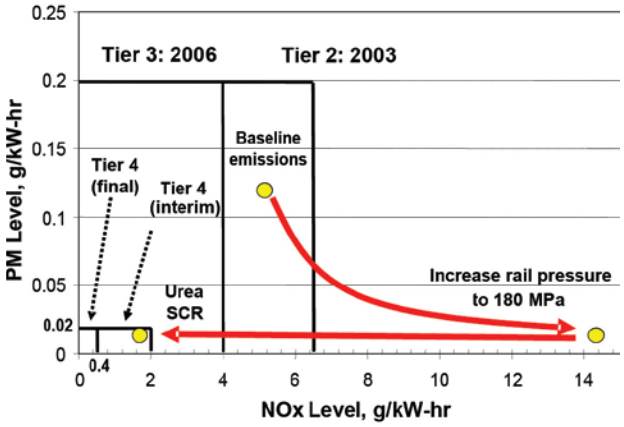
- Caterpillar developed an advanced multi-cylinder engine with compression ratio flexibility and tested it, demonstrating benefits for emissions, efficiency and controls.
- International Truck and Engine redesigned their ITEC 6.4L V8 to support low-temperature or HCCI combustion for high efficiency and low emissions, targeting 2010 federal emission standards using standard diesel fuel.
- John Deere demonstrated that an advanced diesel engine can be operated at stoichiometric conditions with reasonable particulate and NOx emissions at full power and peak torque conditions. Such an engine does not need EGR and will operate at 42% brake thermal efficiency without advanced hardware, turbocompounding, or waste heat recovery.
- Mack Trucks completed a vehicle simulation using air-power-assist (APA) engine technology that showed 4–18% efficiency improvement over a wide range of driving cycles. In addition, they found that low-temperature EGR offered an additional 3-4% efficiency improvement in vehicle simulation tests.
- General Motors completed set up of both gasoline and diesel engines with variable valve actuation systems to enable and test HCCI combustion.

B. Energy-Efficient Emission Controls

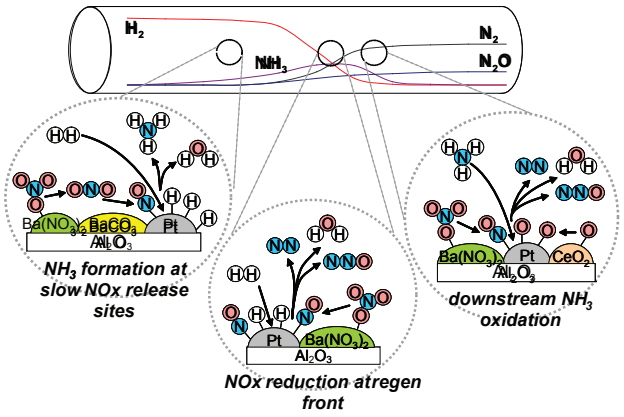
The following project highlights summarize the advancements made in emission control technologies to both reduce emissions and reduce the energy needed for emission control system operation.

- SNL found an optimized, thermodynamically consistent set of kinetic parameters for the regeneration mechanism of lean-NOx traps by fitting model predictions to the results of pseudo-steady-state reactor experiments conducted at ORNL.
- ORNL identified multiple sulfate species on both Ba- and K-based lean-NOx traps that are dependent on time and temperature and demonstrated linear loss in storage sites with sulfation.
- ORNL quantified details of CO regeneration of lean-NOx traps and the function of the water-gas-shift reaction and characterized detection limit of various analytical methodologies for real-time on-engine measurement of oil dilution.
- ORNL achieved interim Tier 4 NOx emissions and final Tier 4 PM emissions for an off-highway diesel engine using a combination of advanced injection control coupled with urea-SCR. This represents a >90% reduction in NOx and PM emissions over the baseline setting.

- ORNL found that when evaluating a lean-NOx trap with low reductant concentrations, the NOx conversion was 11–33% higher at all temperatures with hydrogen engine exhaust compared to conventional CIDI exhaust.
- Pacific Northwest National Laboratory (PNNL) developed tools for digital reconstruction of three-dimensional particulate filter substrate microstructures from a small set of two-dimensional images. They added soot oxidation kinetics to the micro-scale lattice-Bolzmann filter model and developed techniques for observing regeneration on the surface of uncatalyzed and platinum-catalyzed single-channel filter samples.
- ORNL held the 9th Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) workshop at University of Michigan, Dearborn on May 2–4.
- ORNL continued testing and validation of the LNT material characterization protocol in conjunction with the LNT Focus Group, SNL, PNNL and collaborating suppliers, and initiated diffuse reflectance infrared Fourier-transform spectroscopy (DRIFTS) measurements of Umicore reference catalyst to study the relationship of sulfur poisoning to multiple storage sites.



Pathway to Lower Off-Highway Engine Emissions Developed by ORNL



Scenario proposed by ORNL for the stages involved in LNT regeneration as the reductant front progresses axially down the monolith

- ORNL modified LNT regeneration strategies to generate engine-out hydrogen and other reformate products under net-lean conditions and tested them on commercial SCR catalysts using hydrocarbons as the reductant.
- General Motors developed a microwave heating technique that uniformly heats a diesel particulate filter for regeneration and eliminates parasitic soot absorption.
- General Motors tested over 5,600 materials for NOx reduction potential and achieved conversion efficiencies of 92% (Highway Cycle), 76% (US06 Cycle) and 60% (Federal Test Procedure, FTP) using a V6 common rail diesel. Sulfur poisoning has been evaluated, and regeneration strategies have been identified using both reactor studies and engine evaluations.

C. Critical Enabling Technologies

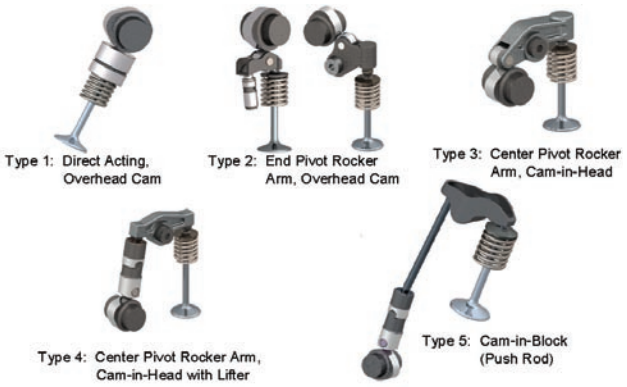
Variable valve actuation and variable compression ratio systems are enabling technologies for achieving more efficient engines with very low emissions. The following highlights show the progress made during FY 2006.

- Envera reduced the hydraulic pressures in their variable compression ratio actuator system by 86% through system optimization.
- Delphi Automotive Systems completed the engine evaluation matrix and selected the diesel engine to be used for testing of their variable valve actuation system. More than 100 research papers were studied and three potential valve motion solutions were identified.

Heavy Truck Engine

With the advent of stringent emission standards, it is necessary to design engines as systems to achieve both high efficiency and low emissions. The following project highlights describe the progress made for both light- and heavy-duty engines during FY 2006.

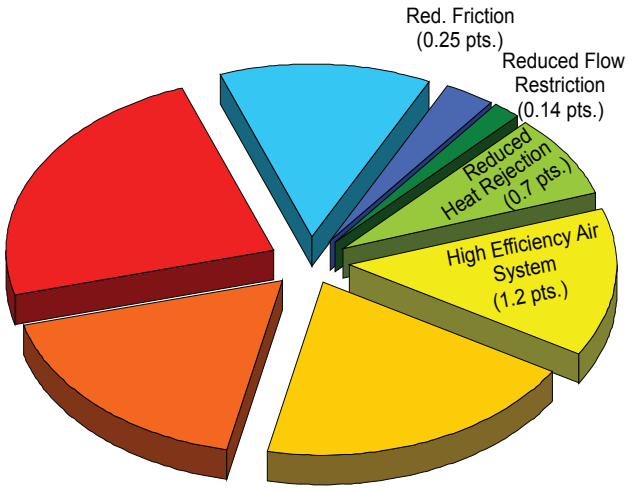
- Cummins demonstrated 50% brake thermal efficiency from a heavy-duty diesel engine while meeting 2010 U.S. EPA legislated emissions requirements.
- Detroit Diesel Corporation demonstrated integrated experimental and analytical technologies capable of achieving 50.2% thermal efficiency at EPA-regulated 2010 emissions levels at a single operating condition in a multi-cylinder engine configuration.



Different Valve System Types Investigated by General Motors for Variable Valve Actuation Systems

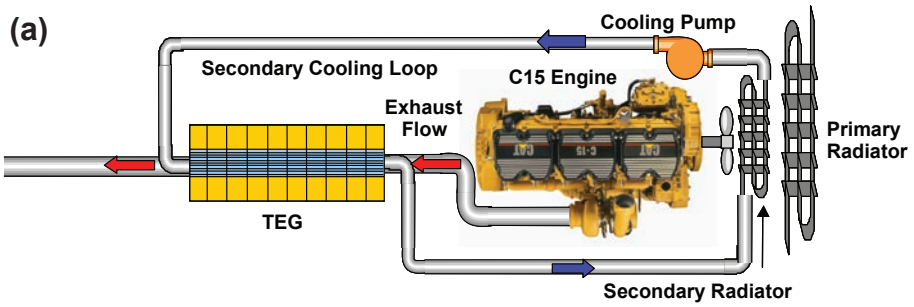
Waste Heat Recovery

Several technologies are being pursued to capture waste heat from advanced combustion engines, including electricity generation from turbochargers, thermoelectrics, and compound/bottoming cycles. Following are highlights of the development of these technologies during FY 2006.



Contribution of 50% Thermal Efficiency Building Blocks Developed by Caterpillar

- General Motors achieved a ZT value of 1.3 at 800 K in nano-composite n-type skutterudites, the highest reported ZT values for n-type skutterudite thermoelectric materials.
- BSST has modeled and designed 20-watt high temperature and 750-watt low temperature thermoelectric generators. A vehicle performance model used to predict fuel efficiency has been developed and validated, and fuel efficiency improvement ranging up to 7.7% has been predicted.
- United Technologies Corporation developed a new thermoelectric generator design that resulted in a 6.5–7.0% fuel economy improvement versus the earlier reported 4–4.5%. A series of bulk boron carbide nanocomposites was fabricated and characterized, and thermoelectric property measurements were acquired up to 400ºC.
- Michigan State University measured properties of known materials for the temperature range of operation and estimated that a segmented couple can provide a 12.3% conversion efficiency. Calculations show estimated improvement of up to 6.2% in fuel economy for a Class 8 truck operating at cruise conditions.
- Cummins has designed and is testing a Rankine cycle to extract waste heat from a heavy-duty truck engine. Recovered waste heat energy will be converted to electricity to assist in driving the vehicle, and powering electrically driven parasitics (such as coolant pumps, fans, etc.) will be explored in addition.

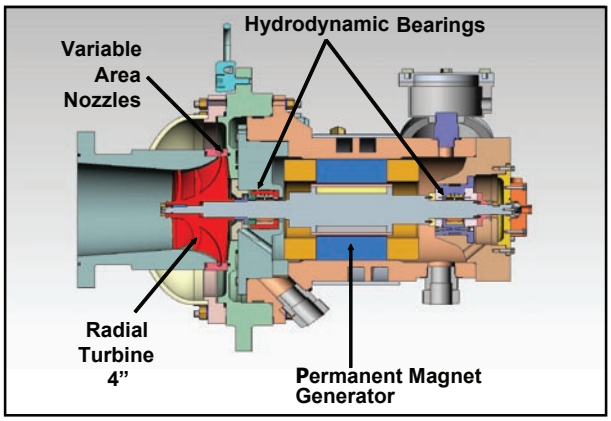


System-Level Thermoelectric Generator Design Developed by United Technologies

- Mack Trucks demonstrated through simulation an engine efficiency increase of 8.2% through use of a continuously variable transmission when operating over a road cycle and 10.5% during steady-state operation at U.S. 2010 NOx levels (0.2 g/bhp-hr).

Off-Highway Engine Efficiency R&D

Off-highway vehicles are coming under more stringent emission controls similar to those for highway vehicles. However, their typical duty cycles place unique demands on emission control systems. Following are highlights of off-highway vehicle emission control development during FY 2006.



Cummins Proposed Turbine/Generator Design

- John Deere completed models that accurately predicted the pressure drop across both a diesel oxidation catalyst (DOC) and a DOC plus a catalyzed particulate filter (DOC+CPF) for various engine speeds and loads under steady-state operation. The models also accurately predicted the amount of mass deposited and oxidized in the CPF as a function of time. The models will next be tested to see if they can indicate when to regenerate.
- In a Cooperative Research and Development Agreement (CRADA) with John Deere, ORNL discovered that the total PM emissions were reduced by 50% by the urea-SCR catalyst in a system without a DPF. This effect was maintained during high rates of urea application.
- John Deere developed and tested a compact 50 kW flywheel-mounted motor/generator system. Through component optimization and turbo system matching, performance goals of 20% power growth and a 10% increase in fuel economy have been demonstrated at Tier 3 emissions levels.

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. Following are highlights of the work conducted in FY 2006.

- ORNL completed a project concentrating on ambient air quality which showed that idling trucks typically dominate the air quality degradation near the roadway despite the large number of trucks traveling on the road per day.

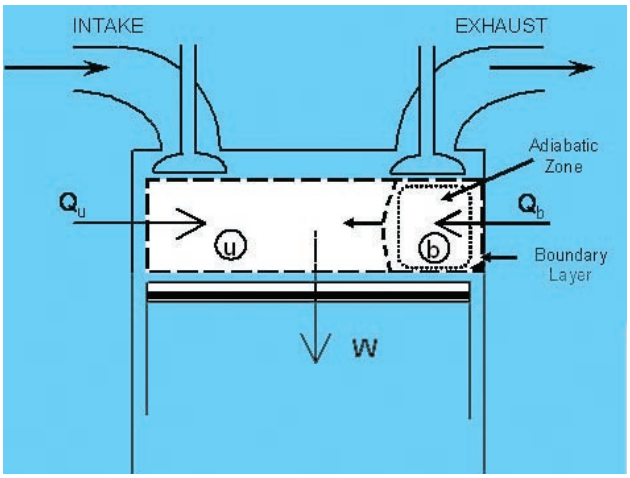
- Lovelace Respiratory Research Institute discovered that used diesel crankcase oil nanoparticles have low lung toxicity, completed a comprehensive study of the effects of repeated inhalation exposure to laboratory-generated gasoline emissions, and discovered that non-particulate emissions from gasoline engines can cause vascular changes in a mouse model of atherosclerosis.
- The Health Effects Institute 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.



UV Remote Sensing Technique Developed by ORNL

University Research

- The University of Wisconsin-Madison has formulated combustion models and reaction mechanisms and applied them to analyze low-emissions operation. A low-emissions window of operation has been identified as a benchmark for further testing.
- West Virginia University developed two models as comparative tools for diesel and low-temperature combustion. The low-temperature combustion model allows for prediction of auto-ignition onset. A general friction model was chosen that includes losses from piston-ring assembly, engine bearing, valvetrain and engine auxiliaries.
- The University of Houston obtained time-averaged NOx conversions exceeding 80% in a lean-NOx trap with cycling protocols of 60 second storage phase and 5–10 second regeneration phase. The byproduct ammonia and nitrous oxide selectivities were determined, with ammonia selectivity as high as 50% depending on the rich pulse composition.
- The University of Kentucky Center for Applied Energy Research determined the effect of ceria on lean-NOx trap NOx storage and regeneration behavior by means of powder reactor and DRIFTS measurements.
- Texas A&M University completed and documented a parametric study of the destruction of availability during the combustion process for simple systems. The availability destroyed during the combustion process decreased with increasing temperatures and varied with the fuel being used under constant conditions.



Texas A&M Engine Cylinder Schematic Depicting Three Zones During Combustion

- The University of Michigan has shown through engine testing and modeling that pilot injection of fuel during negative valve overlap (NVO) can be used to extend the lower load limit of homogeneous charge compression ignition (HCCI) operation. They also found that spark assist has a stabilizing effect on combustion under limiting conditions.

Future Directions

Advanced Combustion and Emission Control Research for High-Efficiency Engines

A. Combustion and Related In-Cylinder Processes

The focus in FY 2007 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. Several labs and universities plan to adopt a common engine research platform that will span optical single-cylinder through multicylinder experiments. Achievement of 42% peak efficiency for the 2007 FreedomCAR goal is expected to be validated at ORNL with this engine.

In FY 2007, LANL will continue their efforts to integrate advanced combustion models into the KIVA-4 computational fluid dynamics model and implement grid converters to improve its accuracy in unstructured grids. LANL will validate their customized version of KIVA against experimental data from both SNL and ORNL for engine operation under HCCI and PCCI conditions. One of their objectives is to develop their model as a predictive tool for engine geometry and fuel injection optimization. SNL will continue to work towards their objective to use high-fidelity science-based simulations in a manner that directly complements select optical engine experiments also being conducted by SNL. The simulations will be carried out using a highly specialized state-of-the-art flow solver designed for turbulent reacting multiphase flows and will be used to study hydrogen combustion. LLNL will extend their fuel combustion model capabilities to additional classes of fuel components, including biodiesel and larger hydrocarbon components, to investigate the effect of fuel molecular structure on sooting under diesel engine conditions.

ANL is continuing their efforts to increase the ambient pressure in their X-ray fuel injector spray measurement device to more closely simulate actual fuel injection pressures. They also plan to incorporate faster data acquisition, processing, and analysis; improved X-ray detector systems; increased X-ray intensity; and greater automation. ANL will also use their endoscope imaging system to acquire images of OH* chemiluminescence from a direct injection hydrogen engine with the objective of characterizing a multiple injection strategy to improve performance while minimizing emissions. This work will be complemented by SNL using planar laser induced fluorescence (PLIF) to obtain a spatially resolved quantitative measure of in-cylinder equivalence ratio. SNL will also apply PLIF imaging to a comparative study of mixture formation using two different gasoline direct injection (GDI) fuel injectors for stratified-charge operation, as well as to a complete investigation of how HCCI progresses through the combustion event, using chemiluminescence spectroscopy and chemical-kinetic analysis for single- and two-stage-ignition fuels. Additional activities at SNL in FY 2007 include evaluating low-temperature combustion, exploring the effects of fuel properties on soot and NOx formation, and studying the effect of fuel spray penetration and equivalence ratio on emissions, all using in-cylinder laser optical techniques.

ORNL will be using parametric engine studies in FY 2007 to resolve multi-cylinder stability and control issues for expanded high-efficiency, controlled combustion (HECC) engine operation. They will also employ combustion and engine models to explain the governing processes that occur during transitions between spark ignition and HCCI combustion using gasoline (i.e., physics, chemistry), explore advanced combustion approaches for achieving improved efficiency and reduced emissions, and investigate potential of waste heat recovery strategies. Cummins plans to complete their multi-cylinder

demonstration of premixed charge compression ignition combustion by employing next-generation turbochargers and controls. They also plan to test biodiesel and conduct single-cylinder engine studies of advanced, multi-pulse injection systems. Caterpillar plans to continue their optical engine tests to refine and validate their computational fluid dynamics submodels to implement HECC on advanced multi-cylinder engines. International Truck and Engine plans to implement variable valve actuation hardware with cylinder pressure feedback software and demonstrate 2010 emissions targets under steady-state at target engine operating points. After proving that their stoichiometric compression ignition concept is viable, in FY 2007 John Deere will further test the concept by building a complete system. Mack Trucks will continue development of their concept to use the engine to convert braking energy into compressed air stored in an on-board tank which is subsequently used to partially power the engine without combustion using a unique variable valve actuation system. SNL plans to initiate design, fabrication, and construction of a two-stroke opposed piston prototype utilizing optimized coupling of Magnequech alternators as a proof-of-concept tool.

General Motors will test variable valve actuation systems on both single- and multi-cylinder engines and assess the potential to lower NOx emissions to meet the Tier 2 Bin 5 standard without the use of aftertreatment devices.

B. Energy-Efficient Emission Controls

In FY 2007, work will continue on lean-NOx traps (LNTs) and selective catalytic reduction using urea (urea-SCR) to reduce NOx emissions. The focus of activities will be on making these devices more efficient, more durable, and less costly. For particulate matter (PM) control, the focus will be on more efficient methods of filter regeneration to reduce impact on engine fuel consumption.

In FY 2007, PNNL will continue fundamental studies of NOx adsorber materials, including BaO morphology studies using temperature programmed X-ray diffraction at the National Synchrotron Light Source and *in situ* transmission electron spectroscopy studies to watch morphology changes in real time. They also will explore the mechanisms of sulfur poisoning of NOx adsorber materials through refining function-specific measures of 'aging' and continuing to improve mechanistic understanding of sulfur removal processes by identifying important desulfation intermediates and the effects of sulfur concentration on Pt accessibility and barium phase changes.

During FY 2007, SNL plans to continue development of their chemical kinetics models for LNTs by augmenting the regeneration mechanism with reactions for additional kinds of reductants, in particular hydrocarbons; repeat the mechanism assembly and parameter optimization process for the NOx storage phase of normal LNT operation; and introduce reactions needed to describe sulfur poisoning and desulfation.

In their CRADA with International Truck and Engine, ORNL plans to continue studying LNT chemistry to improve understanding of sulfation/desulfation and will install a camless engine to explore the interaction between advanced low-temperature combustion modes (lower NOx and PM) and overexpansion (improved efficiency). ORNL also plans to study the fundamental chemistry of LNT sulfation to identify where sulfates form and how best to remove them without damaging the LNT catalyst. In a CRADA with Cummins, ORNL plans to continue evaluation of a range of analytical approaches to assess their applicability for *in situ* oil dilution (caused by operation at certain low-temperature combustion conditions) measurement. ORNL will also, in a CRADA with John Deere, conduct an investigation of particulate formation and chemistry as a function of rail pressure and urea-SCR dosing, optimize the efficiency of a 2007 Deere diesel engine while operating in advanced combustion regimes, assess waste heat recovery potential, and install and evaluate a prototype reformer for a LNT study on the 2007 Deere engine.

While combustion of hydrogen does not result in HCs or CO, it can result in NOx emissions. In FY 2007, ORNL will explore the use of LNTs and urea-SCR catalysts to control NOx emissions. They plan to investigate NO:NO_2 ratios and conduct tests at various temperatures and space velocities.

As part of their CLEERS activities, PNNL plans to extend their micro-scale regeneration model to allow studies of phenomena such as 'NOx recycle' and optimization of catalyst loading and placement, and include coupled heat transfer and oxidation exotherms, allowing studies of 'light-off' conditions during active filter regeneration. They also plan to conduct single-channel experiments with catalyzed and uncatalyzed samples in parallel in order to better quantify the effect of catalyst loading on regeneration behavior.

As part of their CLEERS activities, ORNL plans to 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 organize the 10th CLEERS workshop in the spring of 2007. ORNL also plans to update and post revised global LNT models with input from experimental data as these become available, continue identification of synergies between LNT NH_3 generation kinetics and NH_3-SCR as a potential alternative to urea-SCR NOx control, and coordinate bench reactor studies of the impact of sulfation and desulfation on LNT durability and kinetics.

ORNL plans to evaluate commercial HC-SCR catalysts using bench reactor experiments and tests on an engine dyno. The objective of the bench reactor experiments will be to evaluate the promotional effect of hydrogen, perform temperature sweeps, and investigate CO or HC masking of the catalysts. The engine tests will be used to evaluate high-efficiency clean combustion operation, late-cycle post injection or in-pipe injection of fuel, and individual cylinder control for their effects on HC-SCR catalyst regeneration.

General Motors will examine an alternative diesel particulate filter regeneration technique which builds off the knowledge gained from their microwave regeneration work and may provide an economy benefit over it.

C. Critical Enabling Technologies

The critical enabling technologies activities in FY 2007 include work on variable valve actuation and variable compression ratio systems. In FY 2006, Delphi completed a benchmarking study on competing variable valve actuation (VVA) technologies, prepared a system requirements document, and submitted provisional patent applications covering the VVA mechanism. In FY 2007, Delphi plans to evaluate new dual cam designs, develop detailed packaging designs, and demonstrate and document the performance of the VVA mechanism to enable low-temperature combustion control in CIDI engines. Also in FY 2007, Envera will optimize their variable valve actuator control system, install it in a mule vehicle, and test it.

Waste Heat Recovery

Research will continue in FY 2007 on thermoelectrics and bottoming cycles for capturing and utilizing waste heat from advanced combustion engines. Research on both technologies will focus on development of practical systems that are suitable for future production.

General Motors plans to optimize cost-effective bulk materials, finalize selection of thermoelectric materials for exhaust and radiator heat recovery devices, finalize design of exhaust and radiator waste heat recovery devices including estimated performance, and identify volume-capable and cost-effective manufacturing processes for thermoelectric modules. BSST plans to develop improved low-resistivity electrical contacts to enable weight and cost reductions needed for the target vehicle application; accelerate building of a 750-watt thermoelectric generator module using high-efficiency high-temperature materials; and build a tabletop power generator that displays real-time performance, including energy conversion efficiency. The University of Michigan is planning to conduct design and analysis of the power conditioning system to optimize thermoelectric system performance; explore leg fabrication methods for improving mechanical properties and microstructural characteristics; develop fabrication techniques for scaleable couple/thermoelectric modules; improve results of analytical studies on the full engine system by coupling current simulations to the 3-D heat transfer studies performed at Iowa State University; and improve the coefficient of performance (ZT) by exploring several more promising thermoelectric material compositions.

In the coming year, Cummins will continue development of an effective and efficient Rankine cycle waste heat recovery system by creating specifications for prototype hardware and control software; performing subcomponent testing of prototypes and model-based simulation of integrated systems for vehicle-level performance; defining expected hardware performance in-vehicle; and starting laboratory-based, integrated system testing. Mack Trucks plans to update the design of the compressor and two turbines of their turbocompound system, test the compressor and turbines in special rigs, build prototype high-efficiency turbo and turbocompound units for testing, begin baseline engine development that will include high-efficiency turbo and turbocompound units, and demonstrate the engine and continuously variable transmission system in a test cell environment to determine system efficiency.

John Deere plans to test vehicles under realistic operating cycles to document real-world benefits in both fuel economy and vehicle productivity. They will also develop second-generation hardware with improved performance and greater commercialization potential, define optimal system architecture and power splits for Tier 4 emissions compatibility, and increase the scope of application of turbocompounding by evaluating performance enhancements in both larger and smaller engine platforms. This will be done by starting with modeling to define the potential and then adapting existing hardware to verify advantages.

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.

In FY 2007, the Lovelace Respiratory Research Institute will complete their work to clarify the health importance of nanoparticle (<50 nm) components of diesel emissions and the relative importance of black carbon- vs. non-solid condensate-based particles; complete their study testing the hypothesis that artifactual formation of nitro-aromatic compounds on filter samples is responsible for much of the mutagenicity of diesel particle extracts; and complete their analysis and publication of results from study of gasoline emissions and comparison to effects of diesel emissions. The Advanced Collaborative Emissions Study (ACES) will initiate their 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. The Health Effects Institute, in coordination with the Coordinating Research Council, manages the ACES and will initiate emissions characterization and health effects assessment, as well as solicit and select shorter-term biological screening study contractors to conduct health effects studies.

ORNL will continue their study of health effects of in-use diesel truck emissions by characterizing mobile source air toxics (MSATs) from advanced engine and aftertreatment systems, measuring MSATs at higher time resolutions in order to understand mobile source impacts, and continuing deployment of the remote sensing instrumentation for evaluation of end-use emissions. NREL plans to complete their proximate ozone modeling study in southeast Michigan to answer the question whether the “weekend ozone” effect observed in California also exists in other parts of the country.

University Research

In FY 2007, our university partners will continue their fundamental research into combustion and the chemistry of emission control devices.

The University of Michigan, in conjunction with the University of California at Berkeley, and the Massachusetts Institute of Technology, will simulate the full range of operation of a dual-mode (spark ignition homogeneous charge compression ignition, SI-HCCI) engine and evaluate the fuel economy implications of various control strategies. They will also carry out single-cylinder investigations of upper load combustion limits with super/turbo charging and fast thermal management of intake temperature.

The University of West Virginia will couple their LNT combustion model with a friction model to better evaluate changes that increase indicated mean effective pressure. They will also add a cooling burden model to evaluate waste energy generation. An experimental engine will be identified and procured to conduct experiments.

The University of Houston plans to carry out a comprehensive mechanistic study of the regeneration of model Pt/Rh/Ba NOx storage and reduction (NSR) catalysts with hydrogen and CO reductants. They will also evaluate performance of the model NSR catalysts in a bench-scale NOx trap using synthetic lean-burn exhaust feeds.

The University of Kentucky will evaluate NOx storage/reduction performance of fresh (de-greened) model catalysts using a bench-scale reactor; perform accelerated aging of model catalysts using repeated sulfation-desulfation cycles in a synthetic gas reactor; and perform *in situ* DRIFTS studies in order to relate reactivity at the catalyst surface to catalyst composition (for both fresh and aged catalysts).

Texas A&M will extend their spark ignition engine cycle simulation to include provisions for compression ignition engines; analyze the effects of compression ratio and expansion ratio on engine performance using both the first and second laws of thermodynamics; and investigate the use of exhaust gas energy recovery options from both the first and second laws of thermodynamics.

Michigan State plans to complete baseline testing of their variable cam timing engine for performance and emissions and will conduct experiments with the advanced low-pressure direct injection engine which features the advanced control systems and infinitely variable valves to demonstrate an expected 15% improvement in fuel economy at road load conditions.

Honors and Special Recognitions

- Paul Miles of SNL was awarded the 2005 SAE Harry L. Horning Memorial Award for best paper related to the mutual adaptation of fuels and engines.
- Paul Miles of SNL was invited to give a keynote lecture titled “Thermo- and Fluid Dynamic Processes in Diesel Engines” (September 2006).
- Paul Miles of SNL was invited to give the keynote lecture at the 2nd International Symposium on Clean, High-Efficiency Combustion in Engines (July 2006).
- Lyle Pickett of SNL received the 2005 SAE Horning Award for best technical paper in engine combustion. One award is given each year out of approximately 2,700 SAE papers (SAE 2005-01-3837).
- Lyle Pickett of SNL received an SAE Excellence in Oral Presentation Award for his outstanding technical paper presentation at the 2005 Powertrain and Fluid Systems Conference in San Antonio, Texas (SAE 2005-01-3843).
- Robert Wagner’s work at ORNL was featured as a DOE FreedomCAR Technical Highlight titled “Demonstrated range expansion and estimated potential FTP benefits of HECC operation.”
- Salvador M. Aceves of LANL was invited to deliver a seminar at the SAE 2006 seminar on HCCI (September 2006) in San Ramon, California.
- John Dec of SNL received the SAE Recognition Award for co-organizing the 3rd annual SAE HCCI Symposium in San Ramon, California (September 2006).
- Magnus Sjöberg of SNL was invited to give a presentation at the SAE HCCI Symposium in San Ramon, California (September 2006).
- John Dec of SNL was an invited member of the Technical Committee for the 2nd International Symposium on “Clean and High-Efficiency Combustion in Engines” in Tianjin, China (2006).
- John Dec received an SAE Excellence in Oral Presentation Award, 2006 SAE Congress.
- Magnus Sjöberg received the SAE Forest R. McFarland Award for efforts and leadership in organizing technical sessions on HCCI combustion.
- Bill Pitz of LLNL received an SAE Oral Presentation Award for “Detailed Chemical Kinetic Modeling of Surrogate Fuels for Gasoline and Application to an HCCI Engine,” 2005 Fall Powertrain and Fluid Systems Conference & Exhibition in San Antonio, Texas.

- Bill Partridge of ORNL was invited to give the presentation “Spatially Resolved Capillary-Inlet Mass Spectrometry: Instrument Details and Applications” to the Centre for the Theory and Application of Catalysis (CenTACat), Queen's University Belfast, Belfast, Ireland (June 2006).
- Mike Harold of the University of Houston had the first prize poster at the Southwest Catalysis Society Symposium (May 2006).
- Jerry Caton of Texas A&M University received an SAE 2005 Excellence in Oral Presentation Award for presentation of “Use of a Cycle Simulation Incorporating the Second Law of Thermodynamics: Results for Spark-Ignition Engines Using Oxygen Enriched Combustion Air” at the 2005 SAE International Congress and Exposition, Society of Automotive Engineers, Cobo Hall, Detroit, Michigan (April 2005).
- Chuck Peden (invited presenter), C.M. Wang, J.H. Kwak, D.H. Kim, J. Szanyi, R. Sharma, and S. Thevuthasan, “In-Situ TEM Study of Morphological Evolution of Emission Control Catalysts During Operation”, presentation at the NSF Workshop on "Dynamic in-situ electron microscopy as a tool to meet the challenges of the nanoworld", Tempe, AZ, January 2006.
- Special recognition for collaborative R&D under CLEERS from USCAR was presented to R. Blint (May 2006).

Invention and Patent Disclosures

- Robert Wagner, ORNL: Patent pending, “Device and Method for Inferring Low Particulate Emissions from Nitrogen Oxide Measurements in Low Temperature Diesel Combustion Processes.”
- Daniel L. Flowers of LANL: Patent awarded, “Controlling and Operating Homogeneous Charge Compression Ignition (HCCI) Engines,” United States Patent 6,923,167, August 2, 2005.
- John Dec, SNL: Patent pending, application #11/095,256, “Fuel Mixture Stratification as a Method for Improving Homogeneous Charge Compression Ignition Engine Operation.”
- Caterpillar patents:
  1. Ignition timing control with fast and slow control loops (IVP and EGR).
  2. Mixed high and low pressure EGR in HCCI engine.
  3. Strategy for extending the HCCI operation range using low cetane number diesel fuel and cylinder deactivation.
  4. Recipe for high load HCCI operation.
  5. Power balancing cylinders in HCCI engine.
- Delphi Automotive Systems provisional patents submitted:
  1. System for Continuously Varying Engine Valve Duration
  2. Continuously Variable Valve Actuation System
- Ja Hun Kwak, Do Heui Kim, Xianqin Wang, Janos Szanyi, and Charles H.F. Peden, PNNL: “New Desulfurization Process for Suppression of Pt Sintering of Sulfated Lean NOx Traps.” PNNL Invention Disclosure #15330-E, filed in August 2006.
- Robert Wagner, ORNL: Patent pending, “A Method for Diagnosing and Controlling Combustion Instabilities In Internal Combustion Engines Operating in or Transitioning to Homogeneous Charge Compression Ignition Modes,” IDEAS 05-156.
- Ron Graves, Brian West, Shean Huff, and James Parks: Provisional patent filed, “Advanced Engine Management for Control of Exhaust Species,” 3/30/2006.
- Richard Blint, General Motors: five records of invention were filed based on his work to discover NOx reduction catalysts for CIDI engines.

The remainder of this report highlights progress achieved during FY 2006 under the Advanced Combustion Engine R&D Sub-Program. The following 67 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 internal combustion engines for light-

duty, medium-duty, and heavy-duty vehicles. We are encouraged by the technical progress realized under this dynamic Sub-Program in FY 2006, 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.

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

II.1 Stretch Efficiency in Combustion Engines with Implications of New Combustion Regimes

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- University of Wisconsin, Madison, Wisconsin (Prof. David Foster, Mr. Ben Druecke, Prof. Sandy Klein)
- Texas A&M University, College Station, Texas (Prof. Jerry Caton, Mr. Praveen Chavannavar)

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 low-temperature combustion regimes.
- Establish proof-of-principle of the pathways to stretch efficiency.

Accomplishments

- Utilized in-cylinder phenomenological models for simulating the efficiency effects of low-temperature combustion modes on thermodynamic availability.
- Continued collaboration with Texas A&M in developing and applying a protocol for analyzing the major exergy losses during engine experiments.
- Continued collaboration with University of Wisconsin and Texas A&M in evaluating the fundamental thermodynamic efficiency limits for conventional engines.
- Participated in National Science Foundation workshop on R&D opportunities for hydrogen combustion.
- In collaboration with Texas A&M and University of Wisconsin presented three papers in the 2006 Technical Meeting of the Central States Section of the Combustion Institute (May 21-23 in Cleveland) summarizing the dominant sources of combustion irreversibility in conventional engines and promising directions for future R&D to increase overall combustion engine fuel efficiency.
- Presented overall results from in-house thermodynamic studies and collaborations with Texas A&M and the University of Wisconsin on stretch engine efficiency to DOE project managers during ORNL site visit in September.
- Identified two novel, unconventional approaches for low-irreversibility combustion suitable for experimental proof-of-principle demonstration.

Future Directions

- Implement and experimentally demonstrate at least one low-irreversibility combustion concept at bench-top scale.
- Continue analyses of data from advanced combustion 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 to identify ways in which the potentially lower wall heat loss from low-temperature combustion can be exploited for higher efficiency.
- Continue exercising engine and combustion models to identify combustion modifications that would mitigate exergy losses.

Introduction

The best approach for improving engine efficiency is to understand the causes of losses, then develop ways to mitigate them. Numerous studies over the past 30 years have quantified the thermodynamics of engines (see [1], for example). These studies have demonstrated that both the First and Second Laws of thermodynamics must be taken into accounted in order to understand how efficiently energy is actually utilized. The First Law simply accounts for energy in any form, but the Second Law distinguishes the 'quality' of energy as it relates to producing useful work. For the latter, a thermodynamic property known as availability (or exergy) is tracked as energy is processed by the engine. Because availability directly relates fuel energy to motive work generation, it gives deeper insights into the loss mechanisms for transportation engines than simple energy balances.

In conventional engines the largest efficiency losses (approximately 20-25%) occur in the combustion process itself and are difficult to mitigate. Such losses are not due to unburned fuel, which is a relatively small loss, but they are instead due to the generation of thermodynamic entropy by unrestrained chemical reactions. The net effect is to divert some of the fuel energy into molecular motion and heat. This diverted energy becomes unavailable to produce useful work according to the Second Law of Thermodynamics. Simple energy balances, which reflect the First Law of Thermodynamics, don't distinguish between available energy (energy that can produce work) and unavailable energy (energy that can only make heat). In principle, it is this entropy generating characteristic of unrestrained chemical reactions that gives fuel cells their theoretical advantage over existing combustion engines. However, as we discuss below, it is theoretically possible to carry out our combustion reactions in a more restrained way that produces less entropy and preserves more of the original fuel energy for work.

Typically, 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 [2]. Since these molecules have large energy (i.e., temperature) differences, considerable entropy is generated when they interact. This entropy generation process is depicted schematically in Figure 1.

In general, combustion irreversibility is mitigated if the reactions take place nearer chemical equilibrium.

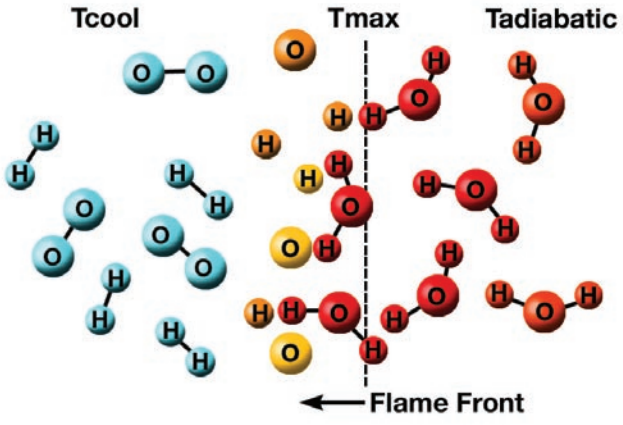


FIGURE 1. Schematic depiction of entropy generation in a flame at the molecular scale. Hydrogen combustion in oxygen is shown for simplicity. Most of the entropy is generated as energetic water molecules share their energy with unreacted oxygen and hydrogen.

This requirement can be accomplished when the reactants are preheated reversibly (slowly, with small temperature gradients) such that they are brought closer to the temperature of the products. We recently published an article describing a theoretical generic isobaric combustion process that could accomplish this near-equilibrium preheating and reaction [3]. It appears that some of aspects of reversible preheating may also be present in combustion processes like homogeneous charge compression ignition (HCCI) or low-temperature combustion (LTC). Thus there has been interest in investigating the combustion reversibility of these advanced combustion modes.

Approach

Through analysis and experiment, we have been investigating the processes in internal combustion engines (ICEs) that produce availability destruction (i.e., conversion of fuel energy into heat rather than useful work). This year, results from internal modeling studies and collaborations with Prof. Jerry Caton at Texas A&M and Prof. Dave Foster at the University of Wisconsin have been combined to yield a global understanding of the dominant exergy losses in conventional engines, including engines operating in advanced combustion modes. Our thinking has also been significantly impacted by discussions with other pioneers in this area, including John Clarke (Caterpillar, retired), Roy Primus (formerly Cummins, now General Electric), Prof. Noam Lior (University of Pennsylvania), John Farrell and Walt Weissman (Exxon-Mobil), and Prof. Chris Edwards (Stanford University).

The cumulative understanding described above has led to specific recommendations for future R&D activities aimed at improving ICE fuel efficiency, including both experimental and analytical components. Some of these recommended investigations include incremental improvements in existing engines, whereas others involve very novel combustion concepts that go well beyond the constraints of current engines. Our current and future efforts involve a mixture of both types of investigations. As before, we anticipated continued collaborations with those mentioned above, as well as additional collaborations with industrial partners as concepts evolve from theory to experimental practice.

Results

During FY 2006, we have continued utilizing the previously developed computational physical property subroutines for both idealized and experimental engine availability balances. These subroutines have been specifically adapted to simulate and analyze low-temperature combustion modes, which are currently a high priority in DOE fuel efficiency activities. We are now using the latter with experimental data from

conventional and homogeneous combustion in the ORNL Mercedes 1.7-L diesel engine. These same routines will be utilized for analysis of results from the ORNL GM 1.9-L engine as it becomes available for experimentation this coming year.

Our updated understanding of the global thermodynamic efficiency limits for conventional engines is based on two types of analyses, one of which considers idealized engine cycles and one of which includes more realistic assumptions about non-ideal engine behavior. As illustrated in Figure 2, our idealized analyses consider global First and Second Law balances around a frictionless conceptual engine that includes a combustion chamber with arbitrarily controlled wall heat losses, isentropic work extraction through a single-stage piston, arbitrarily controlled exhaust gas recirculation (EGR) and/or heat transfer between the exhaust and incoming fuel and air, arbitrary compression ratio, arbitrary air/fuel stoichiometry, and exhaust gas that has fully achieved chemical equilibrium. We consider a large range of fuels (e.g., isooctane, hydrogen, alcohols, etc.) that can burn either homogenously (one zone) or as a propagating flame (two-zone). Burn rates are arbitrarily specified, typically with an adjustable Wiebe function. For more realistic estimates for conventional engines, we add typical non-idealities including mechanical friction, realistic cylinder wall heat transfer, realistic compression ratios, stoichiometric to lean air/fuel mixtures, multi-zone combustion with optimal and non-optimal phasing, and incomplete chemical equilibrium.

An example result coming from the above analyses is illustrated in Figure 3. Here we see a comparison of the net availability changes in an ideal adiabatic engine with stoichiometric, one and two zone combustion of isooctane in air at a fixed global rate. Note that here one-zone combustion is equivalent to the ideal limit for HCCI, while two-zone combustion is equivalent to the ideal limit for propagating flame combustion (e.g., as in a spark-ignited engine). Through such analyses it becomes clear that spatial homogeneity of HCCI does not reduce combustion irreversibility, even though the high spatial gradients of temperature and species surrounding a typical flame are no longer present. This is because the chemical reactions still occur at the same net displacement from equilibrium (as measured in terms of chemical potential), and thus equivalent levels of entropy are generated in the cylinder at the molecular scale. The very slight differences in piston work produced in the two cases here are attributable to slight differences in the

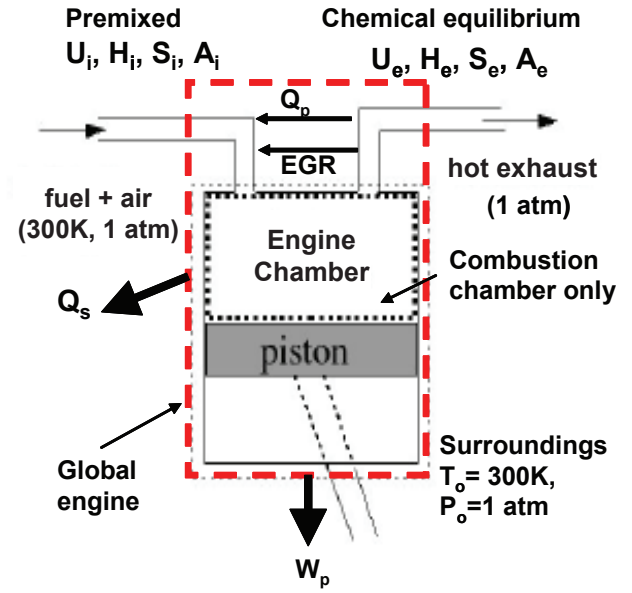


FIGURE 2. Schematic of engine control volumes used for First and Second Law balances. The First Law balances account for overall energy distribution, while the Second Law balances account for thermodynamic availability (which accounts for energy that is converted to entropy and becomes unavailable to do work).

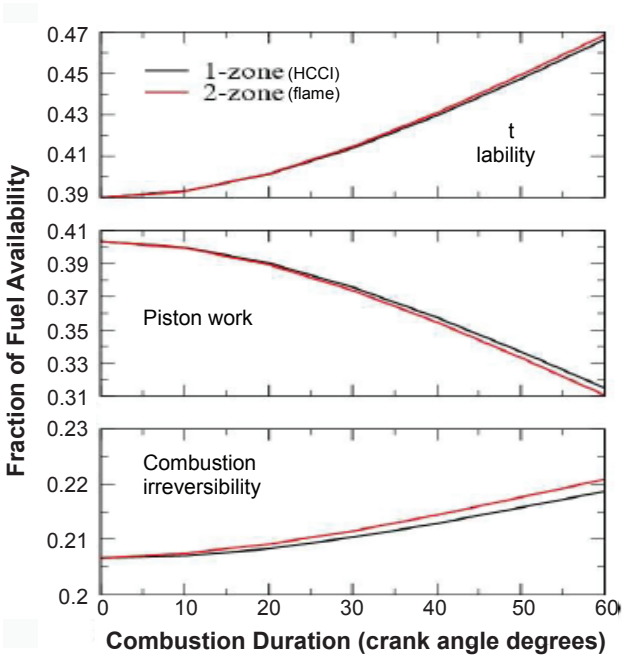


FIGURE 3. Results from an availability analysis of one (HCCI-like) and two-zone (flame-like) combustion simulations for stoichiometric isooctane in air fed to an ideal engine. Here there is no wall heat transfer and burn rate is specified by a Wiebe function. The horizontal axis of each plot is burn duration. The vertical axis is the fraction of the original availability lost on the exhaust, converted to work, and destroyed in combustion, respectively.

effective heat capacity ratios of the gases, which enter into the isentropic work term.

Fuel and air preheating is another parameter expected to reduce combustion irreversibility. Figure 4 illustrates another result from the ideal engine analysis in which the isooctane and air mixture is preheated at constant pressure with recovered exhaust heat before compression in the cylinder. Although combustion irreversibility is reduced as more exhaust heat is recycled, net engine work output is also reduced because more energy is required to achieve the same compression ratio for the expanded inlet charge. The net result of preheating is that the availability lost in the exhaust is increased and overall nothing is really gained. This example illustrates a general trend we have observed repeatedly; reductions in combustion irreversibility in conventional engines are always accompanied by higher losses in the exhaust. This trend points to a fundamental limitation in the ability of single stage engines to extract work from the combustion gases. Ultimately, compound cycles are needed to utilize any additional availability retained by better combustion.

Figures 5 and 6 illustrate how the results of First and Second Law analyses differ from and yet complement each other. In Figure 5, we see the results of a First Law global energy accounting for a non-ideal isooctane-air fueled engine as compression ratio is increased. The output work (at the bottom of the plot) increases with increasing compression ratio, finally becoming almost constant at a compression ratio of about 10. Exhaust energy also decreases with increasing compression ratio, but this decrease is offset by higher heat transfer to the surroundings and more friction. In Figure 6 we see the same type of plot, except that now availability is considered instead of total energy. The exhaust energy now appears in a different light, because it can be seen that only a small portion of this energy is actually available to produce work, especially at higher compression ratios. This implies that attempts to extract this exhaust energy without also reducing availability destruction and/or heat transfer to the surroundings will be less fruitful than one would have otherwise presumed.

As a result of extensive case studies such as those described above, a comprehensive set of conclusions has now been compiled relevant to the fundamental efficiency limits of current engines. Some of the key findings are

- Reduction of combustion irreversibility in single-stage engines will typically cause other losses (e.g., cylinder wall and exhaust heat losses) to increase.
- Cycle compounding is necessary in order to achieve significant benefits from reduced combustion irreversibility.
- Combustion irreversibility is minimized in conventional engines at stoichiometric air/fuel ratios.

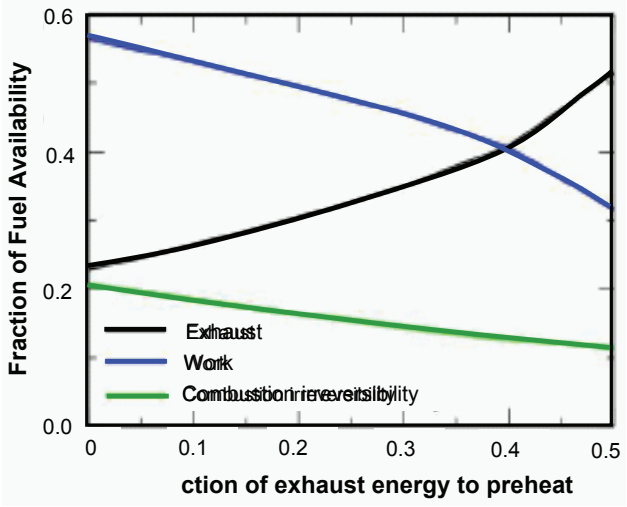


FIGURE 4. Availability results from an ideal engine simulation with recuperative preheating of the isooctane fuel and air. The original fuel availability is accounted for (as fractions) appearing in the exhaust, work, and destruction by combustion irreversibility. The horizontal axis indicates the fraction of the exhaust energy recuperated.

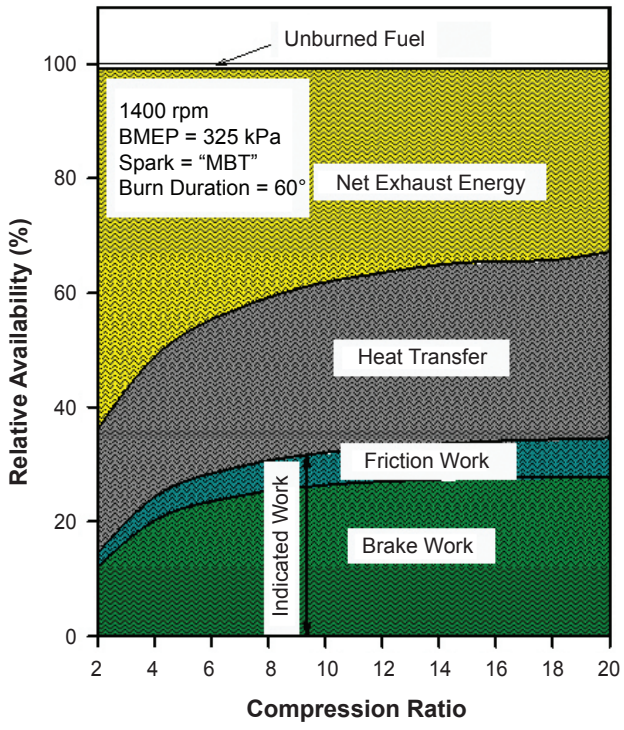


FIGURE 5. Example First Law analysis results for a non-ideal, stoichiometric isooctane-air fuelled spark-ignition engine with varying compression ratio (from Prof. Jerry Caton). As compression ratio increases, work output, friction, and heat transfer all increase.

- Observed benefits in engine work output associated with lean fueling are due to improved gas properties for work extraction (by gas expansion), not because of reduced combustion irreversibility.
- The absence of a flame in HCCI does not reduce combustion irreversibility.
- Observed efficiency advantages associated with HCCI are most likely the result of reduced cylinder wall heat losses.
- Combustion irreversibility is controlled by how far the chemical reactions occur from equilibrium, not how fast the reactions proceed relative the rate of work extraction.

In the longer term, major changes in engine design and mediated combustion chemistry will be required to utilize most of the 20-25% of the fuel energy currently destroyed outright in the combustion process. Radically different combustion approaches such as Staged Combustion with Oxygen Transfer (SCOT) and Counterflow Preheating with near-Equilbirum Reaction (CPER) described in previous reports will probably be required to achieve oxidation reactions that are significantly closer to chemical equilibrium. Shorter-term incremental improvements to existing engines may be possible by judicious use of air and fuel preheating or staging of the combustion reactions (e.g., sequential rich/lean combustion) as long as additional work extraction processes besides the main piston (cycle compounding) are included.

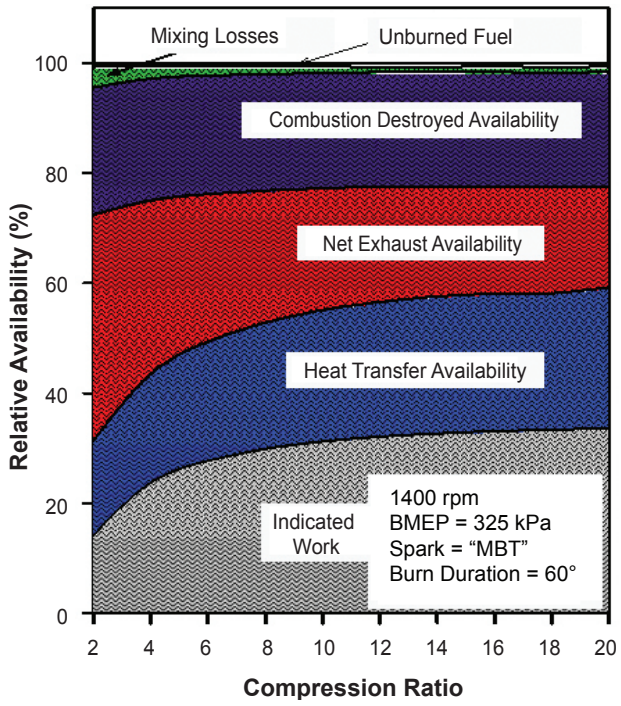


FIGURE 6. Example Second Law analysis results corresponding to Figure 5 (also from Prof. Jerry Caton). Note that much of the energy in the exhaust is actually unavailable to produce work.

Conclusions

Promising engine stretch efficiency concepts which should be considered in the near term include:

- Thermal exhaust heat recuperation combined with compound work extraction;
- Thermo-chemical exhaust heat recuperation with staged gas-phase combustion;
- Low-temperature bottoming cycles for exhaust heat;
- Higher compression ratios;
- Fully expanded engine cycles (e.g., Miller cycles); and
- Exploitation of low-temperature combustion modes with reduced wall heat transfer.

For the longer-term, combustion engines utilizing the following advanced concepts should be considered:

- Heterogeneous combustion reactions (implementations of the SCOT concept);
- Near-equilibrium gas-phase combustion (implementations of the CPER concept);
- Combined cycle systems using both fuel cells and gas-phase reactions;
- High temperature gas-phase combustion with topping cycles (e.g., thermo-photovoltaics); and
- Heterogeneous combustion with mechanical non-gas mechanical work extraction (e.g., piezo-electrics).

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3. J. A. Caton, "Utilizing a Cycle Simulation to Examine the Use of EGR for a Spark-Ignition Engine Including the Second Law of Thermodynamics," accepted for *Proceedings of the 2006 Fall Conference of the ASME Internal Combustion Engine Division*, Sacramento, CA, 5–8 November 2006.

4. J. A. Caton, "First and Second Law Analyses of a Spark-Ignition Engine Using Either Isooctane or Hydrogen," accepted for *Proceedings of the 2006 Fall Conference of the ASME Internal Combustion Engine Division,* Sacramento, CA, 5–8 November 2006.

5. P. S. Chavannavar, and J. A. Caton, "The Destruction of Availability (Exergy) due to Combustion Processes: A Parametric Study," accepted by the *Journal of Power and Energy, Proceedings of the Institution of Mechanical Engineers, Part A*, June 2006.

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7. P. S. Chavannavar and J. A. Caton, "Irreversibilities Associated with Basic Combustion Processes," in the *Proceedings of 2006 Spring Meeting of the Central States Section of the Combustion Institute*, Cleveland, OH, 21–23 May 2006.

8. C. Stuart Daw, V. K. Chakrvarthy, James Conklin, Ron Graves, Minimizing Destruction Of Thermodynamic Availability In Hydrogen Combustion, International Journal of Hydrogen Energy 31 (2006) 728–736.

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

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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 diesel engines.
- Collaborate with modeling groups, providing them with the results of our unique measurements in order to advance the state-of-the-art in spray modeling.

Accomplishments

- In FY 2006 we made the first-ever x-ray measurements of sprays at an ambient pressure of 30 bar. This reproduces the ambient density inside a turbo-charged light-duty diesel engine at the start of injection.
- Robert Bosch GmbH donated new fuel system components to our group, designed, fabricated, certified, and delivered a new pressure vessel for multi-hole nozzles, and sent their employee Thomas Riedel to work with our group for four months. The only expense to Argonne was the cost of Mr. Riedel's lodging. This arrangement represents a significant contribution by Bosch, and enabled our group to make measurements on modern production hardware that is otherwise very difficult to obtain.
- FY 2006 saw the continuation of an important collaboration with General Motors and the Engine Research Center at the University of Wisconsin. One week of x-ray measurements in FY 2006 were dedicated to this collaboration.
- A new x-ray monochromator was used in its first experiments in FY 2006. This new piece of specialized x-ray optics has dramatically improved our spatial resolution and may enable single-shot measurements of sprays.

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. In FY 2006 we achieved 30 bar ambient pressure; in FY 2007 we plan to make measurements at 35 bar. This will be comparable to top dead center (TDC) density conditions inside a boosted light-duty diesel engine.
- 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.

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 diesel fuel injection systems. 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 the x-ray absorption technique 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 make detailed measurements of the fuel distribution in these sprays, extending the existing knowledge into the near-nozzle region. The x-ray measurements were performed at the 1BM-C station of 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

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

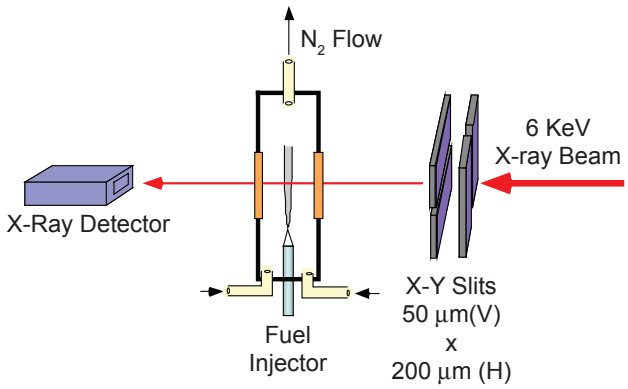


FIGURE 1. Schematic of the Experimental Setup

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 2006 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 under ambient density conditions comparable to those at start-of-injection in a modern light-duty diesel engine. These measurements represent a significant increase in our capability to measure sprays under high-pressure conditions, and enable the results to be directly applied to modern engines and computational models.

A new x-ray monochromator was used in its first experiments in FY 2006. This new piece of specialized x-ray optics was funded by the FreedomCAR office and has already had a significant impact on our ability to make measurements. The device has better focusing capability than our previous optics, and delivers 50 times the x-ray flux. This has enabled us to shrink the size of the x-ray beam used to probe the spray, improving the spatial resolution of our measurements from about 50 microns to 12 microns. This has enabled us to resolve structural features of the spray that were invisible to us even a few years ago. This improvement is reflected in Figure 2, which shows the fuel distribution from nozzles with different internal geometries. Previous measurements in 2004 showed only modest differences between these two sprays, but the improved resolution made possible by the new monochromator reveals striking differences. Measurements such as these are crucial to improved nozzle design, as the two sprays are virtually identical when measured using visible light.

Our group's collaboration with Robert Bosch GmbH was greatly expanded in FY 2005 and FY 2006. Based on a handshake agreement with Gerd Bittlinger of Bosch Corporate Research, Bosch donated new fuel system

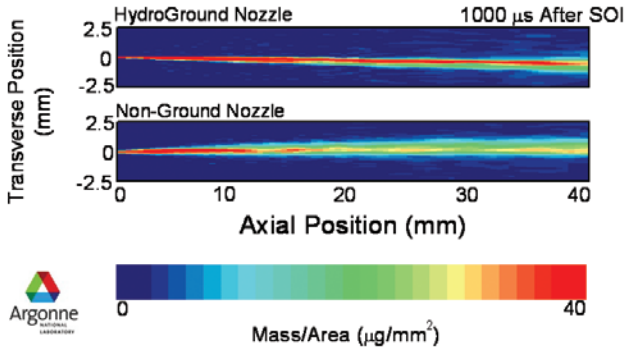


FIGURE 2. Spray images reconstructed from x-ray measurements of sprays from nozzles with different internal geometries.

components to our group, including fuel feed pumps, high-pressure fuel pumps, common rails, fuel lines, injectors, nozzles, and other miscellaneous hardware. Such equipment is very difficult and expensive to obtain otherwise, as commercial suppliers are reluctant to deliver the small quantities needed for a research program. This donation ensured that our group has the hardware required to make measurements, as well as spare equipment in case of failure. We can now make measurements using the latest production hardware from the world's leading fuel injection manufacturer, which maximizes the impact of our work on the engine community. Bosch also designed, fabricated, certified, and delivered a new pressure vessel for multi-hole nozzles. This vessel was built to be compatible with Argonne's x-ray measurements, and Argonne's existing x-ray pressure windows mount to the vessel. Bosch also sent their employee Thomas Riedel to work with our group for four months in FY 2005 and FY 2006 and take part in several experiments. The only expense to Argonne was the cost of Mr. Riedel's lodging. These contributions represent significant support of our research by Bosch (approximately $50,000 of in-kind contributions), and have advanced our work with minimal cost to DOE.

The equipment donated by Bosch was used for experiments which took place in October 2005. The effects of injection pressure, ambient pressure, and nozzle geometry were explored in these experiments. These experiments used multi-hole VCO nozzles similar to those used in diesel passenger cars. The experiments revealed an interesting asymmetry in the sprays from VCO nozzles that had been predicted by spray modeling but not previously measured. We suspect this is a result of the sharp turn the fuel takes inside the nozzle; spray modeling by Bosch will attempt to study this effect. The analysis of the experiments will be performed by Argonne National Laboratory and Bosch, spray modeling will be done by Bosch, and a joint paper will be published.

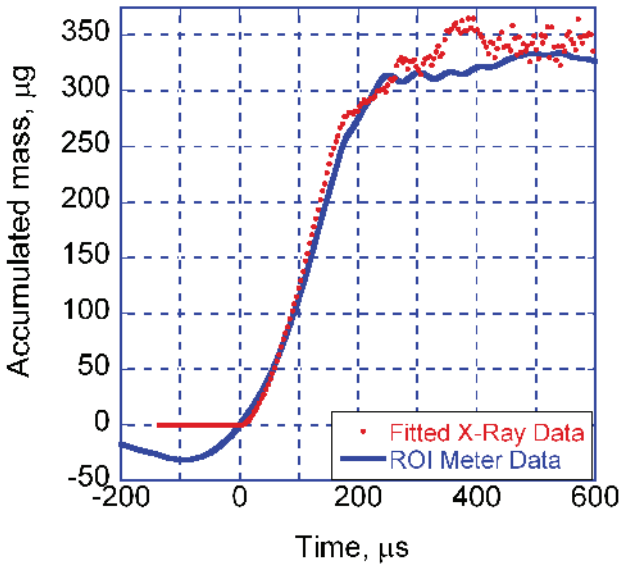


FIGURE 3. Comparison of the rate of injection measured using x-ray radiography and a commercial rate meter.

FY 2006 saw the continuation of an important collaboration with General Motors and the Engine Research Center (ERC) at the University of Wisconsin. One week of x-ray measurements in FY 2006 was dedicated to this collaboration. Measurements were performed at ambient pressures up to 30 bar for several different nozzle geometries. The analysis of the results is being performed by students and faculty at the ERC with funding from General Motors. The collaboration will continue in the future, and the experiments and analysis will form the Ph.D. thesis of Amaury Malave at the University of Wisconsin.

A number of other significant experiments were also performed in FY 2006. Figure 3 shows a comparison of the rate of injection measured using x-rays and compares it with the rate measured using a commercial instrument. The vastly different measurement techniques show good agreement, demonstrating the ability of x-rays to accurately measure the mass flow through the injector.

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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2. "X-Ray Characterization of Light-Duty Diesel Sprays", C. F. Powell, Presentation at DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation, Argonne National Laboratory, May 2006.

3. "Determination of Diesel Spray Axial Velocity Using X-Ray Radiography" A. Kastengren, C. F. Powell, T. Riedel, S. –K. Cheong, Y. Wang, K. –S. Im, X. Liu, J. Wang, Submitted to Society of Automotive Engineers, October 2006.

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II.A.2 Low-Temperature Automotive Diesel Combustion

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Subcontractors:
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Objectives

- Provide the physical understanding of the in-cylinder combustion processes needed to meet future diesel engine emissions standards while retaining the inherent efficiency and low CO_2 emissions of the direct-injection diesel engine.
- Improve the multi-dimensional models employed in engine design and optimization and validate the model predictions against in-cylinder measurements and tailpipe emissions.
- Investigate the effect of various combustion system parameters on engine performance and emissions, thereby generating a knowledge base for optimization efforts.

Accomplishments

- Expanded previous work clarifying the source of CO emissions in highly-dilute, low-temperature diesel combustion regimes. Demonstrated that optimal injection timing for low CO emissions is associated with enhanced mixing early in the combustion process, due to optimal proportioning of fuel in the squish and bowl regions.
- Incorporated new GM 1.9 liter diesel head and GM prototype, Euro-5 intent combustion system into the optically-accessible automotive Low-Temperature Combustion (LTC) facility. With this upgrade, collaboration with GM-sponsored research at the University of Wisconsin and with multi-cylinder testing at Oak Ridge National Laboratory (ORNL) will be greatly facilitated. Optical access into the squish volume was also significantly enhanced over previous designs.
- Obtained first particle image velocimetry (PIV) measurements of flow structures in the bowl of a firing diesel engine.
- Demonstrated potential for direct determination of the locations of heat release in the combustion chamber of a diesel engine from estimates of the velocity field divergence (a measure of local volume expansion).
- Identified the existence of a toroidal vortex at the exit of re-entrant bowl combustion chambers, and the role of this vortex in trapping soot and unburned hydrocarbons. The vortex also prevents mixing of combustion products exiting the bowl with additional squish volume oxidizer.

Future Directions

- Investigate sources of unburned hydrocarbons (UHCs) and CO in highly dilute, low-temperature combustion regimes through cycle-resolved emissions measurements, modeling, and optical investigations.
- Evaluate the effect of engine boost on low-temperature combustion systems and on the fuel conversion efficiency loss typically observed with high dilution levels.
- Examine the influence of combustion system parameters on the formation of the toroidal vortex at the bowl exit, and on the ability of conventional engine simulation codes to capture this phenomenon.

Introduction

Direct-injection diesel engines have the highest fuel conversion efficiency and the lowest CO_2 emissions of any reciprocating internal combustion engine technology. However, this efficiency often comes at the expense of high NOx or particulate matter (soot) emissions. Through adoption of low-temperature combustion techniques, relying on lower compression ratios, large quantities of cooled EGR, and unconventional injection timing and/or strategies, soot and NOx can often be dramatically reduced. Unfortunately, the low combustion temperatures beneficial for inhibiting soot and NOx formation can also lead to significant CO and UHC emissions, due to the slower oxidation of these species and to the more stringent mixing requirements imposed by the low O_2 concentration in the intake charge. Concurrently, a penalty in fuel consumption is also often incurred. Reduction of CO and UHC emissions and recovery of fuel economy through clean, efficient in-cylinder combustion processes is imperative if vehicles powered

by these engines are to be available at a competitive cost and contribute to the abatement of global warming through reduced CO_2 emissions.

Identifying those aspects of the LTC processes which are dominated by mixing processes, understanding the relevant physics controlling these processes, and developing a predictive modeling capability are crucial steps toward the development and optimization of low-emission, fuel efficient engines utilizing low-temperature combustion systems. Each of these components is represented in the research described below.

Approach

The research approach consists of making detailed measurements of flows and thermo-chemical properties in an optically-accessible laboratory test engine, which are then employed to both identify the dominant physical processes governing combustion and emission formation and to formulate and validate multi-dimensional computer models. These measurements are closely coordinated and compared with measurements of engine-out emissions in the optical engine, with emissions measured in identical geometry conventional (non-optical) test engines, and with numerical simulation efforts.

The experimental and numerical efforts are mutually complementary. Detailed measurements of flow variables permit the evaluation and refinement of the computer models, while the model results can be used to clarify the flow physics–a process that is difficult if only limited measurements are available. 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

Efforts in the first part of FY 2006 were aimed at clarifying the physics responsible for the optimal injection timing observed for minimizing CO emissions, that was identified and reported on in FY 2005 [1]. To identify the dominant processes, a comprehensive experimental program was pursued, utilizing experimental heat release analysis, flow measurements, spray and wall-film imaging, imaging of combustion luminosity, and variation of key combustion parameters. The experimental results identified enhancement of early mixing processes as the dominant factor leading to the reduction in CO emissions at early injection timings. Multi-dimensional simulations reinforced this conclusion, and further suggested that a major factor influencing the enhanced mixing was the realization of an optimal split of fuel between the squish volume and the bowl–see Figure 1.

Later efforts were focused on upgrading the facility to incorporate a GM head and a GM-designed, Euro-5 intent combustion system into the optically accessible engine. This engine build has a compression ratio of approximately 16.7:1, more characteristic of low-temperature combustion systems; and a swirl ratio that is variable over a broad range from approximately 1.4–4.5. While incorporating these changes, significant improvement to the optical access was also achieved. By recessing the window retaining structure into the head (Figure 2), a clear view of the squish volume is obtained from the side at all crank angles. This enhanced squish volume access will be crucial for investigating the initial distribution of fuel, which was shown above to be a dominant factor influencing CO

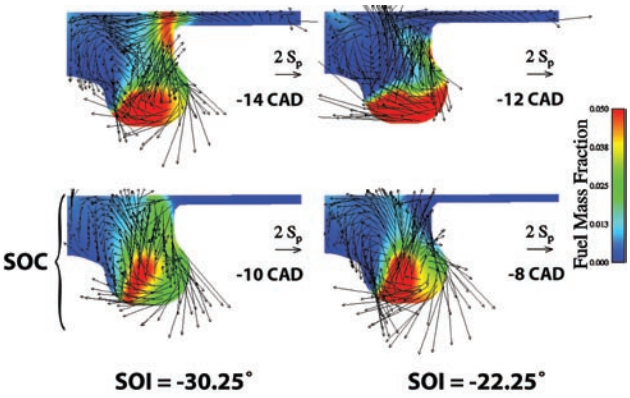


FIGURE 1. With earlier injection, the initial splitting of the fuel between the squish volume and the bowl leads to a broader fuel distribution at the start of combustion (SOC) and less CO formation.

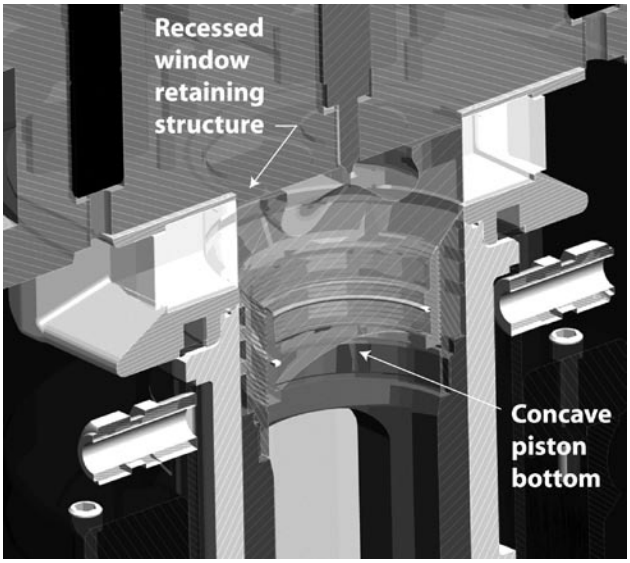


FIGURE 2. Representation of the new optical engine design, incorporating the GM 1.9 liter production head. Significantly enhanced optical access was achieved as compared to previous designs.

emissions. The large top-ring land height further allows imaging of the full-bowl depth at crank angles ±30° from top dead center (TDC). To permit this degree of optical access without compromising the compression ratio, it was necessary to maintain very close clearances (0.18 mm) between the piston sidewalls and the liner. To enhance the imaging capabilities from below, a concave lower surface on the optical piston was incorporated. This surface acts as a negative lens, and allows imaging of the squish volume (with the piston near TDC) to within 3 mm of the cylinder wall.

While this major facility upgrade was taking place, work was performed in collaboration with researchers at the Lund Institute of Technology on techniques for obtaining full-field measurements of flow structures within the bowl–and understanding the influence of these flow structures on the spatial distributions of unburned fuel and particulate matter. As we have shown previously [2], numerical simulations indicate that the formation of beneficial bulk flow structures can significantly enhance late-cycle mixing processes, leading to increased fuel economy and reduced emissions. Until now, however, these structures have eluded experimental observation. By careful application of particle image velocimetry and image correction techniques, we have obtained the first planar velocity field measurements in a firing diesel engine. An example mean flow field, obtained near the time of peak heat release, is shown in Figure 3. With fuel injection and heat release, the flow structure is dominated by a clockwise rotating vortex formed when the spray is deflected by the bowl lip. A smaller vortex is also visible near the center of the cylinder, just above the bowl lip. The false-color background of the images corresponds to an estimate of the flow divergence in the plane of the measurements. Because positive divergence is associated with volume expansion, we anticipate that it will correlate strongly with the locations of heat release. The lower portion of Figure 3 thus clearly shows that the bulk of the heat release during the premixed burning period is taking place in the upper-central region of the bowl.

Later in the cycle, velocity measurements reveal the presence of a toroidal vortex, stabilized just above the bowl mouth (Figure 4). This vortex has been found to form under a variety conditions, corresponding to both highly dilute, early-injection combustion systems as well as late-injection systems. The practical

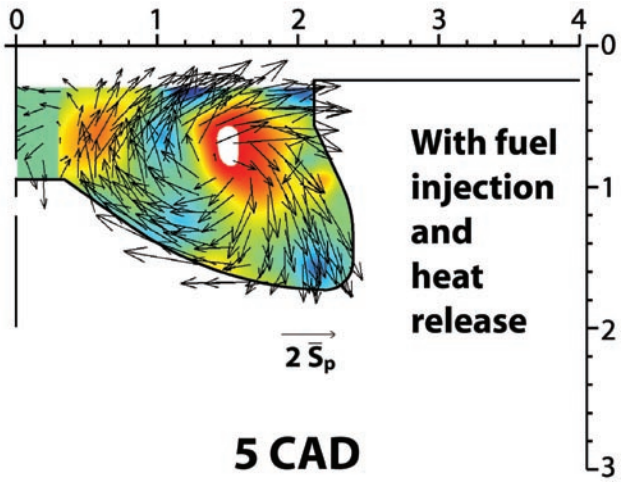


FIGURE 3. Bulk flow structures measured in a fired diesel engine. The flow divergence, indicated by the false color background, identifies regions of large volume expansion (heat release).

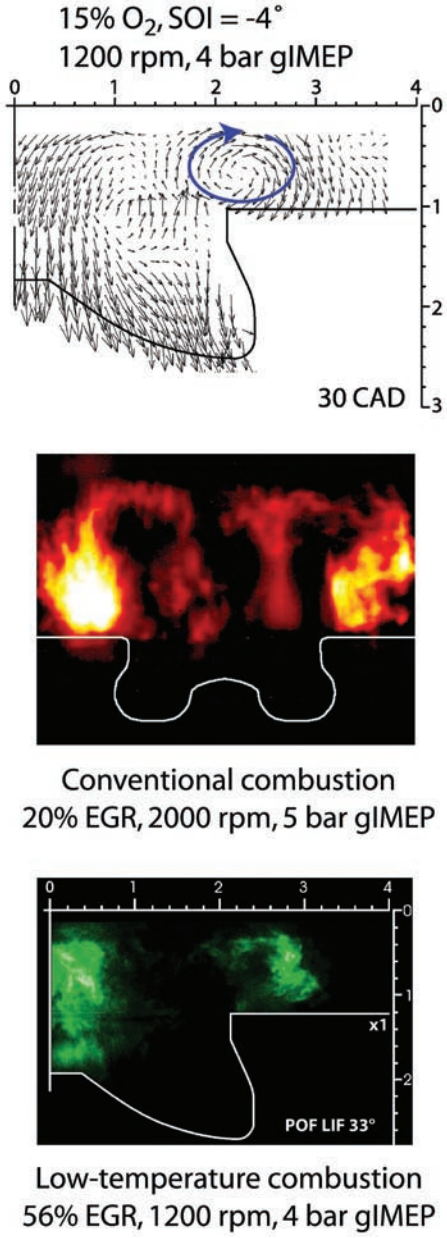


FIGURE 4. Toroidal vortex formed at the bowl exit during the expansion stroke. Either soot or partially-oxidized fuel may be trapped within this vortex for conventional or low-temperature combustion systems, respectively.

consequences of this vortex are two-fold. First, imaging studies of the locations of soot (in conventional diesel combustion systems) and of partially-oxidized fuel (in low-temperature combustion systems) indicate that this vortex can trap pollutants and prevent them from mixing with surrounding fluid–as shown in the middle and lower portions of Figure 4. Second, even if no pollutants are trapped within the vortex, it forms a barrier that prevents partially-oxidized fuel exiting the bowl from mixing with excess air within the squish volume. Understanding how this vortex changes with changes in bowl geometry, swirl, and operating conditions will be one focus of future work in this laboratory.

Conclusions

- Enhancing early mixing processes can significantly improve CO emissions of highly-dilute, low-temperature combustion systems. Changing injection targeting and initial fuel distributions is an effective method of enhancing early mixing.
- Full-field velocity measurements in the combustion chamber of an operating diesel engine are feasible, and show promise for identifying the spatial locations of heat release.
- A toroidal vortex is formed outside the piston bowl during the expansion stroke, which may seriously impede late-cycle mixing processes.
- Full-field imaging of flow structures and distributions of pollutants can offer significant insight into the physics of the late-cycle mixing process, as well as the sources of emissions. The measurements also offer an excellent opportunity to validate the predictions of multi-dimensional simulations.

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3. Miles PC, Collin R, Hildingsson L, Hultqvist A, Andersson Ö (2006) Combined Measurements of Flow Structure, Partially-Oxidized Fuel, and Soot in a High-Speed, Direct Injection Diesel Engine. ***31st Int'l. Symp. on Combustion***, August 6–11, Heidelberg, Germany.

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Special Recognitions & Awards

1. 2005 SAE Harry L. Horning Memorial Award for best paper related to the mutual adaptation of fuels and engines

2. Invited/Keynote Lecture, *Thermo-and Fluid Dynamic Processes in Diesel Engines:* Sept. 2006

3. Invited/Keynote Lecture, *2nd Int'l Symp on Clean, High-Eff. Combustion in Engines:* July 2006

II.A.3 Multi-Diagnostic In-Cylinder Imaging and Multi-Dimensional Modeling of Low-Temperature Heavy-Duty Compression-Ignition Combustion

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DOE Technology Development Manager:
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Objectives

- The overall objective of this project is to understand the spray, combustion, and emissions formation processes of low-temperature combustion (LTC) compression-ignition engines through the application of advanced laser-based and imaging diagnostics in an optically-accessible, heavy-duty, direct-injection diesel engine that is capable of operating under conditions typical of real production engines.
- Specific objectives for FY 2006 include:
  - Use multiple laser/optical diagnostics to broadly characterize in-cylinder processes for multi-mode operating conditions.
  - Develop and improve computer modeling tools for low-temperature combustion by comparing detailed in-cylinder model predictions with experimental images to evaluate three popular prospective engine combustion models.
  - Initiate study of sources of unburned fuel emissions for low-temperature combustion.

Accomplishments

- Studied spray, combustion, and pollutant formation for two conventional and three low-temperature combustion conditions.
  - Use of multiple, simultaneous imaging diagnostics provides understanding and comparison of in-cylinder processes across a wide range of operating conditions on a common platform.
- Extended conceptual model of diesel combustion to multiple low-temperature conditions.
  - Significant differences in spray penetration, liquid vaporization, spatial location of soot formation, combustion reaction and unburned fuel distribution.
- Evaluated detailed in-cylinder performance of prospective state-of-the-art computer models through collaboration with University of Wisconsin.
  - Eight-month student visit to Sandia to collect data for computer model validation.
  - Detailed comparison of model predictions with in-cylinder experimental images, in addition to cylinder pressure, shows failings of some models and validates predictions of others.
- Developed optical diagnostic technique to identify sources of unburned fuel emissions.
  - Evidence of incomplete combustion strongly suggests that lean regions may be formed near the injector after the end of injection.

Future Directions

- Apply optical diagnostics/analyze data for other LTC conditions.
  - Different piston bowl and injector tip geometries
  - Multiple injection schemes, EGR variation
- Maintain modeling collaboration with University of Wisconsin to improve model performance for LTC strategies with different engine and injector spray geometries.
- Develop new diagnostic capabilities to quantify sources of unburned fuel for LTC schemes.
  - Formaldehyde fluorescence showed presence of unburned hydrocarbons (UHC) and suggested lean regions that do not fully ignite.
  - Need quantitative measurement of vapor fuel concentration to confirm.
- Continue to extend the conceptual model of diesel combustion for low-temperature combustion strategies.

Introduction

In efforts to reduce exhaust emissions from compression-ignition engines, a number of researchers have proposed LTC alternatives to conventional diesel combustion. Many LTC schemes use increased pre-combustion mixing (*i.e.,* long ignition delay) along with dilution by exhaust-gas recirculation (EGR) to reduce both particulate matter (PM) and nitrogen oxides (NOx) emissions. Such strategies include:

1. early fuel injection (premixed charge compression ignition) [1,2]
2. late fuel injection (M-K combustion) [3,4]
3. dual (early+late) fuel injections (uniform bulky combustion system, or UNIBUS) [5,6]

Although these LTC strategies reduce both PM and NOx emissions, they generally increase UHC and carbon monoxide (CO) emissions, while engine control becomes more difficult and the load range is reduced. Although the above LTC strategies have been empirically demonstrated, the in-cylinder processes that govern the performance and pollutant emissions of these alternative strategies are not understood. Furthermore, most existing multidimensional computer models have been optimized for conventional diesel combustion, and do not perform well for alternative LTC schemes. In-cylinder experimental data is needed for validation and development of computer models so that they can be used as predictive design tools for engine development for LTC strategies.

The focus of the FY 2006 effort on this project is to use multiple laser and imaging diagnostics to create a knowledge base for three low-temperature and two conventional high-temperature diesel combustion conditions, and to use that data to validate, develop, and improve combustion sub-models for multidimensional computer modeling codes. This investigation, and all of the work on this project, is conducted in cooperation with our industrial partners (including Cummins, Caterpillar, Detroit Diesel, DaimlerChrysler, General Motors, Ford, Mack Trucks, International, John Deere, and General Electric). The results are presented at biannual Advanced Engine Combustion Working Group meetings.

Approach

This project utilizes an optically-accessible, heavy-duty, direct-injection diesel engine for in-cylinder measurements of compression-ignition spray, combustion, and pollutant formation processes. A cut-away cross-sectional schematic of the engine is shown in Figure 1. An extended piston with a large window located in the bowl of the piston provides primary imaging access to the combustion chamber. A portion of the piston bowl-wall is fitted with an optical window that matches the contours of the bowl-rim, in-line with one of the cylinder-wall windows, as shown in Figure 1. This window allows laser-sheet access into the combustion bowl of the piston, along the axis of one of the injector fuel-jets. Windows inserted in the cylinder wall provide cross-optical access for the laser diagnostics.

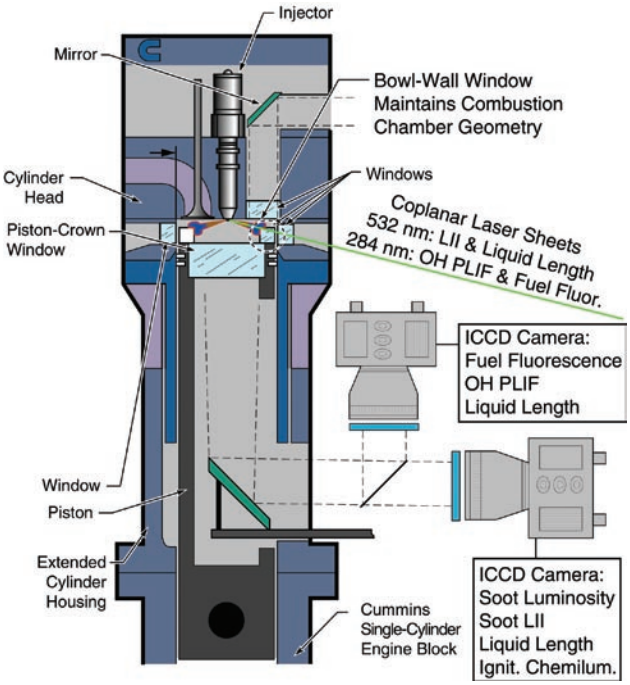


FIGURE 1. Schematic Diagram Showing Optical Engine and Laser/Imaging Diagnostics

In the current study, a suite of optical laser/imaging diagnostics is used: 1) laser elastic scatter to measure liquid fuel penetration, 2) ultra violet (UV) fuel fluorescence for visualizing the vapor-fuel perimeter, 3) chemiluminescence imaging for the spatial and temporal location of ignition, 4) planar laser-induced fluorescence of hydroxyl radicals (OH-PLIF) to study the flame structure and/or hot ignition/combustion, 5) imaging of natural broadband soot luminosity, and 6) planar laser-induced incandescence (LII) of soot. These diagnostics are applied in various simultaneous pairings to study the instantaneous in-cylinder interactions between the measured phenomena.

Three different approaches for modeling diesel engine combustion are examined: 1) A characteristic time combustion (KIVA-CTC) model, 2) a representative interactive flamelet (KIVA-RIF) model, and 3) direct integration using detailed chemistry (KIVA-CHEMKIN). These combustion sub-models were integrated into the same version of the KIVA-3v computer code to provide a common platform for comparing various combustion models.

The engine was operated under five different modes representative of a wide range of conventional and LTC compression ignition engine operating strategies. Space limitations allow data from only one of the LTC operating conditions to be presented here. The late-injection (Modulated Kinetics-type) LTC condition has an inlet oxygen concentration of 12.7% and a load of about 4 bar indicated mean effective pressure. The fuel injection starts at top dead center (TDC).

Results

Shown in Figure 2 are the measured and modeled cylinder pressure and apparent heat release rates (AHRR). Heat release from first-stage ignition in the experiment occurs near 5° after top dead center (ATDC), followed by second-stage ignition, which commences near 10° ATDC. The KIVA-CTC model, which has shown great success for conventional diesel combustion conditions, does not predict the experimental AHRR features well. Very little first-stage ignition is apparent in the AHRR, and the second-stage ignition is much too rapid. The simple timescale formulation of KIVA-CTC combustion model is inadequate for predicting the rates of combustion for the mostly kinetics-controlled LTC conditions. By contrast, both of the other two models predict significant first-stage ignition AHRR, though it is 2-3 crank angle degrees (CAD) earlier than observed in the experiment. The second-stage ignition predictions are 2 CAD early for KIVA-CHEMKIN and 2 CAD late for the KIVA-RIF model. Also, due to its slightly late second-stage ignition, KIVA-RIF predicts a very high peak AHRR compared to KIVA-CHEMKIN. For this operating condition, which is dominated by kinetics, the KIVA-CHEMKIN model gives the best prediction of combustion phasing and magnitude, which is generally true of the other LTC conditions studied (not detailed here).

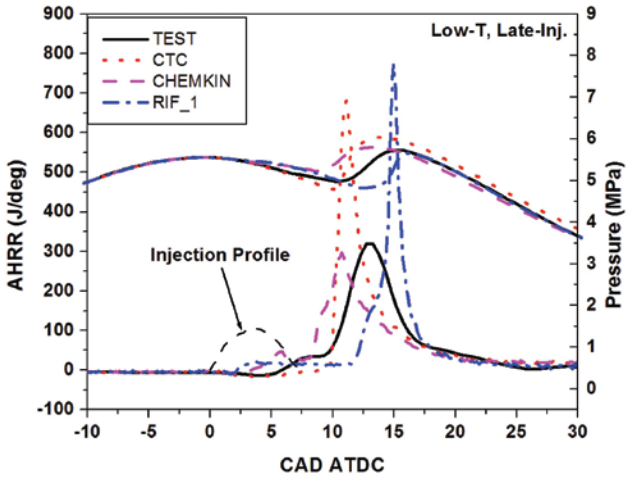


FIGURE 2. Experimentally measured and modeled cylinder pressure (top) and AHRR (bottom), and measured mass rate of injection profile (bottom).

Figure 3 shows a comparison of experimental measurements of liquid- (blue) and vapor-fuel (green) penetration with model predictions. In the experimental images, the injector is indicated by the white dot on the left side of the image, and the piston bowl-rim is indicated by the curved white line on the right side of the images. The model predictions are for a 45 degree sector of the combustion chamber. For all models, the liquid fuel is well predicted until the end of injection, after which all of the models predict residual liquid fuel that was not observed in the experiments. The KIVA-CTC model is worst in this respect, predicting liquid fuel far downstream, mostly due to its lack of first-stage ignition heat release, which would otherwise provide thermal energy to vaporize the fuel. Vapor fuel penetration is predicted well by all three models, lending confidence to the fluid-mechanical predictions of the KIVA platform.

In Figure 4, liquid-fuel penetration (blue) is overlaid with ignition chemiluminescence (green) in the experimental images, and either ignition radical

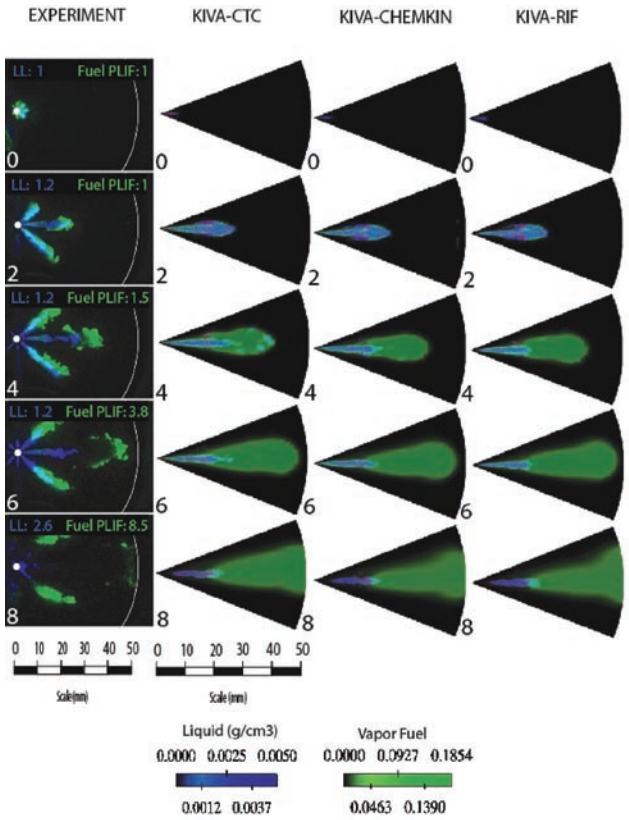


FIGURE 3. Experimentally observed liquid fuel (blue) and vapor-fuel fluorescence (green) and model-predicted liquid-fuel (red circles and blue color) and vapor-fuel mass fraction (green). The relative camera gains are indicated at the top of each experimental image, and the crank angle (°ATDC) is indicated in the bottom left corner of each image.

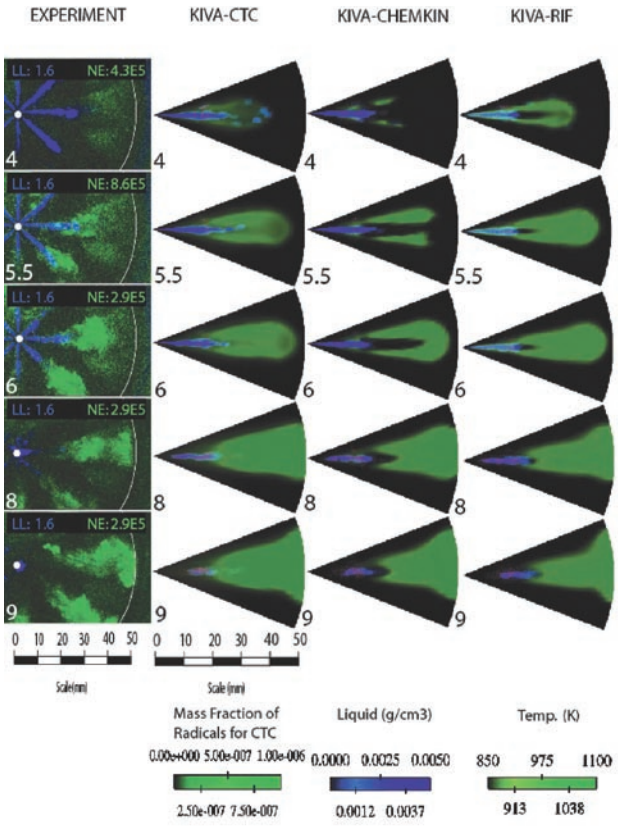


FIGURE 4. Experimentally observed liquid fuel (blue) and natural emission (green) and model-predicted liquid-fuel (red circles and blue color) and either ignition radical concentration (KIVA-CTC, green) or local gas temperature (KIVA-CHEMKIN and KIVA-RIF, green). Labeling is the same as Figure 3.

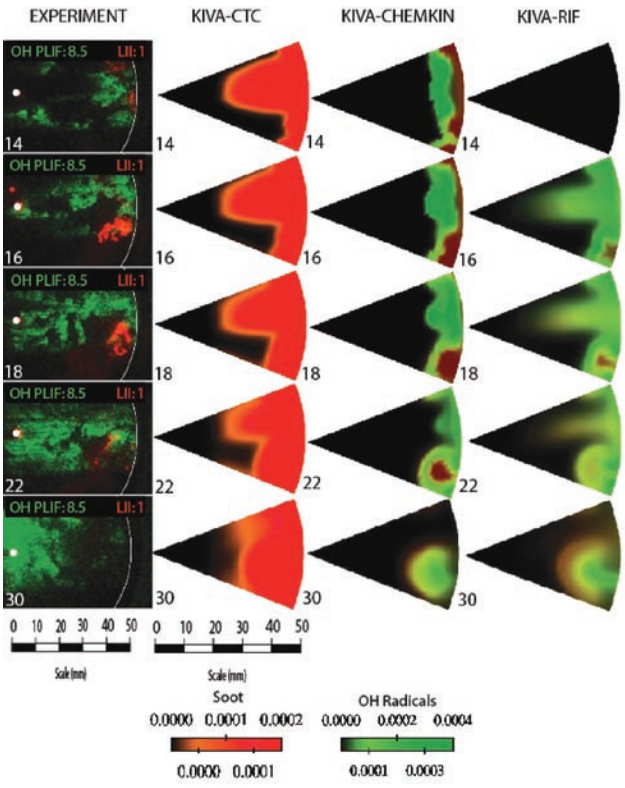


FIGURE 5. Experimentally observed OH-PLIF (green) and soot LII (red) and model-predicted OH (green) and soot (red) mass fractions. Labeling is the same as Figure 3.

concentration (green, for KIVA-CTC) or regions of temperature greater than 850 K (green, for KIVA-CHEMKIN and KIVA-RIF). Chemiluminescence in the experimental images arises from regions that achieve first-stage ignition, which have higher temperatures, and are thus comparable to the model predictions of higher temperature regions. All of the models show the first ignition in a shell on the jet periphery, similar to the experimental observations. The KIVA-RIF model, however, predicts ignition far upstream, near the injector, which was not observed in the experiments. Overall, the spatial distribution of first-stage ignition is predicted reasonably by all three of the models, but the timing is a few crank angle degrees early for both the KIVA-CHEMKIN and KIVA-RIF models (*cf.* Figure 2), and the temperature rise and AHRR (*cf.* Figure 2) for KIVA-CTC is much less than observed in the experiment.

Finally, Figure 5 shows comparisons of the experimental images of OH-PLIF (green) and simultaneous soot LII (red) with the model predictions of OH (green) and soot (red) concentrations (no OH is predicted by KIVA-CTC). KIVA-CHEMKIN and KIVA-RIF predict significant OH downstream, with soot near the head of the jet, similar to the experimental observations. The KIVA-CTC model predicts soot much too early and distributed far too broadly across the width and upstream region of the jet.

Conclusions

The in-cylinder spray, combustion, and pollutant-formation processes for a late-injection, LTC condition were modeled using three different popular combustion modeling approaches, and the model predictions were evaluated by detailed comparison with experimental observations of in-cylinder processes from an optically accessible engine. The data supports the following conclusions:

- State-of-the-art computer models have varying degrees of success for LTC conditions.
  - All models predict initial liquid penetration well, but late vaporization is underestimated.
  - KIVA-CHEMKIN model best predicts ignition, with KIVA-CTC and KIVA-RIF overestimating the spatial extent of ignition.
  - KIVA-CHEMKIN soot and OH distributions were most similar to experiments, while KIVA-RIF showed overlapping soot and OH,

and KIVA-CTC greatly overestimated the soot distribution and underestimated soot oxidation.

Other activities on this project can be summarized as follows:

- In-cylinder processes of three different low-load LTC conditions are not well described by the conceptual model for conventional diesel combustion.
  - Liquid penetration is generally greater, and cool flame reactions may assist vaporization.
  - Hot ignition occurs near the head of the jet, and throughout the jet cross section.
  - Soot forms mostly at the head of jet, and unburned fuel remains after end of injection, near the injector.
  - Conceptual model extension to describe these features is progressing.
- A new optical diagnostic technique has been developed and implemented to identify sources of unburned fuel emissions.
  - Evidence of incomplete combustion strongly suggests that lean regions may be formed near the injector after the end of injection.

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2. "Simultaneous Optical Diagnostic Imaging of Low-Temperature, Double-Injection Combustion in a Heavy-Duty DI Diesel Engine," Satbir Singh, Rolf D. Reitz, Mark P. B. Musculus, and Thierry Lachaux, submitted to Combustion Science and Technology.

3. "In-Cylinder Unburned Hydrocarbon Visualization during Low-Temperature Compression-Ignition Engine Combustion using Formaldehyde PLIF," Thierry Lachaux and Mark P. B. Musculus, accepted for publication at 31st International Symposium on Combustion.

4. "Comparison of the Characteristic Time (CTC), Representative Interactive Flamelet (RIF), and Direct Integration with Detailed Chemistry Combustion Models Against Optical Diagnostic Data for Multi-Mode Combustion in a Heavy-Duty DI Diesel Engine," S. Singh, R. D. Reitz, and M. Musculus, SAE Paper 2006-01-0055, 2006 SAE International Congress and Exposition.

5. "Multiple Simultaneous Optical Diagnostic Imaging of Early-Injection, Low-Temperature Combustion in a Heavy-Duty Diesel Engine," M. Musculus, SAE Paper 2006-01-0079, 2006 SAE International Congress and Exposition, accepted for publication in SAE Transactions.

6. "Two-Stage Lagrangian Modeling of Soot Precursor Formation at Diesel Engine Operating Conditions," L. Pickett, M. Musculus, A. Lutz, and J. Caton, 2006 SAE International Congress and Exposition.

7. "2-Color Thermometry Experiments and High-Speed Imaging of Multi-Mode Diesel Engine Combustion," S. Singh, R. D. Reitz, and M. Musculus, SAE paper 2005-01-3842, SAE Powertrain and Fluid Systems Conference, SAE Transactions 114, No. 4, 1605-21.

8. "Evaluation of the Equivalence Ratio-Temperature Region of Diesel Soot Precursor Formation Using a Two-Stage Lagrangian Model," Lyle M. Pickett, Jerald A. Caton, Mark P.B. Musculus, and Andrew E. Lutz., accepted for publication in International Journal of Engine Research.

9. "Validation of Engine Combustion Models against Detailed In-Cylinder Optical Diagnostics Data for a Heavy-Duty Compression-Ignition Engine," Satbir Singh, Rolf D. Reitz, Mark P. B. Musculus, and Thierry Lachaux, accepted for publication in International Journal of Engine Research.

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11. "In-cylinder Formaldehyde Visualization in a Heavy-Duty Engine," T. Lachaux and M. Musculus, Advanced Engine Combustion Working Group Meeting, September 2005.

12. "Two-Stage Ignition and Unburned Fuel Emissions for Heavy-Duty LTC," T. Lachaux and M. Musculus, Advanced Engine Combustion Working Group Meeting, February 2006.

13. "Laser-Based Imaging of Combustion Processes in the Next Generation of Engines," Invited ASME Tech-Talk Lectures at UC Berkeley, April 2006.

14. "Laser-Based Imaging of In-Cylinder Processes Conventional and LTC HD Diesel Conditions," Invited Seminar at Detroit Diesel Corporation, April 2006.

15. "Laser-Based Imaging of Combustion Processes in the Next Generation of Engines," Invited ASME Tech-Talk Lectures at UC Davis, May 2006.

II.A.4 Fuel Effects on Conventional and Low-Temperature, Compression-Ignition Combustion Processes

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Objectives

- Determine the extent to which near-term and bio-derived fuels can be used to enable a high efficiency clean combustion (HECC) strategy that is not limited by the control and pressure-rise-rate problems that commonly plague homogeneous charge compression ignition (HCCI) strategies.
- Investigate whether fuel composition changes could be used to produce soot with a disordered nanostructure and a correspondingly enhanced oxidation rate.
- Evaluate the validity of prevailing hypotheses that attempt to explain why fueling with biodiesel tends to increase NOx emissions by ~1% for each 10 vol% biodiesel in the blend.

Accomplishments

- Showed that while near-term fuels (*e.g.*, neat biodiesel) can lower smoke emissions by ~50% relative to conventional diesel fuel when high levels of cooled exhaust-gas recirculation (EGR) are used, further reductions of at least an order of magnitude are required to meet the 2010 particulate matter (PM) emission target without using aftertreatment. This indicates that, while fuel composition can strongly affect PM emissions, near-term fuels require additional in-cylinder and/or aftertreatment strategies to simultaneously achieve impending emissions and efficiency targets.
- Demonstrated that fuel changes (*e.g.*, oxygenation) can lead to the production of soot with a disordered nanostructure that could oxidize up to five times faster than highly ordered soot from conventional diesel fuel. Understanding how fuel composition changes can lead to differences in soot nanostructure and reactivity is useful for identifying low-sooting fuel formulations and for facilitating low-temperature diesel particulate filter regeneration with lower catalyst loadings.
- Four of the prevailing hypotheses to explain the higher observed NOx emissions when fueling with biodiesel were evaluated, namely differences in: bulk modulus of the fuel, premixed-burn magnitude, heat-release profile, and stoichiometric adiabatic flame temperature. It was found that there was still an ~10% NOx increase with neat biodiesel even when these effects were removed, indicating that these prevailing hypotheses are inadequate to explain experimental observations. Further experiments are required to determine the underlying cause(s) of the biodiesel NOx increase.

Future Directions

- Quantify fuel effects on transient liquid-fuel penetration length and wall impingement under early direct-injection operating conditions.
- Investigate the hypothesis that increased biodiesel NOx emissions arise because biodiesel produces less in-cylinder soot, which leads to less radiative heat loss from the flame, which leads to higher flame temperatures and thus higher NOx.
- Evaluate a set of oxygenate-water mixtures to determine whether they could enable a HECC strategy without the control problems of HCCI and without requiring the high EGR rates typically necessary for dilute-combustion strategies.
- Upgrade optical-engine hardware to enable operation at 200-bar peak cylinder pressure.

Introduction

Emissions regulations coming into force over the coming decade, increasing costs of imported petroleum, and concerns about global climate change are driving the development of cleaner, more-efficient engine technologies using non-traditional and renewable fuels. One promising approach to achieving the desired efficiency and emissions targets without the use of costly exhaust-aftertreatment systems is high efficiency clean combustion (HECC). HECC is achieved when in-cylinder temperatures are low enough that high nitrogen oxide (NOx) emissions are avoided, and high particulate matter (PM) emissions are avoided by premixing the fuel/oxidizer mixture to overall lean conditions, decreasing in-cylinder temperatures below those

required for soot formation, or enhancing late-cycle soot oxidation. An incomplete understanding of fuel effects on HECC has been one barrier to it being successfully implemented and optimized in production engines. Tasks during fiscal year 2006 (FY 2006) focused on enhancing the understanding of fuel effects on advanced engine processes by: 1) using fuel composition changes to overcome the critical barrier of elevated soot emissions under HECC and conventional combustion strategies, and 2) evaluating the validity of prevailing hypotheses to explain the observed increased NOx emissions with biodiesel fueling, so that this barrier to using this important renewable fuel can be eliminated.

Approach

The experimental work is focused on using advanced diagnostics in the Sandia Compression-ignition Optical Research Engine (SCORE) to investigate the relationships between fuel characteristics, in-cylinder processes, and engine-out emissions. The SCORE is a single-cylinder version of a modern-technology, Caterpillar® 4-stroke, direct-injection (DI) diesel engine that has been modified by Sandia to provide extensive optical access into the combustion chamber [1]. The SCORE is based on the Caterpillar 3176/C-10 engine family used in heavy-duty trucking. A schematic of the SCORE is shown in Figure 1. A large window in the piston bowl enables laser-sheet access and imaging of combustion processes within the engine during operation, as do additional windows in the upper periphery of the cylinder liner and the piston bowl-rim. Specifications of the SCORE are provided in Table 1. The ability to use a wide range of advanced optical diagnostics, coupled with exhaust-gas analysis equipment to measure NOx, smoke, HC, CO, CO_2, and O_2, make the SCORE a versatile instrument for studying the details of fuel effects on in-cylinder processes and corresponding impacts on emissions.

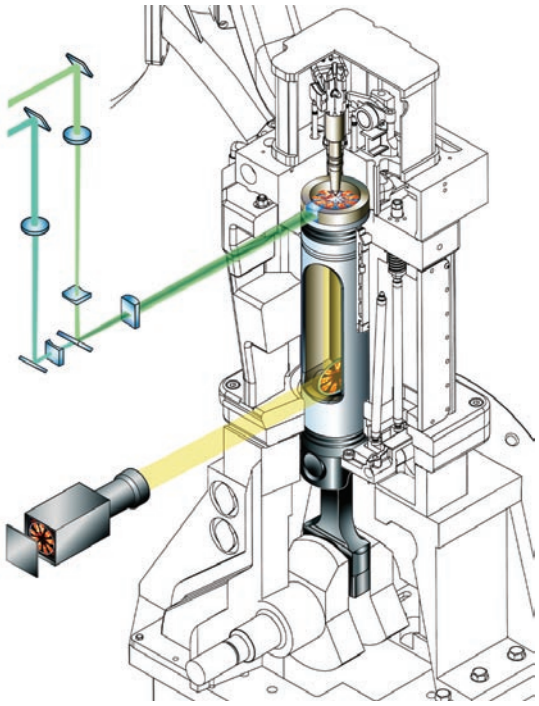


FIGURE 1. Schematic of Sandia Compression-Ignition Optical Research Engine (SCORE)

TABLE 1. SCORE Specifications

Research engine type	1-cyl. vers. of Cat 3176/C-10
Cycle	4-stroke CIDI
Valves per cylinder	4
Bore	125 mm
Stroke	140 mm
Intake valve open[a]	32° BTDC exhaust
Intake valve close[a]	153° BTDC compression
Exhaust valve open[a]	116° ATDC compression
Exhaust valve close[a]	11° ATDC exhaust
Connecting rod length	225 mm
Connecting rod offset	None
Piston bowl diameter	90 mm
Piston bowl depth	16.4 mm
Squish height	1.5 mm
Swirl ratio[b]	0.59
Displacement per cyl.	1.72 liters
Geometric compr. ratio	11.27:1
Simulated compr. ratio[c]	16.00:1

[a] All valve timings are for lift ≅ 0.03 mm
[b] Measured at the Caterpillar Tech. Center using an AVL swirl meter
[c] TDC temperature, pressure, and density in the production engine are matched in the optical engine by preheating and boosting the pressure of the intake air

Results

Can near-term non-traditional fuels enable mixing-controlled HECC? FY 2005 results showed that mixing-controlled HECC (*i.e.*, operation compliant with EPA 2010 on-highway emissions targets and achieving >42% indicated efficiency) is possible without the use of aftertreatment through a strategy employing a highly oxygenated fuel (diethylene glycol diethyl ether, DGE), conventional injection timing, and exhaust gas recirculation (EGR) levels sufficient to drive the oxygen mole fraction in the intake mixture to 10-12% [2,3]. This approach avoids the control, pressure-rise-rate, and light-load emissions problems commonly experienced with premixed HECC strategies like HCCI. FY 2006

experiments focused on determining whether near-term fuels such as neat soy biodiesel (B100) and a Fischer-Tropsch-like paraffinic fuel (CN80) could achieve similar mixing-controlled HECC performance. Figure 2 shows that the smoke emissions for these fuels, while up to a factor of two lower than for the #2 diesel reference fuel (D2), were still at least an order of magnitude higher than the 2010 emissions target at the dilution levels required for NOx compliance. This indicates that additional in-cylinder strategies are required to enable HECC with these near-term fuels [4].

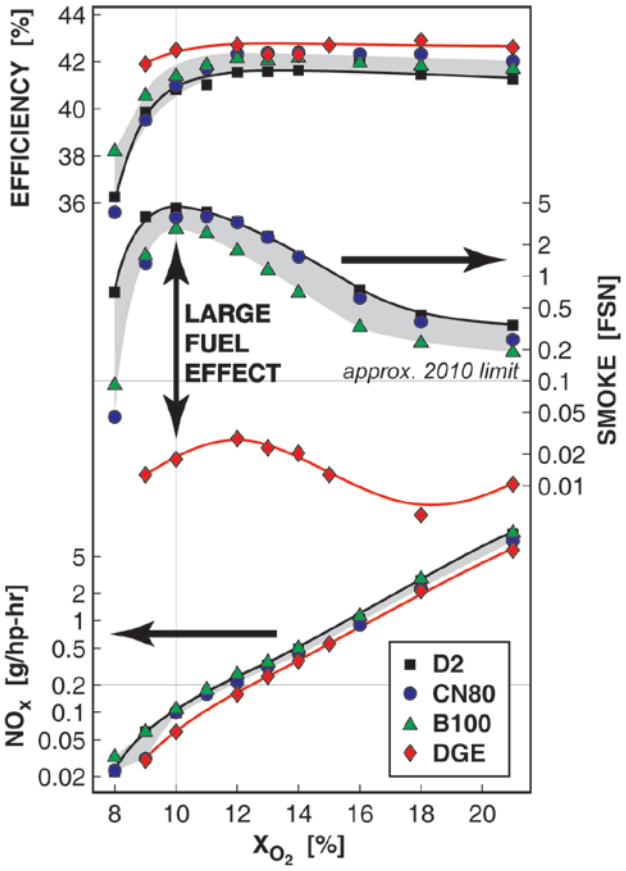


FIGURE 2. Engine-out NOx and smoke emissions, and indicated efficiency, for four different fuels over a range of intake-O_2 mole fractions (X_{02}). The fuels are a low-sulfur #2 diesel reference fuel (D2), an 80-cetane blend of diesel primary reference fuels (CN80 = 76.5 vol% n-hexadecane + balance 2,2,4,4,6,8,8-heptamethylnonane), a neat soy biodiesel (B100 = Nexsol BD-0100 from Peter Cremer NA), and diethylene glycol diethyl ether (DGE). The gray, shaded regions show the ranges achievable with the near-term fuels. It is evident that B100, CN80, and D2 have excessive smoke emissions at dilution levels required for NOx compliance while maintaining reasonable efficiency. X_{02} was adjusted by diluting the intake mixture with nitrogen gas. The injector nozzle had six, 0.163-mm-diameter orifices with a 140° included angle, and the single injection began within 5 crank-angle-degrees before TDC. The engine load was held constant at 6.7 bar gross indicated mean effective pressure (IMEP).

Can fuel-composition changes be used to produce soot that is easier to oxidize? The oxidation rate of soot is related to its nanostructure, that is, to the curvature and relative orientations of its constituent molecular layers. Soot with curved or disorganized layers generally has a higher reactivity than soot with planar, graphitic layers. This study used high-resolution transmission electron microscopy to analyze the soot produced by the combustion of three different fuels in the SCORE, two of which contain oxygen bonded within the fuel molecule. Results show that increasing fuel oxygenation produces lower in-cylinder and engine-out soot levels, consistent with existing studies of the effects of fuel oxygenation on soot emissions from diesel engines. The intriguing new information is that increasing the level of fuel oxygenation produced soot with less graphitic structure, as shown in Figure 3,

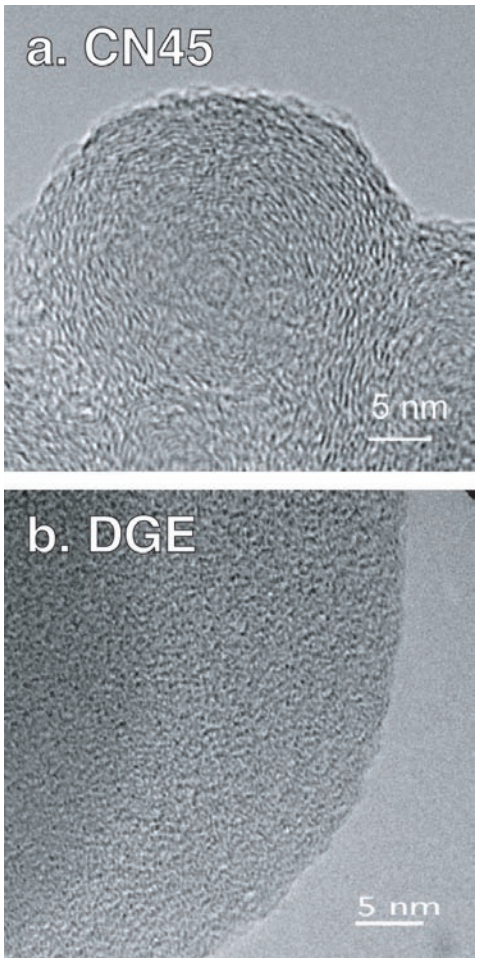


FIGURE 3. High resolution transmission electron micrographs of soot produced by a) CN45 hydrocarbon reference fuel and b) DGE. Note that the DGE soot has a highly disordered nanostructure (*i.e.*, no evidence of concentric carbon layer planes), which is correlated with oxidation rates up to five times greater than those for soot with a more-orderly nanostructure.

which is correlated with higher reactivity. Hence, diesel fuel oxygenation may help curtail soot emissions by enhancing soot oxidation rates as well as by preventing certain fuel carbon atoms from participating in reactions that form soot [5].

Are prevailing hypotheses adequate to explain the observed NOx increase when fueling with biodiesel? Four of the prevailing hypotheses to explain the higher observed NOx emissions when fueling with biodiesel were evaluated. This was accomplished by formulating a blend of the diesel primary reference fuels (PRFs) that had the same start of injection, ignition delay, premixed-burn magnitude, heat-release rate, and stoichiometric adiabatic flame temperature as neat biodiesel (see Figures 4 and 5). Figure 6 shows that there is still an ~10% NOx increase with neat biodiesel even when the above matching is accomplished, indicating that the "accepted" hypotheses are inadequate to explain experimental observations [7]. Further experiments are required to determine the underlying cause(s) of the biodiesel NOx increase.

Conclusions

Significant progress was made in the understanding of fuel effects on soot and NOx formation in advanced combustion modes. The primary conclusions can be summarized as follows:

- While fuel-composition changes such as lowering aromatics and introducing oxygenated compounds

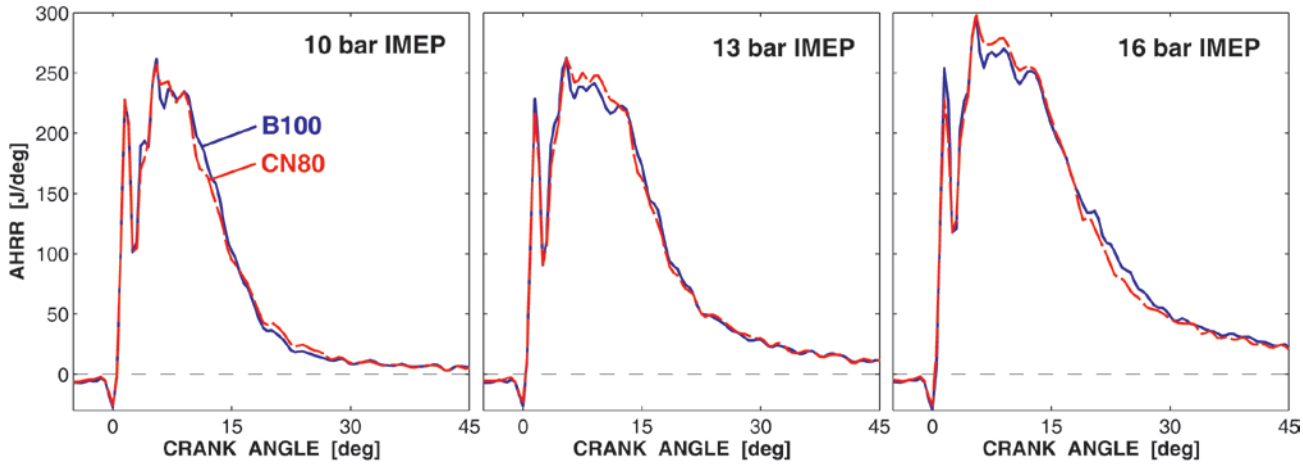


FIGURE 4. Apparent heat-release rate (AHRR) profiles showing matching between B100 and CN80 at three different engine loads.

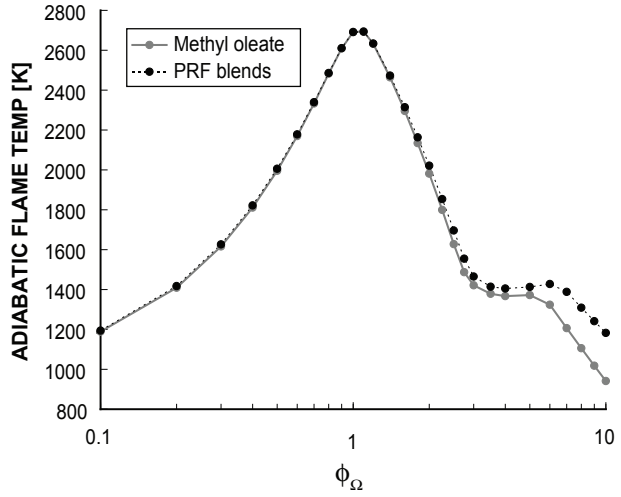


FIGURE 5. Adiabatic flame temperature as a function of mixture stoichiometry for mixtures of diesel primary reference fuels (PRFs) and methyl oleate (a surrogate for B100). The stoichiometric adiabatic flame temperature values are identical for all of the fuels. The oxygen equivalence ratio, ϕ_Ω, is used to correctly quantify the mixture stoichiometry for oxygenated fuels [6].

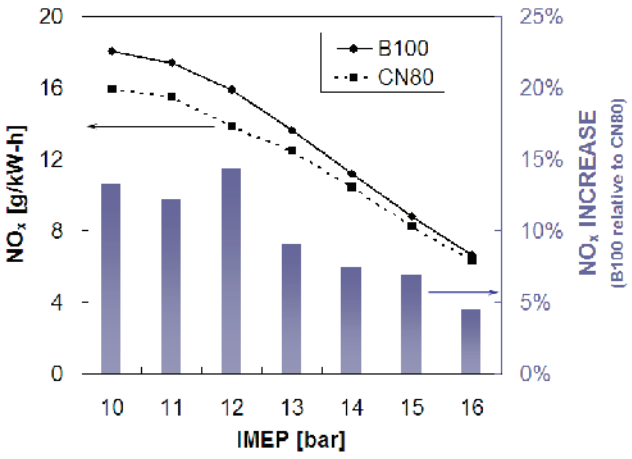


FIGURE 6. Fueling with B100 produces a load-averaged 10.5% NOx increase relative to CN80, even though start of injection, ignition delay, premixed-burn magnitude, heat-release rate, and stoichiometric adiabatic flame temperature are matched between the two fuels at each load.

can enable a highly desirable HECC operating mode, additional in-cylinder strategies are required to attain HECC with near-term fuels like soy biodiesel and Fischer-Tropsch-like paraffinic fuels.

- In addition to curtailing soot *formation*, diesel-fuel changes such as oxygenation can also enhance soot *oxidation* by leading to the production of soot with a more-disordered nanostructure and correspondingly higher reactivity.
- Four prevailing hypotheses were found to be inadequate to explain the increased NOx emissions observed when fueling with biodiesel. Alternative hypotheses such as differences in soot radiative heat transfer, mixture stoichiometry, and prompt-NOx pathways need to be evaluated to determine their roles in increased biodiesel NOx formation.

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3. "Two-Photon Laser-Induced Fluorescence of Nitric Oxide in a Diesel Engine," 2006 SAE World Congress, Detroit, MI (April 5, 2006).

4. "Fuel Effects on Mixing-Controlled Combustion and Emissions under High-EGR Conditions," Advanced Engine Combustion Working Group Meeting, Livermore, CA (Feb. 8, 2006).

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6. "An Overview of Sandia National Laboratories and Activities During My Visit to Caterpillar," Caterpillar Engine Research Division Meeting, Peoria, IL (Dec. 1, 2005).

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II.A.5 Soot Formation under High-EGR LTC Conditions

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Objectives

- Determine how the premixed-burn equivalence ratio changes with the use of exhaust gas recirculation (EGR) by performing quantitative mixing measurements.
- Develop a database for soot volume fraction in reacting sprays including high-EGR, high-density, and high-temperature conditions encountered in engines at conditions where soot emissions are most problematic.
- Investigate how cool flame reactions affect lift-off length and soot formation under low-temperature combustion (LTC) conditions by performing laser-induced fluorescence of formaldehyde.

Accomplishments

- Showed that the premixed-burn equivalence ratio did not decrease with increasing EGR, despite the lengthened ignition delay. Demonstrates that reduced soot formation using extensive EGR is caused by soot kinetics rather than mixture equivalence ratio.
- Generated unique datasets for in situ soot volume fraction in reacting sprays as a function of EGR level, ambient temperature, ambient density, injection pressure, and fuel type. Data are published to http://www.ca.sandia.gov/ECN/ and are currently being used for the development and validation of computational models.
- Found that cool-flame radicals (formaldehyde) exist upstream of flame lift-off, affecting the location of high-temperature reaction, the fuel-rich premixed reaction zone, and the amount of soot formation downstream in the fuel jet.

Future Directions

- Investigate the timing and amount of soot formation for short-injection events at high-EGR conditions.
- Determine the history of liquid penetration at conditions typical of early-injection low-temperature combustion.
- Perform direct measurements of mixing (equivalence ratio) at the time of the premixed burn in constant-injection-duration diesel fuel jets for various EGR levels. This investigation will show how mixing at the end of injection affects the equivalence ratio and location of the premixed burn.

Introduction

Low-temperature diesel combustion concepts generally utilize high levels of cooled EGR. In some combustion strategies, the use of EGR can significantly reduce particulate matter (PM) emissions. The PM emissions reduction appears related to an increase in ignition delay, caused by cooled EGR, which provides more time for mixing before combustion and the potential for a decrease in the equivalence ratio ϕ of the igniting fuel-ambient mixture. The PM reduction is most significant when the ignition delay exceeds the injection duration and there is a high degree of fuel-ambient mixing so as to prevent soot formation and, simultaneously, the EGR and fuel-lean mixtures reduce flame temperatures and suppress NOx formation. Although promising, this type of combustion is currently restricted to low-load conditions, partially because of the requirement that injection end prior to ignition. In practice, high-load conditions are achieved through injection durations that exceed the ignition delay. In addition, use of EGR lowers total in-cylinder oxygen, which can ultimately limit the maximum achievable load.

A reduced oxygen concentration (EGR) can also hinder attainment of low ϕ in the igniting fuel-ambient mixture. This is because the lack of oxygen requires that more ambient mass must be mixed with fuel to achieve the same ϕ. If mixing parameters are left constant, the time required to mix to a given ϕ will be longer. A decrease in ϕ with increasing EGR is possible only if the increase in ignition delay can compensate for this longer-mixing-time requirement. Therefore, it is unknown if the longer ignition delay is primarily responsible for the reduction in soot formation and

ϕ or if additional measures that increase mixing, like shortened injection duration, are needed to reduce ϕ. We assessed this question by performing measurement of ϕ in the premixed-burn region of a fuel spray while varying the EGR level. The injection duration exceeded the ignition delay to keep mixing parameters constant up until the time of premixed burn and to focus on conditions needed to extend low-emission, low-temperature combustion to higher engine load.

Approach

Research was performed in an optically accessible combustion vessel using a common-rail diesel fuel injector as shown in Figure 1. The experimental ambient and injector conditions are carefully controlled in this facility, thereby facilitating investigation of the effects of fundamental parameters on diesel combustion. With full optical access, advanced mixing, combustion, and soot formation measurements can be performed. Quantitative equivalence ratio measurements in the vaporizing fuel jet were made using planar laser Rayleigh scattering (PLRS) [1]. The light source was an Nd:YAG laser (532 nm) with pulse energy of 150 mJ. The laser beam was formed into a collimated 40 mm wide, 0.3 mm thick sheet and passed through the fuel jet center.

The PLRS technique is illustrated in Figure 2, which is a composite image of a vaporizing n-heptane fuel jet visualized using two different techniques. The left image (till 16 mm) shows Mie scattering from the liquid-phase

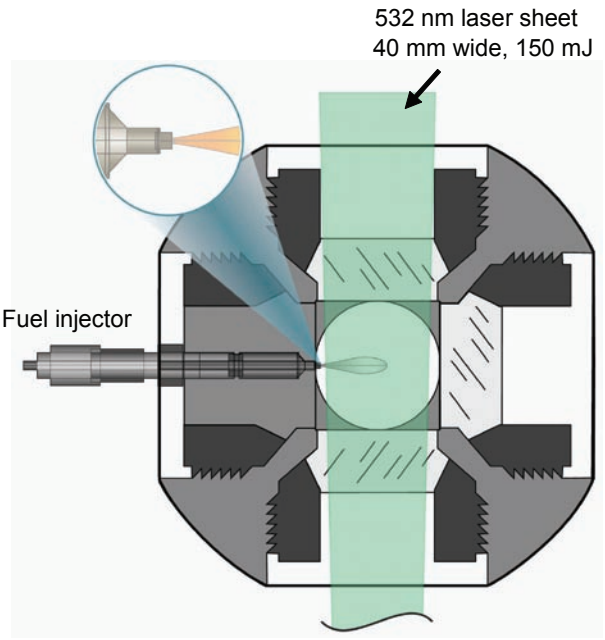


FIGURE 1. Schematic of the combustion vessel and optical setup for planar diagnostics. A 532 nm, 40 mm wide, collimated laser sheet is used for Rayleigh scattering measurements.

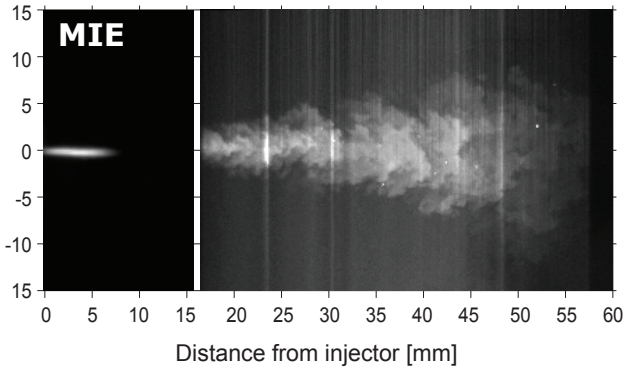


FIGURE 2. A diesel spray injected into the constant-volume combustion vessel visualized using two diagnostic techniques. On the left is the liquid phase visualized using Mie scattering and on the right is the vapor phase visualized by Rayleigh scattering. The two images are obtained from separate injection events. **Ambient conditions: 14.8 kg/m^3**, 1,000 K. Injector conditions: 150 MPa injection pressure, 0.1 mm nozzle.

of the vaporizing fuel jet. The right image is Rayleigh scattering from the ambient and the vapor-phase of the fuel jet. Scattering from liquid fuel extends only to 9 mm. Positioning of the PLRS laser sheet and camera field-of-view downstream of the liquid penetration ensured no interference from liquid droplets. The method for conversion to equivalence ratio is given in Ref. [1].

Results

Figure 3 shows the composite-average (left) and instantaneous (right) images of equivalence ratio for different EGR conditions. The time after the start of injection (ASI) of image acquisition is the ignition delay for a particular EGR condition, corresponding

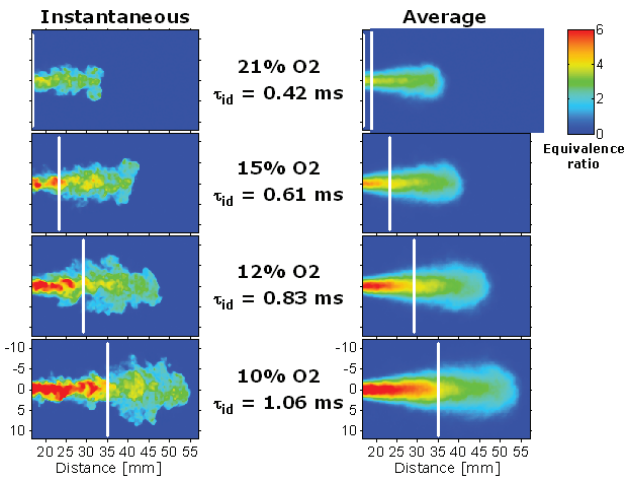


FIGURE 3. Mean (left) and instantaneous (right) equivalence ratio images for the different EGR conditions at time of ignition. Dashed line is lift-off length. (Conditions of Fig. 2)

to the time of the premixed burn. The region of the fuel jet that burns during the premixed burn is the region downstream of the lift-off length, shown as a dashed white line. Figure 3 shows that there are richer mixtures at the same axial location for lower ambient oxygen concentration. This is expected because of the reduced entrainment of oxygen into the jet in a high-EGR environment. However, since the premixed-burn region (distances greater than the lift-off length) shifts downstream as EGR is varied, the peak equivalence ratio of the mixtures doesn't necessarily change (mean centerline values of 2 to 3).

To better compare the fuel-ambient distributions in the premixed-burn region, a histogram for the fuel mass at a given ϕ was computed for the region extending from the lift-off length to the head of the jet (Figure 4). The fuel mass distributions in the premixed-burn region exhibit a monotonic behavior of increasing fuel mass over the range of ϕ with increasing EGR. Despite an increasing fraction of fuel available for premixed burn with increasing EGR, the ϕ of this mixture does not decrease. The average mass-weighted equivalence ratio is relatively unchanged with increasing EGR.

The mass of soot in the fuel jet, on the other hand, remains dependent upon EGR (Figure 5) [2], indicating that factors other than equivalence ratio are important to soot formation at high-EGR conditions. The total mass of soot in the jet actually increases, reaches a peak at 15% O_2 and then decreases to zero at 8% O_2. This trend in soot formation is caused by competition between soot formation rates and increasing residence time. Soot formation rates decrease with decreasing oxygen concentration because of the lower combustion temperatures. Simultaneously, the residence time for soot formation increases, allowing more time

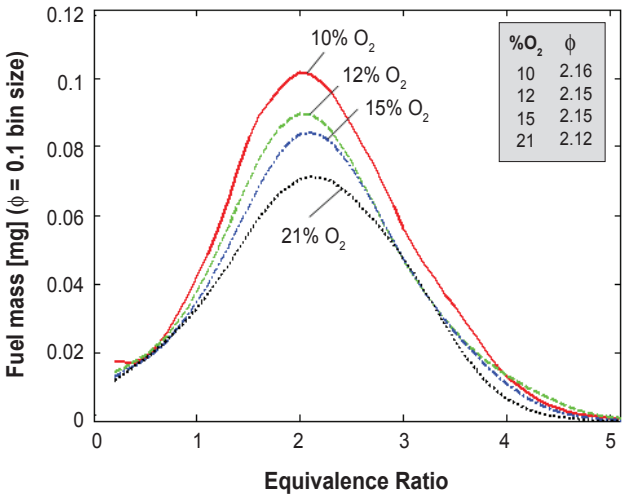


FIGURE 4. Fuel mass distributions in the premixed-burn region for different EGR conditions. The bin size used was $\Delta\phi$=0.1.

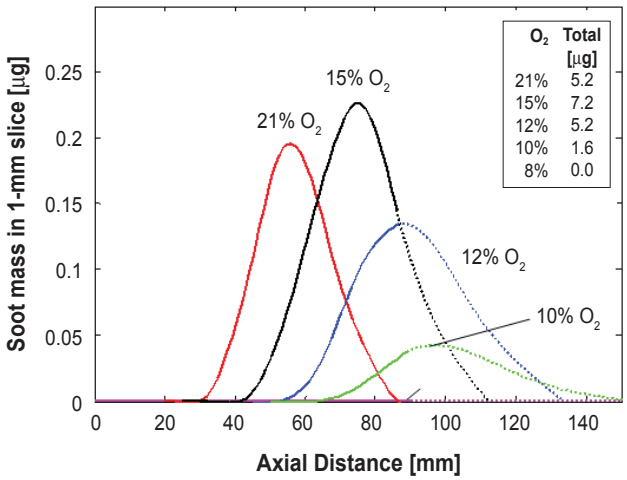


FIGURE 5. Soot mass in thin (1 mm) radial cross-sections of the jet as a function of axial distance. (Fig. 2 conditions)

for accumulation of soot. The tradeoff between an increased residence time and a reduced rate of soot formation determines the ambient oxygen concentration for which soot formation is maximum. For these typical engine temperatures and densities, this maximum is 15% O_2. These results show that soot formation kinetics, in addition to mixture equivalence ratio, have a strong effect on soot production at diesel LTC conditions.

Conclusions

Rayleigh scattering measurements were made in a vaporizing fuel jet to quantify the equivalence ratio distribution during the premixed burn. Results show that the equivalence ratio values in the premixed-burn region does not vary with EGR (peak values of 2-3). Fuel-oxygen mass distributions show a larger mass in the premixed-burn region for higher EGR conditions, implying higher potential for heat release during the premixed burn. For the experimental conditions in this study, an increasing ignition delay with increasing EGR does not decrease the equivalence ratio as would be desired for reducing soot formation. However, soot levels vary considerable with EGR, indicating soot formation kinetics play a major role in soot production at LTC conditions, in addition to the effect of equivalence ratio.

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Special Recognitions & Awards/Patents Issued

1. 2005 SAE Horning Award for best technical paper in engine combustion. One award given each year out of approximately 2,700 SAE papers. (SAE 2005-01-3837).

2. SAE Excellence in Oral Presentation Award for outstanding technical paper presentation at 2005 Powertrain and Fluid Systems Conference, San Antonio, TX. (SAE 2005-01-3843).

II.A.6 Achieving High Efficiency Clean Combustion (HECC) in Diesel Engines

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Objectives

- Expand speed-load operation in HECC modes while achieving improvements in efficiency and emissions.
- Estimate potential benefits of HECC for efficient emission compliance in light-duty operation through modal experiments.
- Develop computer simulations for experimental guidance and interpretation of results. Simulations also used to identify efficiency opportunities.
- Initiate acquisition and installation of more modern light-duty diesel engine platform.

Accomplishments

- Expanded HECC speed-load operation using combinations of high- and low-pressure exhaust gas recirculation (EGR) methods.
- Characterized potential emissions reduction of using fuel injectors with reduced orifice diameters for improved atomization and mixing.
- Developed multi-cylinder model of Mercedes Benz (MB) engine used in this activity and thermodynamic analysis routines for identifying efficiency opportunities.
- Acquired more modern engine platform from General Motors (GM) and are in the processes of installing and developing control system.

Future Directions

- Resolve multi-cylinder stability and control issues for expanded HECC operation.
- Characterize effects of EGR methods on HECC operation.
- Identify efficiency opportunities for expanded HECC operation.
- Complete transition to GM 1.9-L engine for improved collaboration with University of Wisconsin and Sandia National Laboratories.

Introduction

Advanced combustion modes such as premixed charge compression ignition have shown promise as potential paths for meeting 2010 and beyond efficiency and emissions goals. Oak Ridge National Laboratory (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 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 low-temperature combustion (LTC), premixed charge compression ignition (PCCI), homogeneous charge compression ignition (HCCI), Modulated Kinetics (MK), and many more acronyms were in use, but conveyed nothing about the advantages and/or were aligned with certain companies.

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 highly modified MB 1.7-L common rail four-cylinder diesel engine. This engine is equipped with a full-pass engine control system, allowing complete control of all engine parameters including EGR and fuel injection parameters (timing, duration, number). This engine is also outfitted with a low-pressure EGR system which is used in conjunction with a high-pressure EGR system to control the level, composition, and temperature of EGR introduced into the intake system. Physical parameters of the fuel injectors were changed by replacing the tips (167 μm diameter orifices) with custom manufactured tips (100 μm diameter orifices). HECC operation was evaluated at four speed-load conditions which were originally defined by an industry working group to be representative of light-duty diesel engine operations.

Results

Major challenges to evaluating HECC strategies on an engine dynamometer are selecting representative experiment conditions and then relating the results to drive cycle emissions. Four 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 [1-2]. The working group also assigned weights to each mode for estimating the magnitude of drive cycle emissions. 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 four modes used in this study are summarized in Table 1.

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

We performed experiments on a MB 1.7-L diesel engine with conventional and HECC strategies for the modal conditions in Table 1. The engine is equipped with low-pressure and high-pressure EGR systems. The low-pressure system enabled the expansion of the HECC operating range on this engine to include the highest modal speed-load condition as shown in Figure 1. Also shown in Figure 1 are the estimated emissions benefits of HECC based on the light-duty Federal Test Procedure (FTP) modal points described above. Note that BSFC for HECC operation is the same as for conventional operation for all four conditions. This is a requirement for HECC operation as defined for ORNL strategies.

The effect of injector orifice size on drive cycle emissions was also investigated for HECC operation. Experiments were performed at each condition for conventional operation, HECC operation with an OEM orifice diameter of 169 μm, and HECC operation with a custom orifice diameter of 100 μm. Estimated drive cycle emissions are shown in Figure 2 and show that

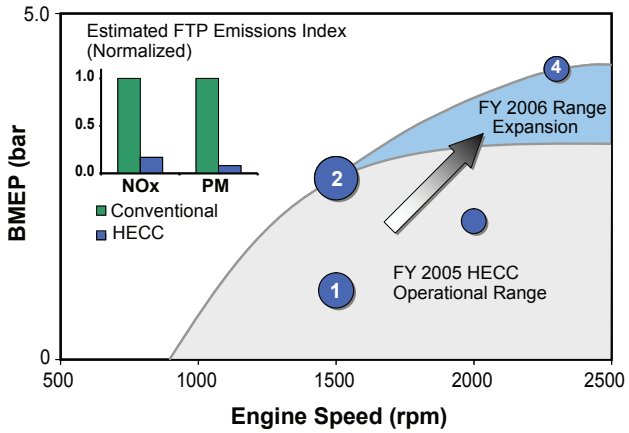


FIGURE 1. Expansion of Usable HECC Speed-Load Range Using Low-Pressure EGR

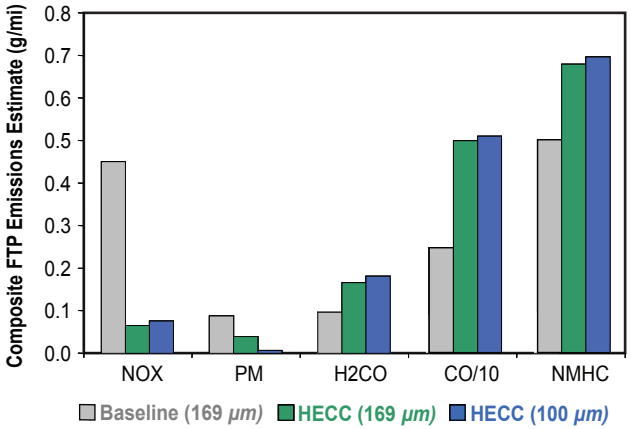


FIGURE 2. Composite Emissions Estimates Based on Light-Duty FTP Modal Conditions (Injector orifice diameter in parentheses.)

HECC operation is successful at reducing NOx and PM emissions but at the expense of CO and HC emissions. In addition, a smaller injector orifice size resulted in a further reduction in PM emissions but was not able to mitigate the elevated CO and HC emissions which are characteristic of advanced combustion operation. These results are important to consider for the successful implementation of aftertreatment technologies with advanced combustion operation. Specifically, achieving high oxidation effectiveness for reducing the elevated CO and HC emissions may be a challenge due to low exhaust temperatures. Another potentially valuable observation was that the NO_2/NO ratio in the exhaust exceeded two for HECC operation whereas the value is one or less for conventional diesel operation as shown in Figure 3. The higher NO_2/NO ratio may be beneficial to some NOx aftertreatment technologies while being detrimental to others.

The composite emissions estimates for HECC operation are compared to U.S. Tier 2 Bin 5 regulatory standards in Table 2. Recall that these emissions estimates are based on steady-state data from a fully warm engine and do not include important effects associated with cold-start and transient load-speed operation. Examination of Table 2 indicates some form of aftertreatment will most likely still be required for the form of HECC used in this activity. While significant in-cylinder NOx reduction was achieved and dramatically reduces the NOx aftertreatment requirement, HC and CO emissions were increased in the processes resulting in the need for increased aftertreatment oxidation as compared to conventional operation. Also note that a diesel particulate filter was used in the low-pressure EGR system and will corresponding be required to meet the HECC values shown in Table 2.

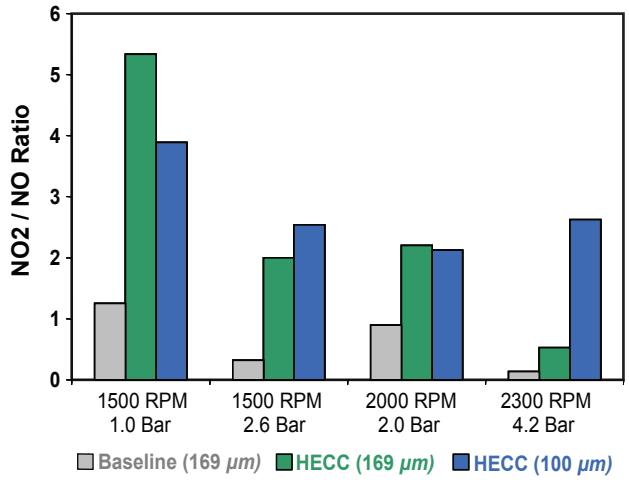


FIGURE 3. NO_2/NO Ratio for Conventional and HECC Operating Conditions (Injector orifice diameter in parentheses.)

TABLE 2. U.S. Tier 2 Bin 5 Emissions Standards, HECC FTP Drive-Cycle Emissions Estimates, and Required Aftertreatment Effectiveness Estimates.

Pollutant	Tier 2 Bin 5 g/mi	HECC g/mi	Required Effectiveness
NOx	0.07	0.075	7%
NMHC	0.09	0.694	87%
CO	4.2	5.08	17%
H_2CO	0.018	0.181	90%
PM	0.01	0.007	Required for LPEGR

Due to the concise nature of this report, we were not able to discuss all of the research performed during this activity in FY 2006. Please see the publications/presentations list for more information.

Conclusions

This activity has provided new information for expanding the usable speed-load range of advanced combustion operation and to better understanding the potential benefits and limitations of this technology for achieving HECC in light-duty diesel engines. Specific observations are as follows:

- Combinations of low- and high-pressure EGR allow improved control of intake mixture conditions and consequently provide a path for expanding the speed-load range of HECC operation.
- Advanced combustion strategies for achieving HECC are successful at reducing NOx and PM emissions but at the expense of CO and unburned HC emissions.
- Aftertreatment oxidation will be a challenge for reducing higher CO and HC emissions associated with HECC operation.
- Aftertreatment solutions for NOx emissions used with HECC operation will need to be more tolerant of a wider range of NO_2/NO ratios.

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5. C. S. Sluder, R. M. Wagner, S. A. Lewis, and J. M. E. Storey, "Fuel Property Effects on Emissions from High Efficiency Clean Combustion in a Diesel Engine", SAE 2006-01-0080 (Detroit, MI; April 2006).

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Special Recognitions & Awards/Patents Issued

1. Patent pending. "Device and method for inferring low particulate emissions from nitrogen oxide measurements in low temperature diesel combustion processes".

2. FreedomCAR Technical Highlight in 2006. "Demonstrated range expansion and estimated potential FTP benefits of HECC operation".

II.A.7 Large Eddy Simulation Applied to Low-Temperature and Hydrogen Engine Combustion Research

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Objectives

- Combine unique state-of-the-art simulation capability based on the large eddy simulation (LES) technique with Advanced Engine Combustion R&D activities.
- Directly complement optical engine experiments being conducted at the Combustion Research Facility (CRF) by performing identical companion simulations.
- Focus initially on optical hydrogen-fueled internal combustion engine (H2-ICE) experiment, and then systematically extend focus to low temperature combustion (LTC) applications.

Accomplishments

- Established suite of validation studies aimed at simultaneous treatment of turbulence and combustion phenomena in ICE environments (Oefelein 2005, 2006a-c, and Oefelein et al. 2006)
- Time-varying ICE grid refined to eliminate local resolution errors and grid-conditioning constraints
- Simulation of H2-ICE in progress (premixed operation for preliminary staging runs, direct injection operation next)
- Systematic model validation being conducted in collaboration with the DOE Office of Science (International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames www.ca.sandia.gov/tnf)
- Two postdoctoral research associates hired to support our simulation efforts (split between current project and Office of Science activities)
- Established "Computational Combustion and Chemistry Laboratory" specifically dedicated to IC-engine calculations (256 processor Beowulf cluster)
- Two special journal issues prepared to establish state-of-the-art in 1) modeling needs for LES, 2) high pressure (supercritical) combustion

Future Directions

- Continue high-fidelity simulations of optical H2-ICE
  - Move to direct-injection, match experimental activities
  - Validation through comparison of measured, simulated results
    - Chemiluminescence imaging
    - Particle image velocimetry (PIV)
    - Planar laser induced fluorescence (PLIF)
  - Analysis of complementary data extracted from validated simulations
  - Enhance basic understanding
  - Improve engineering models
  - Perform H2-injector pattern optimization studies
- Systematically extend to homogeneous charge compression ignition (HCCI) and LTC diesel engine experiments
  - Perform detailed studies of low temperature combustion processes
  - Work toward treatment of complex hydrocarbon processes
- Continue leveraging between DOE Office of Science and Office of Energy Efficiency and Renewable Energy activities
  - Detailed validation, analysis of key combustion phenomena
  - Access to high-performance "leadership-class" computers

Introduction

This research combines a unique high-fidelity simulation capability based on the large eddy simulation (LES) technique with the Advanced Combustion Engine R&D activities at Sandia National Laboratories. The objective is to use high-fidelity science-based simulations in a manner that directly complements select optical engine experiments. Each of the proposed tasks requires considerable high-level expertise, labor, and computational resources. They significantly exceed the time and resources available in industry and academia and are consistent with a National Laboratory's role of using high-performance computing to enable fundamental exploration of complex combustion phenomena. The simulations are being carried out using

a highly specialized state-of-the-art flow solver designed for LES of turbulent reacting multiphase flows. This software provides a unique enabling capability well suited for the proposed set of tasks.

In theory, a hydrogen-fueled direct-injection IC-engine can provide 15% more horsepower than the identical engine fueled with gasoline. The challenge, however, is that in-cylinder injection requires that hydrogen and air mix in a very short time (i.e., approximately 4 ms at 5,000 rpm). Since mixture formation at the start of combustion is critical to engine performance and emissions, a fundamental understanding of the effects and optimization of in-cylinder hydrogen-air mixture formation is necessary before commercialization is possible. The collaborative experimental-numerical research being conducted by White and Oefelein are designed to systematically address these issues. Experimental results acquired by White are complemented with a closely coupled set of numerical calculations using LES. These simulations are conducted using a highly specialized massively parallel flow solver designed to treat the turbulent reacting flow processes typically encountered in IC-engines.

Detailed LES calculations of the full engine geometry are performed in a manner directly synchronized with the progression of experimental tasks to first validate the numerical models, and then perform joint complementary analysis of key in-cylinder engine processes. In addition to advanced software, performing the detailed calculations requires significant computational resources. In particular, each case takes on the order of 500,000 CPU hours on contemporary supercomputer platforms. To facilitate routine application of LES for this purpose, the CRF is currently engaged in a pilot project aimed at establishing dedicated computational resources for high-fidelity combustion simulations. These dedicated resources enable implementation of both production level simulations and porting of larger simulations to high-end "capability-computing" DOE supercomputer facilities for larger grand-challenge applications.

Approach

Application of LES provides the formal ability to treat the full range of multidimensional time and length scales that exist in turbulent reacting flows in a computationally feasible manner. The large energetic scales are resolved directly. The small "subgrid-scales" are modeled. This provides a way to simulate the complex multiple-time multiple-length scale coupling between processes in a time-accurate manner and facilitates analysis of all dynamic processes simultaneously. Treating the full range of scales is a critical requirement since phenomenological processes are inherently coupled through a cascade of nonlinear interactions. The baseline theoretical-numerical framework employed at the CRF combines a general treatment of the governing conservation and state equations with state-of-the-art numerical algorithms and massively-parallel programming paradigms. Recent results with detailed formulations are given by Segura et al. (2004), Oefelein (2005, 2006a-c) and Oefelein et al. 2006.

The approach involves four key components: 1) application of unique software capabilities and computational resources, 2) implementation of a sophisticated set of subgrid-scale models that are consistent with the direct numerical simulation (DNS) technique in the limit as the grid cut-off is refined toward smaller scales, 3) rigorous validation of models using high-fidelity data acquired from the carefully selected target experiments, and 4) detailed characterization of complex turbulent combustion processes through combined-analysis of experimental and numerical data. Once validated against experiments, the high-fidelity simulations offer a wealth of information that cannot be measured directly. They provide a detailed description of intricately-coupled processes, information required to improve and/or develop advanced control strategies, and the composite data required for development of advanced engineering models that provide the fast turn-around times required by industry designers.

Results

Efforts in FY 2006 have been focused on completing the time-varying grid of the CRF H2-ICE configuration and beginning a set of target simulations that identically match the baseline operating conditions selected by White et al. in the Advanced Hydrogen Engine Laboratory. A series of verification studies have been completed to insure that the appropriate grid quality exists and we have conducted a concurrent set of validation studies to demonstrate the accuracy of the current subgrid-scale model implementation. The modeling approach employs a sophisticated set of subgrid-scale models that converge to a DNS as the local grid cut-off is refined. This approach is fundamentally different than models typically employed in engineering frameworks such as KIVA. Unlike the conventional modeling approaches, chemistry is treated directly. The filtered energy and chemical source terms are closed by selecting an appropriate chemical kinetics mechanism and employing a moment-based reconstruction methodology that provides a modeled representation of the local instantaneous scalar field.

The baseline grid of the CRF H2-ICE is shown in Figure 1. The corresponding valve and spark timing profiles are shown in Figure 2. We have now refined the grid to include the port and valve configuration that identically matches the experimental geometry in

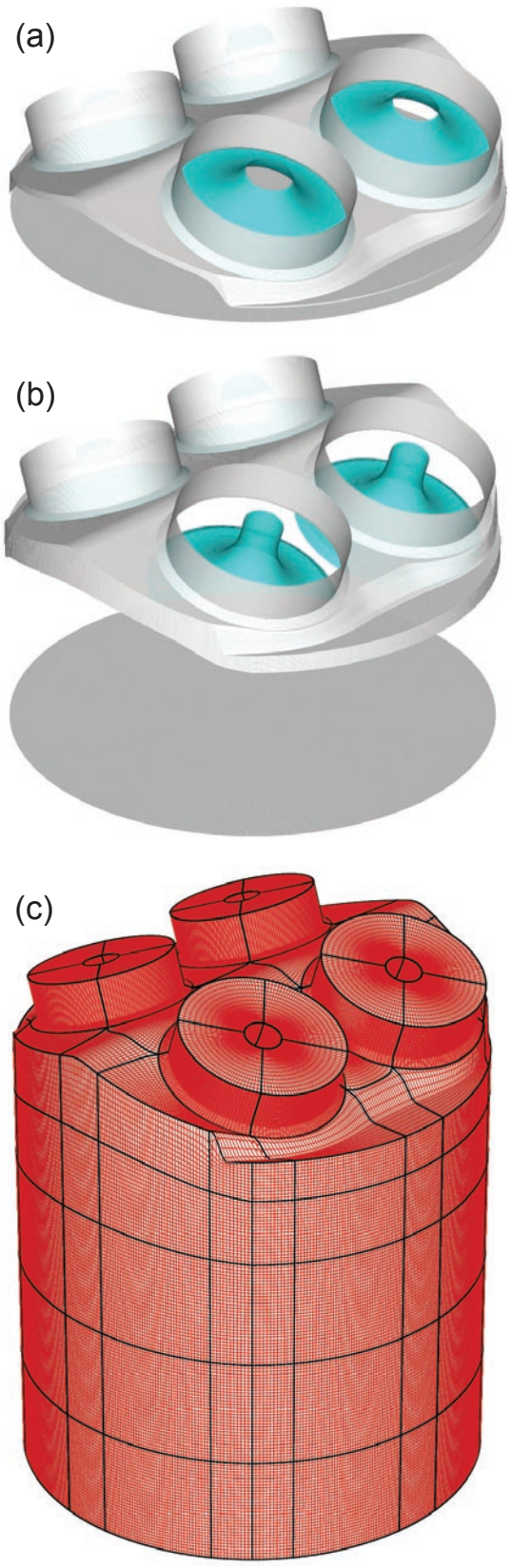


FIGURE 1. Generalized time-varying multiblock grid at 360, 432, and 540 CAD (intake stroke) used for LES of the CRF H2-ICE engine (3-million cells, 137 blocks, ports removed from images).

a time-accurate manner. The refitted direct-injection engine configuration employs a flat-piston with a four-valve pent-roof head and has been designed to handle a range of compression ratios from 9.5 to 12.5. Here, the ports have been removed to show details in the vicinity of the valves. The ports are included in the calculations, however. The valve topology is shown in the images at 360 and 432 crank angle degrees (CAD). The multiblock grid topology is shown in the image at 540 CAD. The black lines highlight a typical generalized multiblock decomposition (137 blocks for this case), where one block per processor is run on a high-performance massively parallel computer platform. The current baseline LES case is being performed using 3.2-million cells. Subsequent calculations will approach on the order of 10-million cells.

To facilitate routine application of LES for this purpose, the CRF is currently engaged in a project aimed at establishing dedicated computational

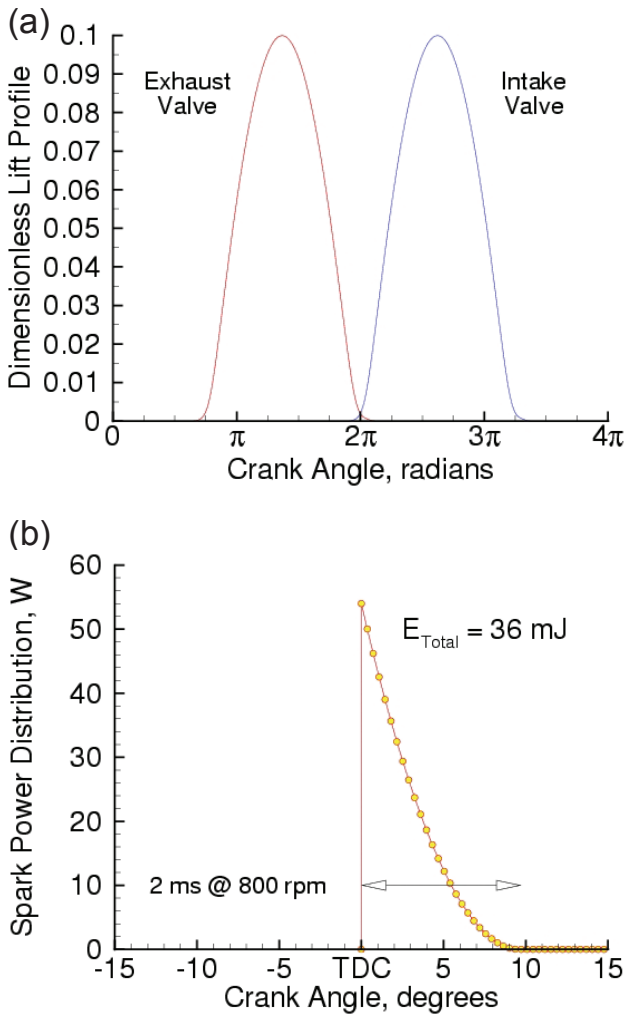


FIGURE 2. Valve and Spark Timing Profiles

resources for high-fidelity combustion simulations. The "Computational Combustion and Chemistry Laboratory" (established in FY 2005) houses two state-of-the-art "Beowulf" clusters. One is funded by the DOE Office of Basic Energy Sciences (BES) to support joint simulations of experiments being conducted in the Turbulent Combustion Laboratory. The second is funded by the DOE Energy Efficiency and Renewable Energy (EERE) office. These platforms leverage open-standards technology and provide a highly scalable, massively-parallel, computational capacities. The base systems provide 284 and 256 AMD Opteron™ (Model 246, 2.0 GHz) processors, respectively, with approximately 20 terabytes of RAID 5 disk storage. These dedicated resources enable implementation of both production level simulations and porting of larger simulations to high-end "capability-computing" DOE supercomputer facilities for larger grand-challenge applications. Figure 3 shows one of the baseline cluster configurations housed at Sandia National Laboratories.

As one example of the experimental-numerical research being conducted, White has applied OH* chemiluminescence to assess the effect of injection variables on engine operation. Since OH* chemiluminescence is known to track heat release and increase in intensity with increasing fuel-air ratio, it is used as a qualitative measure of both flame development and mixture formation. To-date, three injection strategies have been investigated: (i) premixed (ii) early direct injection and (iii) late direct injection. Initial numerical experiments corresponding to case (i) have been performed in the full engine geometry to complement the experimental results. In turn, the experimental results are used to systematically validate key numerical processes. Figure 4 shows representative numerical results from the LES, which shows the instantaneous H_2O production rate at 4, 8, and 12 CAD, respectively, after spark. These data were extracted from the full three-dimensional dataset in the same axial plane as the experimental results acquired by White. Since H_2O production is known to peak in the vicinity of the flame, the ring structure observed in Figure 4 is used as a measure of the instantaneous flame front, similar to



FIGURE 3. Baseline cluster configuration housed at Sandia National Laboratories (284 AMD Opteron™, Model 246, 2.0 GHz) processors with InfiniBand interconnect and 20 terabytes of RAID 5 disk storage.

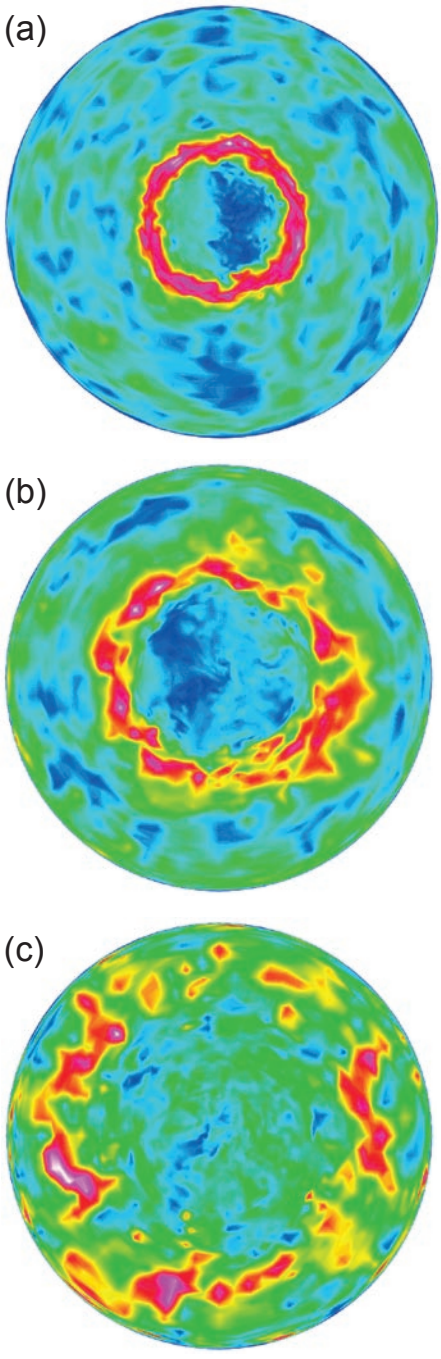


FIGURE 4. Instantaneous H_2O production rate at 4, 8, and 12 CAD, respectively, after spark.

the OH* signal measured in the experiments. The flame speed can be estimated by calculating the time it takes for the peak in the H_2O production rate to reach the cylinder wall. For case (i) from the LES results the flame speed is estimated at 17.6 m/s and from the experiments it is estimated at 16 ± 2 m/s. The agreement between the independent measures of the flame speed obtained experimentally and numerically is promising for the end objective of extracting fundamental physics from the numerical experiments that can not be measured by experimental diagnostics.

Conclusions

Future work will be focused both on hydrogen fuel injector pattern optimization and on the critical needs and challenges associated with the use of hydrogen as a fuel. These needs include obtaining a clearer understanding of power density limitations, maximum fuel efficiency, in-cylinder NOx formation, turbulent mixing characteristics, turbulence-chemistry interactions, and the effects of mixture stratification as a function of local in-cylinder processes over full engine cycles. Information from the simulations, combined with detailed laser-based experiments at well-defined target conditions, will provide the science-base needed by engine companies to develop fuel efficient, low-emissions H2-ICEs. Through interdisciplinary leveraging with other projects, we will continually perform assessments of the base model and select chemical kinetics mechanisms to 1) verify that the chemical mechanisms selected for the IC-engine work are capable of representing important phenomena such as ignition and extinction, and 2) build a validated level of confidence in the overall accuracy of the coupled LES model framework.

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9. Special triple issue on Supercritical Fluid Transport and Combustion by J. C. Oefelein and V. Yang (guest editors). Combustion Science and Technology, 178(1-3), 1-621 (20 topical papers), 2006.

10. Special sections on Combustion Modeling and Large Eddy Simulation, Development and Validation Needs for Gas Turbines by F. F. Grinstein, N.-S. Liu and J. C. Oefelein (guest editors). AIAA Journal, 44(3), 417-468 and 44(4), 673-750 (20 topical papers), 2006.

Presentations at Conferences and Project Meetings

1. BES 26th Annual Combustion Research Conference, Warrenton, VA, June 2005.

2. 41st AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Tucson AZ, July 2005.

3. Ford Motor Company, Detroit MI, July 2005.

4. DOE Headquarters, September 2005.

5. Ford Motor Company, Detroit MI, September 2005.

6. 27th Meeting of the IEA Implementing Agreement on Energy Conservation & Emissions Reduction in Combustion, Zurich Switzerland, September 2005.

7. ORNL Workshop on High Performance Computing, Fall Creek Falls TN, October 2005.

8. Supercomputing 2005, Seattle WA, November 2005.

9. DOE Distributed Energy Peer Review, Arlington VA, December 2005.

10. 44th AIAA Aerospace Sciences Meeting, Reno NV, January 2006.

11. Penguin Computing Advisory Board Meeting, San Francisco CA, January 2006.

12. Interagency Workshop on the Future of Modeling and Simulation for Combustion Applications, Pittsburgh PA, February 2006.

13. Ford Motor Company, Detroit MI, March 2006.

14. BMW, Sandia CRF, March 2006.

15. Ford Motor Company, Sandia CRF, May 2006.

16. DOE Merit Review of Advanced Combustion, Emissions & Fuels Research, ANL, May 2006.

17. SciDAC 2006, Denver CO, June 2006.

II.A.8 Detailed Modeling of HCCI and PCCI Combustion and Multi-Cylinder HCCI Engine Control

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DOE Technology Development Manager:
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Subcontractors:
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- University of Wisconsin-Madison, Madison, WI

Objectives

- Obtain low emissions, high efficiency operation of homogeneous charge compression ignition (HCCI) and premixed charge compression ignition (PCCI) engines.
- Advance our analysis techniques to learn the fundamentals of HCCI and PCCI combustion and to make accurate predictions of combustion and emissions.
- Conduct experiments to determine strategies to control multi-cylinder HCCI engines. Test new instruments for determining HCCI combustion timing.

Accomplishments

- Developed a very fast methodology for analysis of HCCI combustion. This methodology uses a fluid mechanics code and a neural network-based chemical kinetic model. The methodology can analyze HCCI combustion runs while taking only ~10% longer computational time than a motored (non-firing) case.
- Developed an efficient methodology for analyzing gaseous injection within the framework of KIVA. The methodology extends to gaseous injection the well-developed and validated KIVA models for liquid fuel injection, achieving great practical advantages.
- Demonstrated innovative control strategies and applied them to the Caterpillar 3406 experimental HCCI engine, demonstrating accurate cylinder balancing and fast load and ignition timing adjustment.

Future Directions

- *Validate our KIVA-based multi-zone analysis code (KIVA3V-MZ-MPI) against experimental data under partially stratified conditions:* we are working with engine researchers at Sandia Livermore (John Dec and Dick Steeper) to conduct validations of our code at PCCI conditions.
- *Use KIVA3V-MZ-MPI as a predictive tool for engine geometry and fuel injection optimization:* A well validated KIVA3V-MZ-MPI code should be applicable for improving and optimizing engine characteristics in an HCCI or PCCI engine.
- *Analyze spark-assisted HCCI experiments:* we are working with engine researchers at Oak Ridge National Laboratory (Robert Wagner) for analyzing SI-HCCI transition experiments at high EGR conditions.

Introduction

Modeling the premixed charge compression ignition (PCCI) engine 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 PCCI modeling approach, but is computationally very expensive. As a result, modeling assumptions are required in order to develop tools that are computationally efficient, yet maintain an acceptable degree of accuracy. Multi-zone models have been previously shown by the authors to be accurate to capture geometry-dependent processes in homogeneous charge compression ignition (HCCI) engines [1]. We have been testing methodologies for multi-zone analysis of PCCI combustion that show promise for delivering accurate results within a reasonable computational time. We are also developing new tools of analysis that apply to different aspects of HCCI/PCCI operation.

Approach

Our approach is to collaborate with national laboratories and universities conducting experimental work as a part of DOE's Advanced Combustion in Engines (ACE) program. Our role in these collaborations is to provide analytical support that complements the very high quality experimental work being conducted at other places. Although most collaboration to date is HCCI/PCCI centric due to the great importance of this combustion mode, we are working on extending our work to other areas of interest to the DOE ACE program, such as low-temperature combustion and hydrogen engines.

Results

In our ongoing search for efficient and accurate computational tools that can be of interest to engine researchers and manufacturers, we have now developed a neural network based chemical kinetic model and linked it to a fluid mechanics code. The new analysis tool (titled KIVA3V-ANN) can yield accurate HCCI predictions at very low computational cost. The neural network predicts ignition delay as a function of operating parameters (temperature, pressure, equivalence ratio and residual gas fraction). KIVA3V-ANN keeps track of the time history of the ignition delay during the engine cycle to evaluate the ignition integral and predict ignition for each computational cell. After a cell ignites, chemistry becomes active, and a two-step chemical kinetic mechanism predicts composition and heat generation in the ignited cells (Figure 1).

KIVA3V-ANN has been validated by comparison with iso-octane HCCI experiments in two different engines. The neural network provides reasonable predictions for HCCI combustion and emissions that, although typically not as good as obtained with the more physically representative multi-zone model (also developed at LLNL), are obtained at a much reduced computational cost. KIVA3V-ANN can perform reasonably accurate HCCI calculations while requiring only 10% more computational effort than a motored (non-firing) KIVA3V run. It is therefore considered a valuable tool for evaluation of engine maps or other performance analysis tasks requiring multiple individual runs.

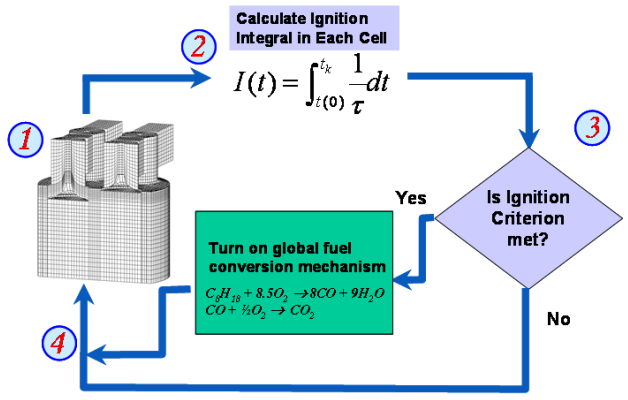


FIGURE 1. Schematic of the analysis procedure used for neural network based analysis of HCCI/PCCI combustion. The neural network is trained for predicting combustion delay. Ignition in individual cells is predicted through the use of the autoignition integral. Ignited cells then react according to a 2-step chemical kinetic mechanism [2].

We have recently developed an innovative methodology for analyzing gaseous fuel injection. While liquid fuel injection is routinely analyzed with standard fluid mechanics codes (e.g. KIVA); gaseous injection in engines is not as simple to model. Typically, gas injection is modeled by specifying boundary elements where a fuel inlet pressure or speed is assigned. This is difficult to implement in the code, requires remeshing for changes in injection parameters (i.e. number of injectors or direction of injection) and it may require fine grid resolution at the nozzle, increasing the computational expense.

Searching for new methodologies for analysis of gaseous fuel injection we conducted a literature survey that revealed an important concept: when modeling gas jets, the momentum injection rate must be reproduced if one wants to reproduce the mixing rate [3, p. 189]. Accepting this to be true, it should be less critical which modeling technique is used to get the gas into the chamber, as long as the gas enters the chamber with the correct mass and momentum rate.

This basic concept can be advantageously used to reduce the computational effort of simulating gaseous fuel injection. Recognizing that the KIVA3V CFD code has extensive capabilities for liquid fuel injection, it is a good idea to take advantage of these capabilities for gaseous fuel injection. The benefits of this approach include:

- Most coding is already in place, which reduces development time.
- A gas inlet does not have to be specified on the computational domain boundary, therefore re-meshing is not required when representing different injectors (number of holes, hole size, hole orientation, etc.) or different flow conditions.
- A fine mesh whose cell size is some fraction of the injector hole size is not required to resolve the inflow boundary, which reduces simulation run time (hole diameters can be less than 1 mm).

The approach consists of injecting the gaseous fuel using the KIVA3V liquid injection model. The resulting

"gaseous spheres" evaporate after a short distance, producing a gaseous jet. The gaseous spheres are fully coupled with the gas phase species with respect to energy and momentum, and therefore simulate entrainment and mixing. "Evaporation" of the gaseous spheres, i.e., their transition from being treated as distinct entities to being part of the combustion chamber gas is based on gas dynamics and empirical relations.

The model was validated by comparison with experimental results for both correctly expanded (subsonic) and underexpanded (sonic) gaseous jets. The results show good agreement in the maximum velocity reached at any point along the jet (Figure 2). However, the model overpredicts the time necessary for the jet to reach the given points. Further research is necessary to improve the arrival time estimations.

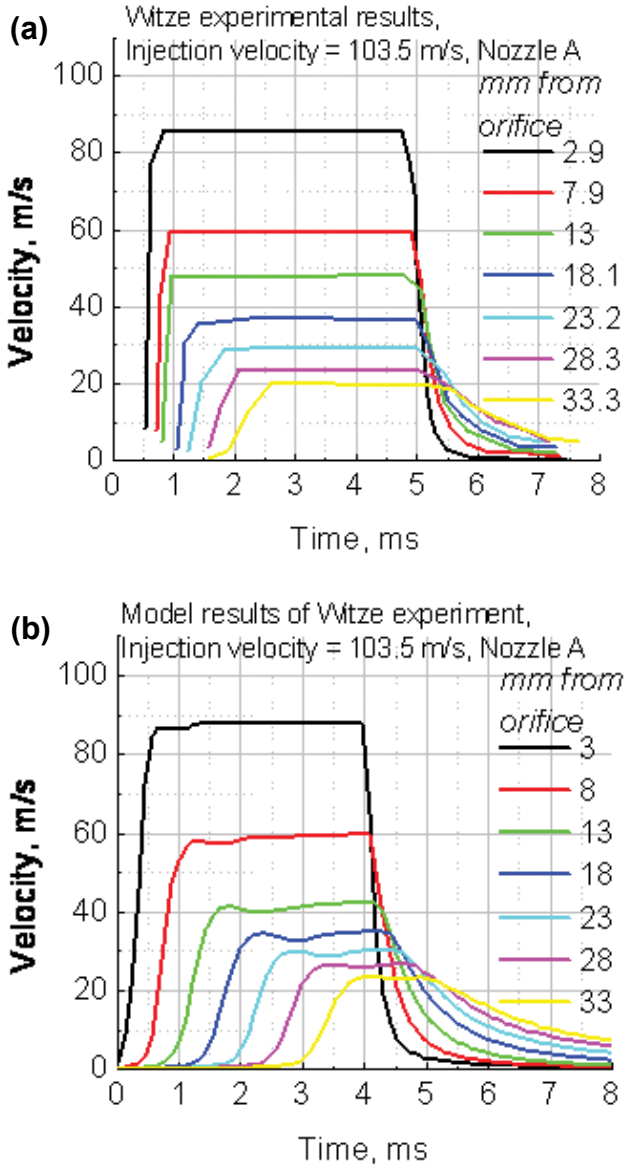


FIGURE 2. Measured (top) and calculated (bottom) velocity histories at seven locations downstream of the injector, for fully expanded experiments with air injected into air.

We have also developed and implemented control technologies for ignition timing in a Caterpillar 3406 HCCI engine prototype (6 cylinder, 14.6 liters total displacement). In this application, combustion control is achieved by blending hot and cold intake with control valves (Figure 3). This control system has the advantage of independently regulating the intake temperature of each cylinder, to obtain optimum ignition timing in all cylinders. The mixing valves are computer controlled. A real-time control system based on Labview's real-time software is used. This system utilizes a dedicated PC running on the Labview real-time operating system as the target, which allows deterministic closed-loop control. Control algorithms can then be easily developed on a host computer connected to the target PC via an ethernet connection and downloaded onto the target PC for implementation. The control algorithm computes the combustion timing based on the pressure signal from each cylinder. The valve position is then scheduled by the control algorithm to yield the desired combustion timing. The hardware side of this control system consists of an electric motor teamed with a rotary position sensor per each cylinder to control the valve position. The control system inputs consist of pressure signals from each cylinder in conjunction with the output from a crankshaft encoder. This control system has demonstrated to be an efficient and robust control strategy for HCCI combustion.

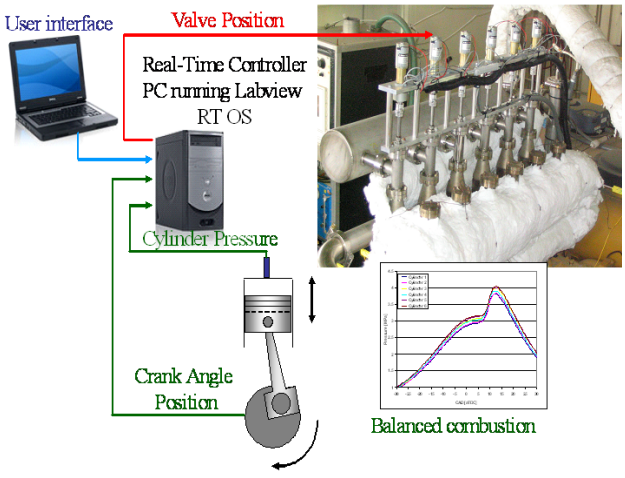


FIGURE 3. Control system for experimental Caterpillar 3406 HCCI engine based on blending a hot stream and a cold stream in a cylinder-by-cylinder basis.

Conclusions

- We have developed a neural network based chemical kinetic model that enables very fast analysis of HCCI combustion at a computational expense only ~10% higher than necessary with a motored run.
- Our gaseous injection model greatly simplifies the analysis of natural gas or hydrogen fueled engines. The model uses the framework of the liquid injection existing in KIVA, enabling straightforward modeling of gaseous direct injected engines.
- We demonstrated the possibility of obtaining consistent combustion in all six cylinders of a Caterpillar 3406 experimental HCCI engine through fast control techniques for cylinder balancing and for load and ignition timing adjustment.

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13. Fast Prediction of HCCI Combustion with an Artificial Neural Network Linked to a Fluid Mechanics Code, Salvador M. Aceves, Daniel L. Flowers, Jyh-Yuan Chen, Aristotelis Babajimopoulos, SAE Paper 2006-01-3298, 2006.

14. A Simple HCCI Engine Model for Control, Nick Killingsworth, Salvador Aceves, Daniel Flowers, Miroslav Krstic, Proceedings of the IEEE International Conference on Control Applications, Munich, Germany, 2006.

15. A Comparison on the Effect of Combustion Chamber Surface Area and In-Cylinder Turbulence on the Evolution of Gas Temperature Distribution from IVC to SOC: A Numerical and Fundamental Study, Randy P. Hessel, Salvador M. Aceves, Daniel L. Flowers, SAE Paper 2006-01-0869.

16. Effect of Charge Non-uniformity on Heat Release and Emissions in PCCI Engine Combustion, Daniel L. Flowers, Salvador M. Aceves, Aristotelis Babajimopoulos, SAE Paper 2006-01-1363, 2006.

Special Recognitions & Awards/Patents Issued

1. Salvador M. Aceves invited to deliver a seminar at the SAE 2006 seminar on HCCI, September 2006, San Ramon, CA.

2. Controlling and Operating Homogeneous Charge Compression Ignition (HCCI) Engines, Daniel L. Flowers, United States Patent 6,923,167, August 2, 2005

II.A.9 HCCI and Stratified-Charge CI Engine Combustion Research

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DOE Technology Development Manager:
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Objectives

Project Objective

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

FY 2006 Objectives

- Apply chemiluminescence imaging to investigate the relative importance of thermal stratification across boundary-layers vs. that in the bulk-gas for slowing heat-release rates at high loads.
- Conduct chemiluminescence imaging and analysis to investigate how the chemiluminescence intensity and uniformity vary with fueling rate and swirl intensity.
- Investigate the potential of two-stage-ignition fuels to operate stably with greater timing retard than single-stage-ignition fuels, and thus, allow higher loads without knock.
- Setup fuel planar laser induced fluorescence (PLIF) imaging diagnostic for investigations of fuel/air mixture preparation, and obtain preliminary PLIF images of fuel stratification at low loads.
- Support chemical-kinetics and computational fluid dynamics (CFD) modeling work at Lawrence Livermore National Laboratory (LLNL) to help develop improved kinetic mechanisms and advance the understanding of in-cylinder processes.

Accomplishments

- Showed that thermal stratification must extend into the bulk gases to be effective in reducing the maximum pressure-rise rate to allow higher loads without knock.
  - Boundary-layer thermal stratification was found to have only a secondary effect.
- Found that the HCCI combustion process consists of a series of distinct phases, each with its own unique chemiluminescence spectral and spatial signature, indicating different key reactions.
- Determined that chemiluminescence intensity tracks the heat-release rate well during the main high-temperature combustion for higher fueling rates, but it is not a reliable marker of the heat-release rate at low loads.
- Showed that two-stage-ignition fuels have advantages over single-stage fuels for acceptable operation at high loads, including improved cycle-to-cycle stability that allows operation with greater timing retard, which reduces pressure-rise rates.
- Completed setup of a PLIF imaging system for in-cylinder fuel/air mixture images. Applied technique to obtain preliminary images of fuel-stratified operation, which can improve low-load combustion efficiency.
- Acquired preliminary in-cylinder temperature data using a novel laser-based technique involving water-vapor absorption, in cooperation with Stanford University.

Future Directions

- Apply PLIF imaging to a comparative study of mixture formation using two different gasoline direct injection (GDI) fuel injectors for stratified-charge operation.
- Complete investigation of how HCCI progresses through the combustion event, using chemiluminescence spectroscopy and chemical-kinetic analysis for single- and two-stage-ignition fuels.
- Investigate the effects of exhaust gas recirculation (EGR) and its constituents (CO_2, H_2O, and N_2) on combustion phasing for various fuels.
  - Isolate the effects of EGR on the heat-release rate to determine its potential benefits for high-load operation.
- Complete detailed exhaust-speciation study over a range of fueling rates and for mixture stratification at low loads, in cooperation with an analytical chemistry group at LLNL.
  - Work with LLNL on CFD modeling to better understand the sources of emissions.
- Complete development of an electro-hydraulic variable valve actuation system and begin initial studies.

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 these barriers is that high-load operation is limited by excessive cylinder-pressure rise rates (PRR) and engine knock. Other issues are improving combustion efficiency and controlling hydrocarbon and carbon monoxide emissions at low loads, and controlling autoignition timing. As outlined under the accomplishment bullets above, several studies have been conducted over the past year (FY 2006) that provide significant new understanding related to overcoming these technical barriers.

Approach

The majority of investigations conducted during FY 2006 involved optical diagnostics and were conducted in our optically-accessible HCCI engine. However, complementary measurements and one study were also made in the matching all-metal engine in our dual-engine HCCI laboratory, using conventional cylinder-pressure and exhaust-emissions diagnostics. This facility is designed to allow operation over a wide range of conditions, and it has several features to provide precise control of operating parameters such as combustion phasing, intake temperature and pressure, mass flow rates of supplied fuel and air, and in-cylinder swirl.

Investigations corresponding to the first three bullets in the accomplishments section above involved quantitative chemiluminescence imaging and spectral analysis. To accomplish this, an intensified camera was calibrated over a wide range of intensifier gains, and various image-analysis programs were written to extract the necessary data. Two different camera mounting locations were used as shown in Figure 1. For the side view, a long depth-of-field imaging technique was developed to image across the combustion chamber for studies of boundary-layer combustion. To investigate changes in the combustion process through the various temporal phases of HCCI autoignition/combustion, this camera was replaced with a spectrometer. The bottom view shown in Figure 1 was used for investigations of the changes in combustion chemiluminescence with operating conditions and for fuel PLIF imaging.

Metal-engine experiments provided more realistic engine-performance data for the conditions investigated in detail in the optical engine. For investigations of the high-load potential of two-stage-ignition fuels, performance and emissions measurements were made for representative single- and two-stage-ignition fuels, while the combustion phasing was systematically retarded.

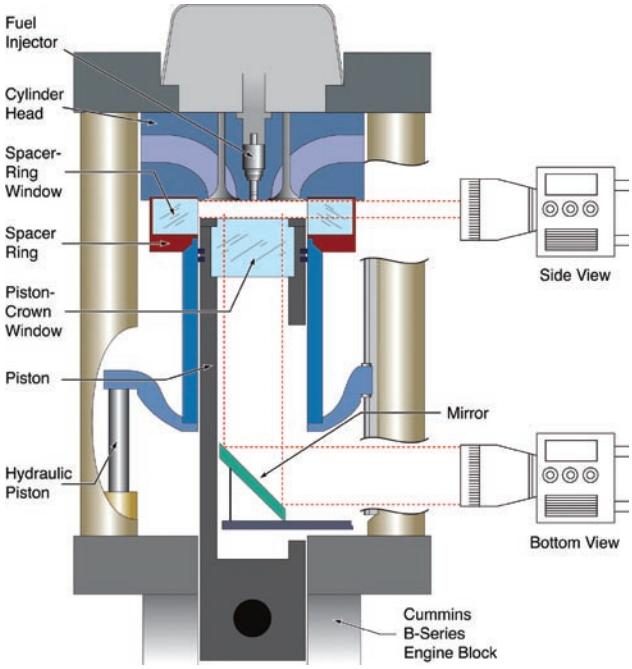


FIGURE 1. Schematic of the optically accessible HCCI engine showing camera views.

In addition to these investigations, other efforts involved working cooperatively with other research organizations. These efforts included: providing data and working with chemical-kinetic and CFD modeling groups at LLNL, working with an analytical chemistry group at LLNL to develop better methods for making detailed exhaust-species measurements, collaborating with researchers at Stanford University on adapting and testing a new in-cylinder temperature measurement diagnostic, and continued interactions with the International Truck and Engine Co. on the development of a variable valve actuation system.

Results

Previous research in our laboratory showed that the naturally occurring charge stratification in HCCI engines results primarily from thermal stratification due to heat transfer from the hot compressed-charge gases to the combustion-chamber walls. This stratification slows the heat release rate (HRR), extending the high-load operating range significantly compared to that of a truly homogeneous charge engine. Because of its importance for high-load operation, and the potential for increasing the high-load limit of HCCI with relatively modest increases in the thermal stratification [1], it is important to understand the spatial distribution of the thermal stratification. Temporally resolved chemiluminescence imaging provides a means of visualizing the sequential autoignition of various parts of the charge, resulting from

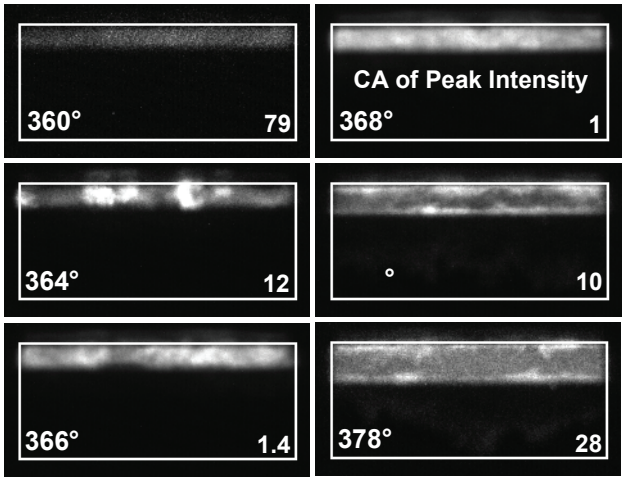


FIGURE 2. A sequence of side-view chemiluminescence images (each from a separate cycle) of HCCI combustion. The crank angle degree ATDC-intake appears in the lower left corner, and the relative intensifier gain is in lower right.

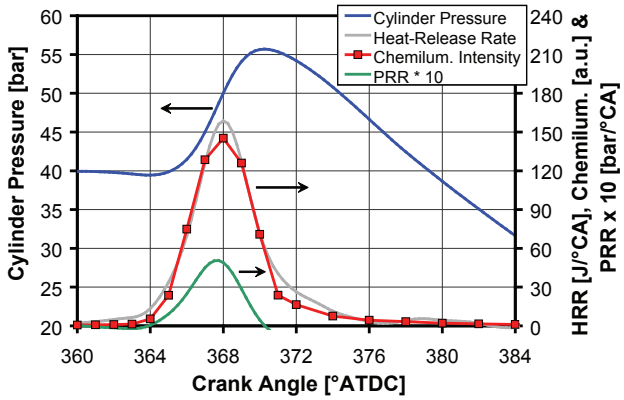


FIGURE 3. Cylinder pressure, HRR, average chemiluminescence intensity and PRR for the same conditions as the images in Figure 2 ($\phi = 0.38$, CA50 = 368°). The data are ensemble-averaged over 20 engine cycles.

this thermal stratification. However, it is important that these images distinguish between the combustion in the bulk gas and combustion in the thermal boundary layers, the latter of which are thought to be a main source of thermal stratification since heat transfer occurs at the in-cylinder surfaces. Near top dead center (TDC), the boundary layers occur primarily along the cylinder-head and piston-top surfaces. Using the side view depicted in Figure 1 (with a long depth-of-field imaging system) the chemiluminescence in the bulk gas and boundary layers can be distinguished.

Figure 2 presents a sequence of these images (each from a separate cycle). The corresponding cylinder pressure, HRR, and PRR are plotted in Figure 3. The images show that the early stages of autoignition (360° crank angle, CA) produce a weak emission which is nearly uniform over the entire chamber. Then at 364° CA, hot ignition begins in localized regions near the vertical center of the combustion chamber. Over the next several crank-angle degrees, more and more regions in the central part of the charge autoignite and burn intensely until the path-averaged side-view images appear nearly uniform in intensity. This sequential autoignition indicates that the naturally occurring thermal stratification extends into the bulk gases. (This occurs as a result of convective transport by in-cylinder flows.) Eventually, the intense combustion in the central part of the charge begins to burn out, and the cooler boundary-layer regions along the cylinder-head and piston-crown surfaces ignite and burn (see the 372° CA image). However, this boundary-layer combustion does not begin until well after the time of maximum PRR, which occurs at 367.7° CA (see Figure 3). Therefore, it is the thermal stratification in the bulk gases that is primarily responsible for controlling the maximum PRR, and thermal stratification in the boundary layer has only a secondary effect. Based on these results, for enhanced thermal stratification to be effective in further reducing the maximum PRR and allowing higher loads, it must also be distributed throughout the bulk gas. A complete discussion can be found in Ref. [2].

As also shown in Figure 3, the total chemiluminescence intensity from the images correlates well with the HRR during the main combustion event for this relatively high load ($\phi = 0.38$) HCCI condition. However, chemiluminescence images acquired with progressively lower fueling rates show that this correlation breaks down at low loads, as evident in the examples shown in Figure 4. At $\phi = 0.2$, the chemiluminescence has begun to significantly phase-lag the heat release, and the peak intensity is proportionally less compared to the peak HRR. This trend progresses rapidly as fueling is further reduced to $\phi = 0.16$, and then to an idle fueling rate of $\phi = 0.12$ (not shown). Therefore, chemiluminescence intensity is not a reliable marker of the HRR at low loads.

A comparative study of the high-load potential of single-stage and two-stage ignition fuels was also conducted. As discussed above, natural thermal stratification slows the HRR allowing higher fueling rates without knock. Moreover, retarding the combustion phasing amplifies the benefit of a given thermal stratification further extending the high-load limit [1]. Thus, one of the key parameters affecting the high-load limit is the amount of timing retard allowable before combustion becomes unstable or a misfire occurs. These stability limits are not well understood and depend on the autoignition characteristics of the fuel. One of the main differences between fuels is whether or not they have early cool-flame reactions that result in a two-stage-ignition process. Therefore, fuels having both single- (iso-octane) and two-stage-ignition (PRF80, 80%

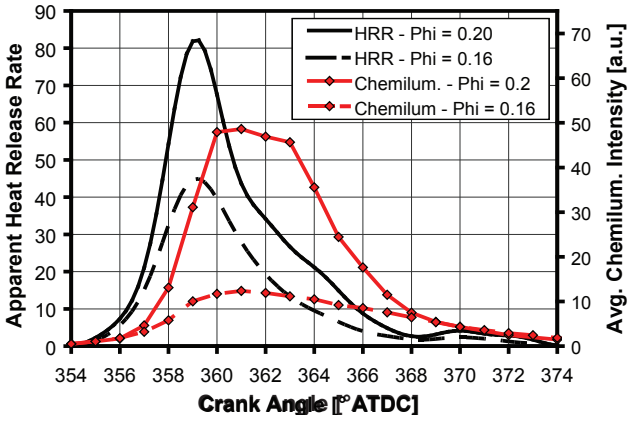


FIGURE 4. Comparison of chemiluminescence intensity and HRR for $\phi = 0.2$ and 0.16. The data are ensemble-averaged over 20 cycles.

iso-octane and 20% *n*-heptane) were investigated for stability under highly retarded conditions.

Figure 5a shows that both fuels exhibit an increased standard deviation in the power output (indicated mean effective pressure, IMEP) from cycle to cycle as the timing is progressively retarded by reducing the intake temperature. However, PRF80 allows significantly more timing retard before reaching the acceptable limit of 2%. This greater allowable timing retard is beneficial for reducing the HRR and allowing higher loads without knock. Additionally, Figure 5b shows that a greater change in intake temperature is required to shift the phasing for PRF80 compared to iso-octane. This means that for PRF80, combustion-phasing control can be made more robust, which is important for practical operation at highly retarded conditions. Finally, the lower intake temperatures with PRF80 increase the initial charge density (*i.e.* the charge mass inducted), which has the potential to increase the power density of the engine. The required intake temperature for iso-octane can be reduced by increasing the compression ratio (CR) from 14 to 18 as shown in Figure 5b. However, to achieve the same intake temperature as PRF80, the CR would have to be well above 18, which is above the range of typical engines and could result in reduced efficiency due to excessive heat-transfer losses and friction [3], unless special care is taken in the engine design. Taken together, these results indicate that two-stage-ignition fuels potentially have significant advantages for high-load HCCI operation. Additional information may be found in Refs. [4,5].

Conclusions

- Side-view chemiluminescence images show that thermal stratification must extend into the bulk gas to strongly reduce the maximum PRR and allow higher loads without engine knock. Boundary-layer thermal stratification has only a secondary effect.

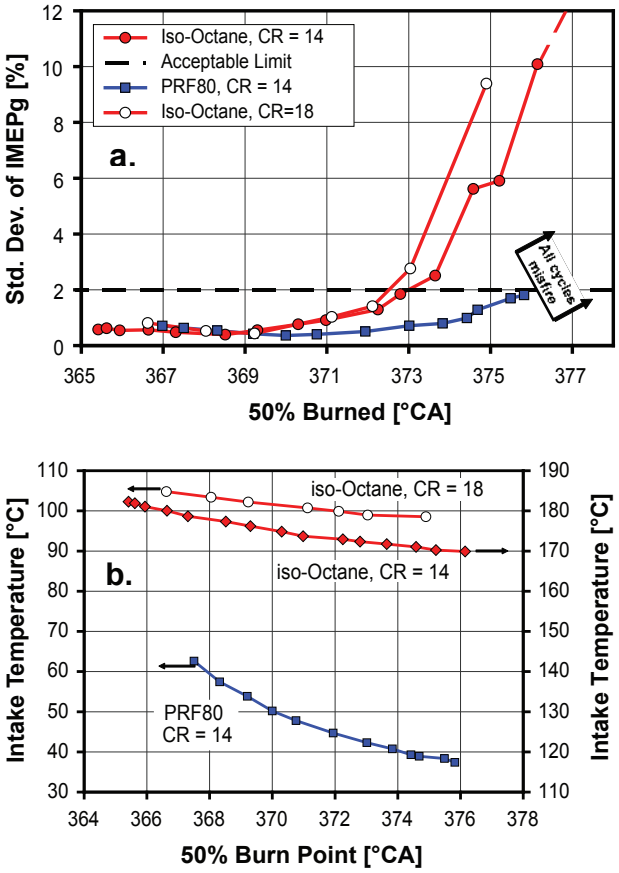


FIGURE 5. Standard deviation of the IMEP (a) and intake temperatures (b) as a function of combustion phasing (50% burn point) for PRF80 and iso-octane.

- The intensity of the chemiluminescence emission correlates well with the HRR during the main combustion event for higher fueling rates (*e.g.* $\phi = 0.38$), making it a good marker of the HRR, and therefore, an indicator of the location of reaction zones.
- Chemiluminescence intensity is not a good marker of the HRR at low fueling rates. For equivalence ratios less than about 0.24, it significantly phase-lags the HRR, and the chemiluminescence intensity is proportionally lower compared to the HRR.
- PRF80 fuel (which has two-stage autoignition) shows a smaller increase in cycle-to-cycle variations of combustion phasing and IMEP with timing retard than does iso-octane (a single-stage-ignition fuel). This allows operation at greater timing retard with PRF80, which provides a greater reduction in the HRR, allowing higher fueling rates without knock.
- For retarded combustion phasing, the two-stage-ignition fuel (PRF80) requires a larger change in intake temperature to achieve a given change in combustion phasing, making it easier to maintain a steady combustion phasing for retarded operation.

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4. Sjöberg, M. and Dec, J. E., "Smoothing HCCI Heat-Release Rates using Partial Fuel Stratification with Two-Stage Ignition Fuels," SAE paper no. 2006-01-0629, 2006.

5. Sjöberg, M., and Dec, J. E., "Comparing Late-cycle Autoignition Stability for Single- and Two-Stage Ignition Fuels in HCCI Engines," Proceedings of the 31st Symposium (International) on Combustion, 2006.

FY 2006 Publications/Presentations

1. Naik, Chitralkumar V., Pitz, W. J., Sjöberg, M., Dec, J. E., Orme, J., Curran, H. J., Simmie, J. M., and Westbrook, C. K., "Detailed Chemical Kinetic Modeling of Surrogate Fuels for Gasoline and Application to an HCCI Engine," *SAE Transactions*, Vol. 114, Sec 4, pp. 1381-1387, paper no. 2005-01-3741, 2005 SAE Fall Powertrain and Fluid Systems Meeting.

2. Dec, J. E., Hwang, W., and Sjöberg, M., "An Investigation of Thermal Stratification in HCCI Engines using Chemiluminescence Imaging," accepted for *SAE Transactions*, SAE paper no. 2006-01-1518, 2006 SAE Congress.

3. Sjöberg, M. and Dec, J. E., "Smoothing HCCI Heat-Release Rates using Partial Fuel Stratification with Two-Stage Ignition Fuels," accepted for *SAE Transactions*, SAE paper no. 2006-01-0629, 2006 SAE Congress.

4. Mattison, D., Jefferies, J. B., Hanson, R. K., Steeper, R. R., De Zilwa, S., Dec, J. E., Sjöberg, M., and Hwang, W., "In-Cylinder Gas Temperature and Water Concentration Measurements in an HCCI Engine Using a Multiplexed-Wavelength Diode Laser System: Sensor Development and Initial Demonstration," Proceedings of the 31st Symposium (International) on Combustion, 2006.

5. Sjöberg, M., and Dec, J. E., "Comparing Late-cycle Autoignition Stability for Single- and Two-Stage Ignition Fuels in HCCI Engines," Proceedings of the 31st Symposium (International) on Combustion, 2006.

6. Hwang, W., Dec, J. E., and Sjöberg, M., "An Investigation of the Stages of HCCI Autoignition and Combustion using Chemiluminescence Spectroscopy," Advanced Engine Combustion Working Group Meeting, February 2006.

7. Sjöberg, M., and Dec, J. E., "EGR and Intake Boost for Managing HCCI Low-Temperature Heat Release over Wide Ranges of Engine Speed," Advanced Engine Combustion Working Group Meeting, February 2006.

8. Sjöberg, M., and Dec, J. E., "Comparing Late-cycle Autoignition Stability for Single- and Two-Stage Ignition Fuels in HCCI Engines," HCCI University Working Group Meeting, February 2006.

9. Dec, J. E., Sjöberg, M., and Hwang, W., "HCCI and Stratified-Charge CI Engine Combustion Research," Advanced Combustion Engine R&D Peer Review, May 2006.

10. Sjöberg, M., Dec, J. E., and Hwang, W., "Thermodynamic and Chemical Effects of EGR and its Constituents on HCCI Autoignition," Advanced Engine Combustion Working Group Meeting, June 2006.

11. Sjöberg, M. and Dec, J. E., "Extending High-Load HCCI Operation using Partial Fuel Stratification with Two-Stage Ignition Fuels," invited presentation, SAE HCCI Symposium, San Ramon, California, September 2005.

Special Recognitions & Awards/Patents Issued

1. SAE Recognition Award (John Dec) for co-organizing of the 3rd annual SAE HCCI Symposium, San Ramon, California, September 2006.

2. Invited presentation (Magnus Sjöberg) at the SAE HCCI Symposium, San Ramon, California, Sept. 2006.

3. Invited member (John Dec) of the Technical Committee for the 2nd International Symposium on "Clean and High-Efficiency Combustion in Engines" Tianjin, China, 2006.

4. SAE Excellence in Oral Presentation Award (John Dec), 2006 SAE Congress.

5. SAE Forest R. McFarland Award (Magnus Sjöberg) for efforts and leadership in organizing technical sessions on HCCI combustion.

6. Patent pending, application #11/095,256, "Fuel Mixture Stratification as a Method for Improving Homogeneous Charge Compression Ignition Engine Operation."

II.A.10 Automotive HCCI Combustion Research

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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 FY 2006 include:

- Quantify the relationship between charge preparation and NOx emissions for low-load, late-injection HCCI operation. Prior work developed a probability density function (PDF) method to correlate laser-induced fluorescence (LIF) measurements of fuel mixing with carbon-based emissions; this work extends the method to include NOx emissions.
- Include the effect of combustion phasing in PDF-emissions correlation. Prior work considered only the equivalence-ratio parameter; this work adds combustion phasing as a parameter.
- Evaluate the NOx-CO_2 (i.e., NOx-combustion efficiency) trade-off for late-injection HCCI operation using alternative injection strategies.
- Test laser-based temperature diagnostics developed at Stanford University for in-cylinder temperature measurements in the Sandia HCCI research engines.
- Facilitate development and application of automotive HCCI engine simulations.

Accomplishments

- Uncovered correlation between LIF-based PDF statistics of fuel-air mixing and measured engine-out NOx emissions during low-load, late-injection HCCI operation. Taken together with earlier data for carbon-based emissions, these results indicate that the developed PDF method could be a useful tool for formulating and assessing advanced mixture-preparation strategies.
- Measured and incorporated combustion-phasing data into the PDF method. As a result, the required lookup table was expanded to quantify emissions as a function of both equivalence ratio and location of 50% heat release.
- Investigated various mixture-preparation strategies for their effect on the NOx-CO_2 trade-off. Determined that neither split-injection nor enhanced-intake-charge-motion strategies improved the trade-off for the swirl-type injector tested. In contrast, tests using a multi-hole injector revealed distinctly improved emissions performance. Increasing injection pressure for the multi-hole injector improved the trade-off modestly. Optical experiments were conducted to understand the observed trends.
- Analyzed *spatial* fuel distribution as an indicator of emissions performance to supplement the PDF analysis, which ignores spatial information.
- Development of multiple in-cylinder temperature diagnostics continued at Stanford as part of Sandia's HCCI engine program. Measured crank-angle-degree-resolved temperatures using Stanford diode-laser absorption sensor in Sandia's optical HCCI engines.
- Continued development of HCCI simulation tools. The UW-LLNL-SNL KIVA/Multi-zone code achieved full-cycle simulation of motored operation in agreement with Sandia optical-engine pressure data. A Sandia WAVE model matched to experimental data provided initial- and boundary-condition estimates. Finally, a Sandia CHEMKIN routine was developed to provide NOx emission predictions for the PDF method described above.

Future Directions

- Install negative-valve-overlap cams to enable use of recompression strategies in the HCCI optical engine.
- Investigate the use of alternative injection strategies, including injection during the recompression period, to accomplish advanced fuel-air mixing strategies.
- Examine the benefits of spark-assisted HCCI operation.
- Computationally evaluate effect of spatial fuel distribution using a Linear Eddy Model in a 1-D direct numerical simulation of HCCI combustion.
- Test Stanford wavelength-modulation tunable diode laser (TDL) sensor and wavelength-ratioing LIF sensor in Sandia HCCI engines.

- Continue development of KIVA/Multi-zone model for simulation of fired HCCI operation. Exercise the model to aid in interpreting and guiding experiments.

Introduction

Major challenges to the implementation of HCCI combustion–including phasing control, operating-range extension, and emissions control–will require advanced, non-homogeneous, fuel-air mixing 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 were applied to obtain information about HCCI in-cylinder processes. In-cylinder spray imaging allowed assessment of spray evolution, penetration, and wall-wetting. LIF imaging produced vapor-fuel-distribution data, and PDF statistics derived from the images quantified the state of mixing just prior to low-temperature heat release. Chemiluminescence imaging provided information about the combustion process that could be related to corresponding mixture-preparation images. Finally, engine-out emission measurements enabled an assessment of correlation between mixture-preparation strategies and combustion/emission performance. Development of new diagnostics for in-cylinder temperature measurements, a critical need for HCCI research, continued at Stanford University, with testing taking place in Sandia's optical engines. Development of a KIVA simulation of the automotive HCCI engine continued at the University of Wisconsin and Lawrence Livermore National Laboratory, with Sandia providing supporting experimental data. Technical exchanges with original equipment manufacturers, national labs, and academia provided feedback and guidance for the research program.

Results

In prior work, a PDF method has been demonstrated that correlates fuel-distribution statistics derived from LIF images with engine-out carbon emissions during low-load, late-injection HCCI operation. The method is potentially useful as a tool for assessing injection strategies, and our industrial partners requested that we enhance the method to include NOx emissions. A look-up table of emissions versus equivalence ratio is required by the PDF method–in the case of carbon-based emissions, the tabular data were generated by homogeneous-charge experiments. The same could not be done for NOx, since, for homogeneous operation, significant NOx emissions are generated only at loads that exceed the limits of our optical engine. Instead, a multi-temperature-zone CHEMKIN model was developed to estimate NOx as a function of equivalence ratio. Figure 1 illustrates the agreement achieved between experimental and simulated pressure traces for homogeneous operation. In addition, estimated carbon-based emissions agreed acceptably well with experimental values, building confidence that the model could provide reasonable estimates of NOx for use in the required look-up table.

The PDF method, as described in earlier reports, uses look-up tables to convert LIF-based PDFs into emission predictions. Figure 2 compares measured CO, CO_2, and NOx emissions with values predicted using the above method. The figure indicates that the predictions capture emission trends well for the injection-timing sweep. The obvious limitations of the technique, e.g., using a single planar measurement to estimate the statistics of fuel distribution for the whole cylinder, explain the modest offset of predictions and

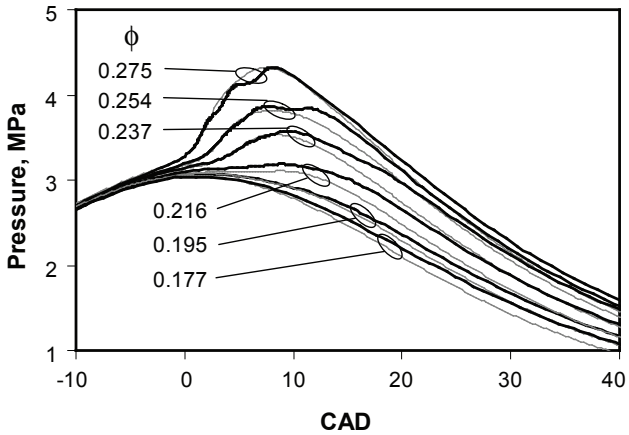


FIGURE 1. CHEMKIN predictions (dark lines) compared to measured pressure data (light lines) for homogeneous HCCI operation over a range of equivalence ratios. Fuel = PRF50, intake pressure = 120 kPa, intake temperature = 120°C, speed = 1200 rpm.

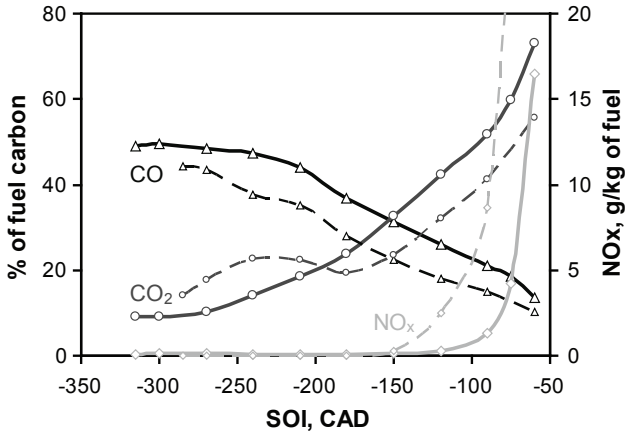


FIGURE 2. Emission predictions (dashed lines) from LIF-based PDF statistics compared to low-load HCCI measurements (solid lines) for CO, CO_2, and NOx. Data are plotted as a function of start-of-injection timing. Swirl injector; global equivalence ratio = 0.2; other conditions as in Fig. 1.

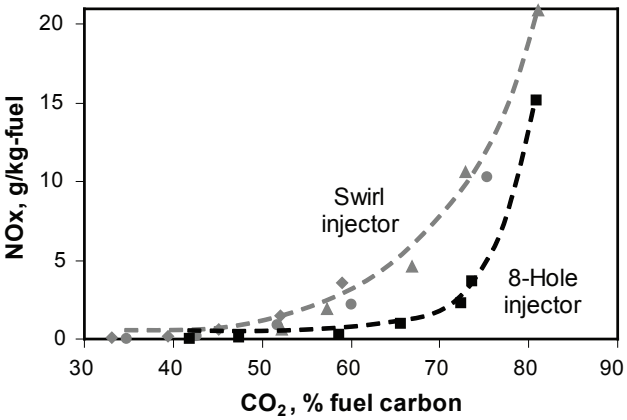


FIGURE 3. NOx-CO_2 trade-off plot for swirl and 8-hole injectors. Different shaped symbols for the swirl injector represent different injection strategies mentioned in the text. Dashed lines are visual aids only. Conditions as in Fig. 2.

measurements. But the correct trends produced by the method suggest that it can be used to assess and guide mixture-preparation strategies for low-load, stratified operation.

As mirrored in the trends of Figure 2, retarding injection timing dramatically improves combustion efficiency (CO_2 conversion) at light loads, but eventually leads to exponential increase of NOx emissions. These conflicting trends are referred to as the NOx-CO_2 trade-off. Experiments were conducted using a range of charge-preparation strategies to examine the trade-off. The upper curve in Figure 3 plots NOx versus CO_2 emissions for a hollow-cone swirl injector. Several strategies using this injector are represented, including enhanced intake charge motion and split injections, yet it is clear that all data fall on the same trade-off curve. In contrast, tests of a newer, 8-hole injector demonstrated superior performance. The lower curve in Figure 3 displays emission measurements for this injector, and its position below and to the right of the swirl-injector curve indicates higher CO_2 conversion and lower NOx emissions compared to the swirl injector. This is a potentially important result for the optimization of late-injection HCCI strategies.

In an attempt to reveal reasons for this improved performance, we applied multiple diagnostics to compare engine operation for the two injectors. In-cylinder spray imaging documented substantial differences in spray patterns. At the conditions of these late-injection experiments, the swirl spray collapses axially, leading to minimal radial penetration and large axial penetration, with substantial fuel deposited on the piston top. These fuel films caused brief pool fires observed using high-speed video—this liquid burning likely contributes undesirable emissions in the case of the swirl injector. The 8-hole sprays, in contrast, penetrated axially to fill more of the cylinder volume with no significant fuel impingement on the piston top.

LIF imaging was used to compare fuel distributions for the two injectors. Based on PDF statistics of the LIF images, fuel distributions for comparable points were surprisingly similar, providing no explanation for the difference in NOx performance. However, it is important to note that PDF statistics contain no spatial information, and for the swirl and 8-hole injectors, a significant difference in spatial fuel distribution was evident from visual examination of the LIF images. This difference was quantified by defining a spatial-mixing statistic; this metric indicated a 50% increase in the number of fuel packets spread through the cylinder for the 8-hole injector. Further work will investigate the importance of this spatial statistic of mixing on emissions performance.

A final fuel-injection parameter investigated by request of industry was fuel-supply pressure. Combustion and emission performance of the 8-hole injector was measured for fuel pressures of 50, 100, and 150 bar over a range of injection timings and global equivalence ratios. Results in Figure 4 show that the injection-timing and fuel-pressure data all collapse on the same curves, indicating that decreasing fuel pressure has the same effect on fuel mixing as retarding injection timing, i.e., both increase stratification. LIF-based statistics of fuel distribution led to the same conclusion. NOx-CO_2 trade-off data collected and presented in Figure 5 suggest there is a small emissions advantage to be gained at a fuel pressure of 150 bar.

Two projects conducted by Ron Hanson's group at Stanford University in collaboration with Sandia target the development of in-cylinder temperature diagnostics for HCCI engines. The first project involves imaging of temperature variations prior to heat release, using a

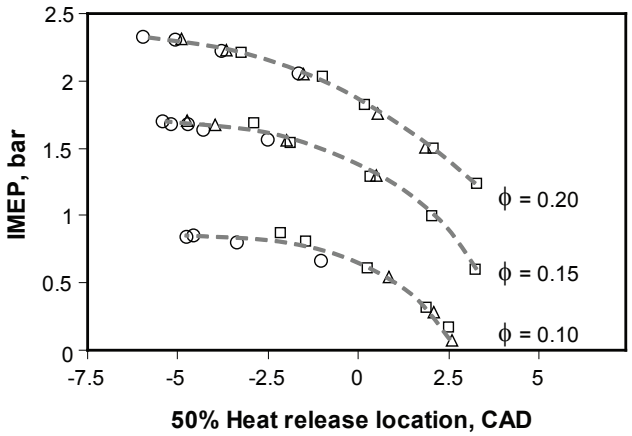


FIGURE 4. Combustion performance of the 8-hole injector for a range of fuel pressures, global equivalence ratios, and start-of-injection timing. Dashed lines are visual aids only. Fuel-pressure symbols: circles = 50 bar; triangles = 100 bar; squares = 150 bar. Other conditions as in Fig. 1.

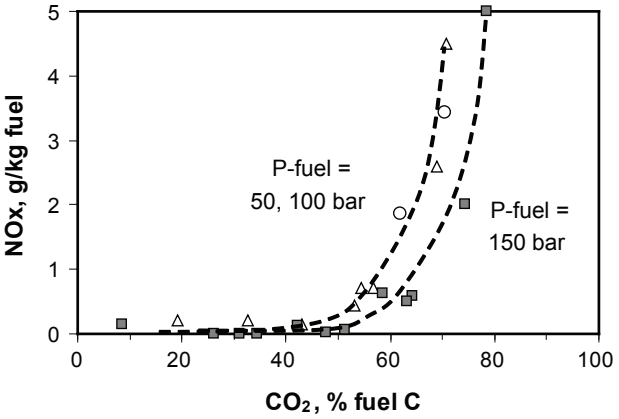


FIGURE 5. NOx-CO_2 trade-off plot for 8-hole injector operating at different fuel pressures. Dashed lines are visual aids only. Symbols as in Fig. 4, with 150-bar symbols filled for visibility.

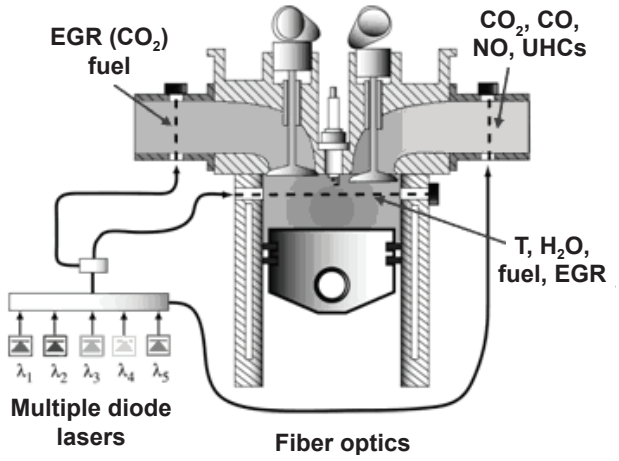


FIGURE 6. Wavelength-multiplexed, TDL sensing for internal combustion engine applications.

PLIF diagnostic with toluene as a tracer. Photophysics experiments at Stanford have shown that toluene's fluorescence signal after Nd:YAG-excitation at 266 nm is highly sensitive to temperature, making it suitable for resolving temperature variations of 10-20 K. To take advantage of this temperature sensitivity, an excitation light sheet whose intensity is spatially uniform and reproducible from pulse-to-pulse is required. Thus, recent work has focused on creating a more uniform, repeatable laser intensity distribution and monitoring the sheet uniformity for image corrections. This research has taken two directions: evaluation of excitation from excimer lasers at 248 nm and 308 nm, and use of specialized optical trains to provide uniform laser light intensity, e.g., homogenizers and remappers.

The second Stanford project comprises tunable-diode-laser absorption measurements of in-cylinder crank-angle-resolved gas temperature and water vapor concentration. A wavelength-multiplexed TDL sensor was designed at Stanford and then used for the first-ever cross-cylinder measurements of water-vapor absorption in the Sandia optical HCCI engines. Light outputs from three diode lasers were combined onto a single optical fiber and transmitted across the cylinder, collected, dispersed, and detected with crank angle resolution. Two of these lasers were tuned for absorption by water vapor transitions and the third corrected for variations in transmitted intensity due to beam steering and light scattering. A spectroscopic line selection process was used to select the most appropriate pair of water absorption transitions for thermometry during the compression portion of the engine cycle. During the demonstration, the spectroscopic design and optical engineering of the sensor were shown to significantly reduce noise from beam-steering, engine vibration, and polarization-related interference. The flexibility of the wavelength-multiplexed architecture allows the straightforward addition of wavelengths to potentially measure other important engine parameters as illustrated in Figure 6.

More recent work at Stanford is focused on an improved sensor that includes additional absorption transitions to enable more precise temperature measurements over a wider range of temperature and pressure, and to provide a measure of the temperature non-uniformity along the laser line-of-sight. Specifically, this new sensor will use a wavelength-modulation strategy that provides a separate monitor of the transmitted laser light from each of the multiplexed lasers. This signal normalization will suppress the intensity noise of the transmitted laser beams that was the dominant source of errors in the earlier engine measurements. A prototype of this new sensor has been

designed and built. Initial laboratory tests have begun at Stanford and the results show a remarkable ability to suppress temporal variations in the laser transmission.

Conclusions

- A correlation has been demonstrated between PDF fuel-distribution statistics and corresponding engine-out emissions for low-load, stratified HCCI operation.
- The PDF method includes only non-spatial details of fuel distribution – an additional, spatial-mixing statistic may help explain differences observed in combustion and emissions performance.
- New GDI-type injector designs such as multi-hole injectors may improve the NOx-CO_2 trade-off encountered when adopting late-injection strategies. Multiple optical diagnostics can provide evidence necessary to understand differences in injector performance.
- The Stanford collaboration provided the first demonstrations of a promising new laser-based sensor for crank-angle resolved measurements of in-cylinder temperature capable of quantifying cycle-to-cycle variations.

FY 2006 Publications/Presentations

1. De Zilwa, S. and Steeper, R. R., "Predicting NOx Emissions from HCCI Engines Using LIF Imaging," SAE Technical Paper 2006-01-0025, 2006.

2. White, C. M., Steeper, R. R. and Lutz, A., "The Hydrogen-Fueled Internal Combustion Engine: A Technical Review," *International Journal of Hydrogen Energy* **31**(10):1292-1305, 2006.

3. Mattison, D. W., Jeffries, J. B., Hanson, R. K., Steeper, R. R., De Zilwa, S., Dec, J. E., Sjoberg, M. and Hwang, W., "In-Cylinder Gas Temperature and Water Concentration Measurements in HCCI Engines Using a Multiplexed-Wavelength Diode-Laser System: Sensor Development and Initial Demonstration," *Proc. Combust. Inst.*, **31**, 2007, in press.

4. Steeper, R. R. and De Zilwa, S., "Improving the NOx-CO_2 Tradeoff of an HCCI Engine using a Multi-Hole Injector," submitted to 2007 SAE World Congress, 2006.

5. De Zilwa, S., "Acquisition of Corresponding Fuel Distribution and Emission Measurements in HCCI Engines," SAE Powertrain and Fluid Systems Conference, San Antonio, TX, October 25, 2005.

6. Steeper, R. R., "Predicting Emissions from HCCI Engines using LIF Imaging," SAE Powertrain and Fluid Systems Conference, San Antonio, TX, October 25, 2005.

7. Steeper, R. R., "Sandia Automotive HCCI Engine Project," DOE AEC Working Group Meeting, Sandia, Feb. 7, 2006.

8. De Zilwa, S., "Predicting NOx Emissions from HCCI Engines using LIF Imaging," 2006 SAE World Congress, Detroit, April 6, 2006.

9. Steeper, R. R., "Automotive HCCI Combustion Research," DOE Advanced Combustion Engine Program Review," Argonne National Laboratory, May 16, 2006.

10. Steeper, R. R., "HCCI Tests of a Multi-hole GDI-type Injector," DOE AEC Working Group Meeting, USCAR, Detroit, June 27, 2006.

11. Hanson, R. K., "In-Cylinder Gas Temperature and Water Concentration Measurements in HCCI Engines Using a Multiplexed-Wavelength Diode-Laser System: Sensor Development and Initial Demonstration," 31st International Combustion Symposium, Heidelberg, Germany, August 6, 2006.

II.A.11 Spark-Assisted HCCI Combustion

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Objectives

- Investigate the potential of nonlinear control methods to stabilize the transition between spark ignition (SI) and homogeneous charge compression ignition (HCCI) combustion modes as well as to stabilize intermediate hybrid combustion modes.
- Further understanding of physics of combustion at intermediate conditions and during SI-HCCI transitions.

Accomplishments

- Confirmed that instabilities observed during transition from SI to HCCI are deterministic and predictable.
- Determined nonlinear pattern recognition and feedback control strategies are likely to be useful for improving HCCI utilization.
- Identified hybrid combustion modes which may have the potential for achieving HCCI-like emissions and efficiency with reduced pressure rise rate, and expanding the practical engine load range.

Future Directions

- Employ combustion and engine models to explain the governing processes that occur during the SI-HCCI transition (i.e., physics, chemistry).
- Develop low-order engine and systems models and strategies that can be used for real-time analysis of stability, prediction, and control.
- Improve industry interaction through establishment of a Cooperative Research and Development Agreement (CRADA) partnership.

Introduction

An improvement in the fuel efficiency of gasoline engines is necessary to realize a significant reduction in U.S. energy usage. Homogeneous charge compression ignition (HCCI) in internal combustion engines is of considerable interest because of the potential reductions in flame temperature and nitrogen oxide 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 expanding the operational range and the ability to switch between HCCI and traditional propagating flame (e.g., spark ignition) 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.

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. Data as well as new information derived from modeling is also being shared with Lawrence Livermore National Laboratory.

SI-HCCI operation was investigated on a 0.5-L single-cylinder AVL research engine with an 11.34:1 compression ratio. The engine has two intake valves and one exhaust valve and is equipped with a full-authority hydraulic variable valve actuation (VVA) system. Only a single intake valve was used in this study to promote swirl and mixing. The transition from SI to HCCI is achieved in this engine with high

levels of exhaust gas retained in the cylinder through manipulation of the intake and exhaust valve events. All experiments were performed at stoichiometric fueling conditions and a range of speeds and loads.

Results

In our research, the transition, and hence HCCI, 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 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. Four distinct modes of operation were observed and are labeled in Figure 1. This report will focus on observations from the transition region.

Recall the primary objective of this activity is to investigate the potential of nonlinear control methods to stabilize the transition between SI and HCCI combustion modes as well as to stabilize intermediate hybrid combustion modes. Achieving this objective requires an improved understanding of the deterministic nature (i.e., cycle-to-cycle interactions) of the combustion processes during the transition from SI to HCCI combustion modes. Due to the concise nature of this report, we are not able to discuss all of the research performed during this activity in FY 2006 but instead will focus on an example which highlights some of the more important observations. Please see the publications/presentations list for more information.

The deterministic nature of the behavior within the transition region is evidenced by the recurrence of certain patterns or trajectories in the heat-release data such as those shown in Figures 2, 3, and 4. The repeating sequences in Figure 2 are superimposed combustion event sequences observed at different times for the same operating condition. Note that only a few examples of the repeating sequences are shown for illustration. The frequency of occurrence for these patterns was typically quite high within the 2,800-cycle data sets. In Figure 2(a) we observe a distinctive 3-state pattern or trajectory, which shows an increase in combustion energy for three consecutive events followed by a low-energy or partial misfire event. An example of this 3-state pattern is shown in relation to the first return map in Figure 3 along with the heat-release profile for each of the three characteristic cycles in the sequence. Cycle 1 appears to represent incomplete SI combustion. The residuals from this cycle produce in-cylinder conditions on cycle 2 which are again not conducive to SI combustion but with further compression now support HCCI combustion. However, the total heat release for cycle 2 is below average suggesting that combustion is incomplete.

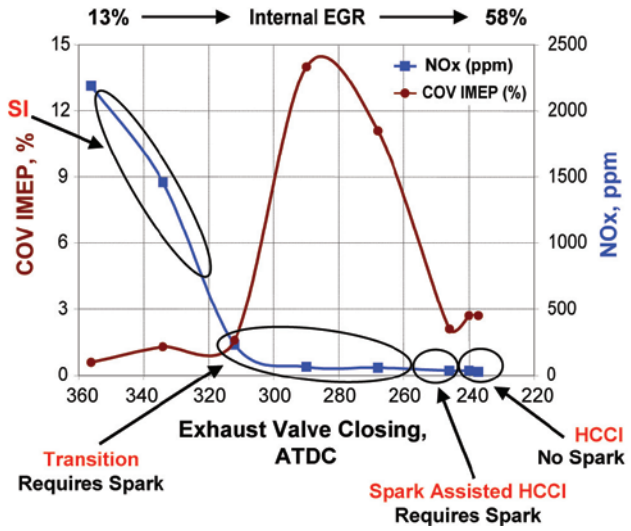


FIGURE 1. Stability and NOx emissions during the transition from SI to HCCI combustion using internal EGR. Engine conditions were 1,600 rpm, 3.4 BMEP.

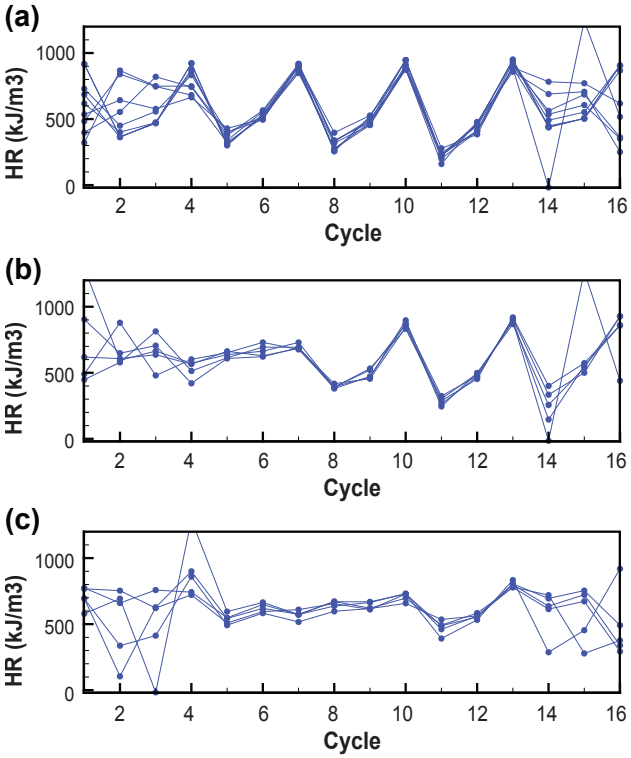


FIGURE 2. Repeating patterns observed for an intermediate EGR level corresponding to the transition region. Engine conditions were 1,600 rpm, 3.4 bar BMEP.

On cycle 3, conditions finally appear conducive to proper SI combustion but as the flame front progresses across the cylinder compressing the unburned reactants, we suspect that the high concentration of unburned fuel and/or intermediate species from the previous two incomplete cycles leads to auto-ignition of the remaining unburned zone. While the resulting intense combustion event no doubt produces a high-temperature residual, we suspect that all the intermediate species needed for HCCI (or SI) combustion are consumed leading to another incomplete combustion and a repeat of the 3-step pattern.

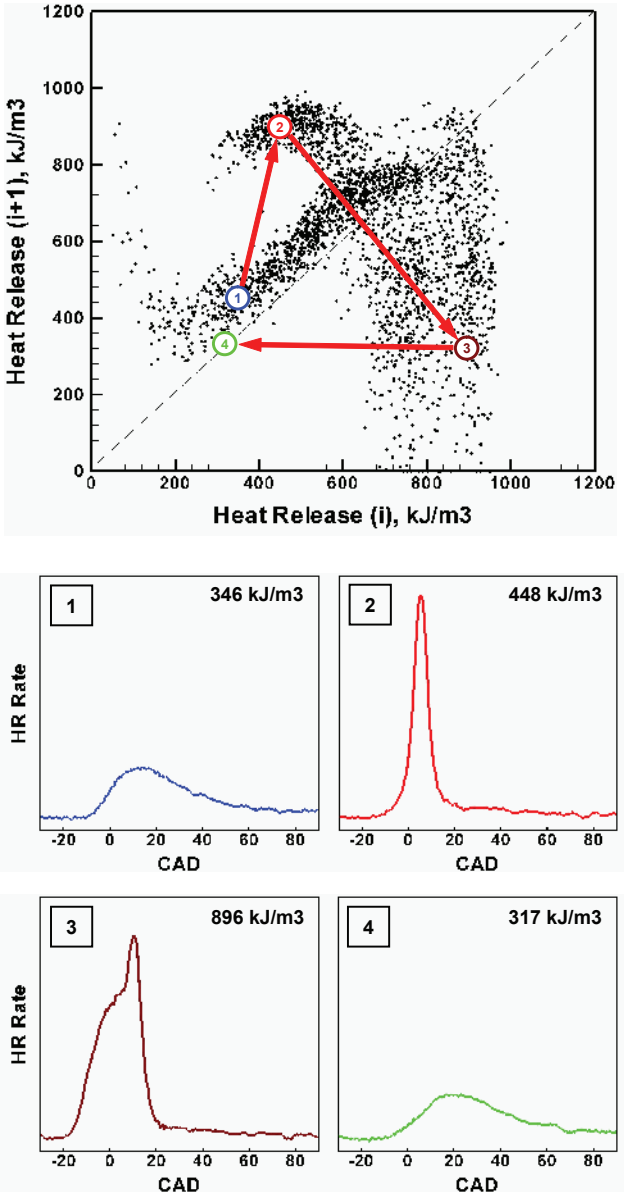


FIGURE 3. Example of the trajectory of the 3-step heat release pattern shown and corresponding heat release rate profiles. Engine conditions were 1,600 rpm, 3.4 BMEP.

Figure 2(b) illustrates a precursor to the 3-state pattern in which the engine oscillates near a single

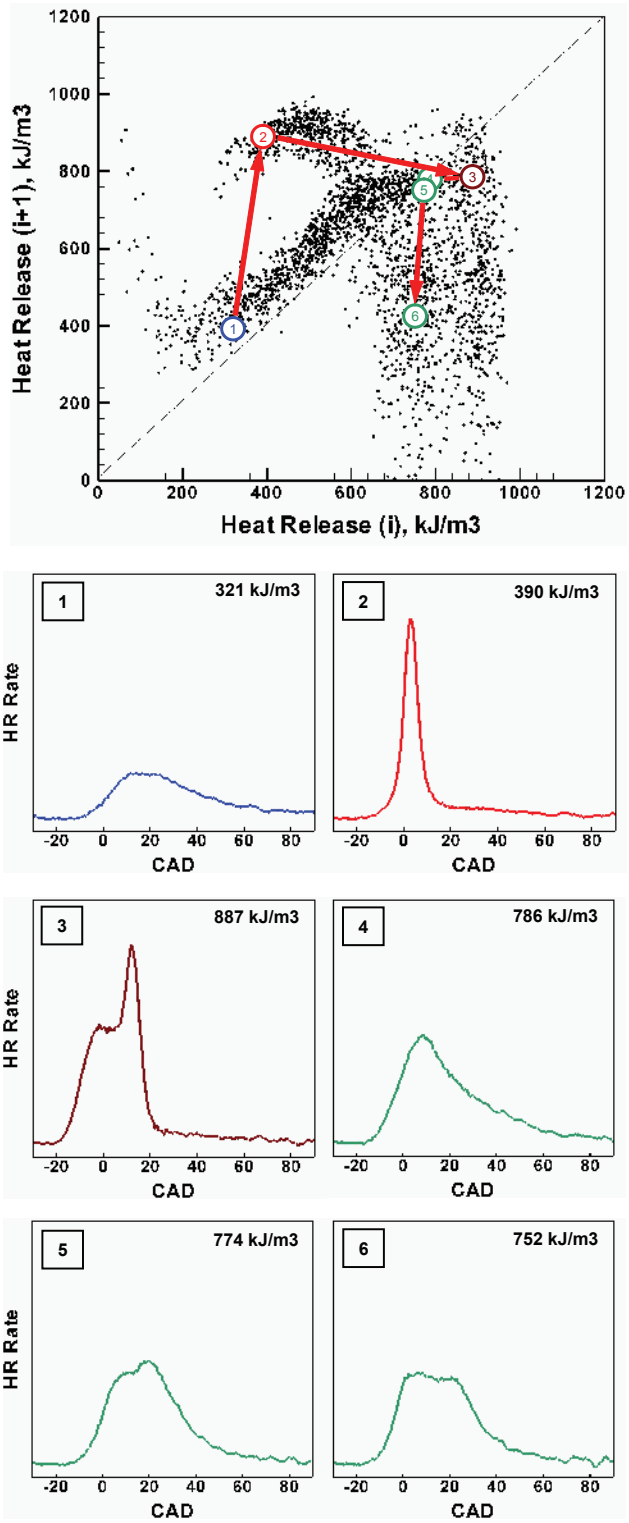


FIGURE 4. Example of temporary entrainment around an unstable fixed point. The unstable fixed point corresponds to a hybrid combustion mode as illustrated in the heat release profiles. Engine conditions were 1,600 rpm, 3.4 BMEP.

value before diverging into ever increasing oscillations. Figure 4 shows an example of this behavior in relation to the first return map. In this example, the engine combustion exits the 3-step pattern and becomes briefly entrained in the vicinity of an unstable period-1 fixed point (cycles 4, 5 and 6) before diverging back to the 3-step pattern (following cycle 6). We hypothesize that some slight difference in the temperature and/or composition of the residual products following cycle 3 of this example provides just the right conditions for cycle 4 to be more complete and self-sustaining than in the previous example. A more stable example of this behavior is illustrated in Figure 2(c) where the engine combustion oscillates near a single heat release value for approximately 10 cycles before diverging and entering the 3-state pattern. This entrainment of the combustion behavior about the unstable fixed point suggests the presence of stable manifolds which could be used to control engine behavior about the fixed point.

The hybrid (or mixed-mode) combustion mode which corresponds to the stable manifold is a combination of SI and HCCI combustion within a single cycle. This mode is thought to have the emissions benefits of HCCI without the penalty of higher pressure rise rates, providing an alternate operating mode when pure HCCI operation is not possible, such as at high load or when in-cylinder charge preparation is not sufficient to produce HCCI combustion. The hybrid combustion mode also has dynamic characteristics which appear to be conducive to control. Specifically, the existence of these stable manifolds allows for the potential control of the cycle-to-cycle combustion trajectory, in effect rate shaping the combustion process. We are currently developing low-order engine models to capture the phenomena observed in our experiments and for use in the development and evaluation of control methodologies.

Conclusions

This activity has provided new information on hybrid combustion modes which have the potential for improving the transition from SI to HCCI combustion modes and achieving HCCI-like benefits when pure HCCI modes are not possible or practical. Hybrid modes have reduced pressure rise rates as compared to pure HCCI modes which may allow for higher load operation and an expansion of the practical load range. Another potential use is for a system with limited VVA and charge preparation capability for achieving pure HCCI. We are currently constructing low-order combustion models to simulate the experimental observations for developing and evaluating new control concepts as well as to provide new insight into the physics and chemistry of the transition dynamics.

FY 2006 Publications/Presentations

1. R. M. Wagner, K. D. Edwards, C. S. Daw, J. B. Green, and B. G. Bunting, "On the Nature of Cyclic Dispersion in Spark Assisted HCCI Combustion", SAE 2006-01-0418 (Detroit, MI, USA; April 2006).

2. K. D. Edwards, C. S. Daw, R. M. Wagner, "Cyclic Variability During the Transition Between Spark-ignited Combustion and HCCI", Central States Technical Meeting of the Combustion Institute (Cleveland, Ohio; May 2006).

3. C. S. Daw, R. M. Wagner, K. D. Edwards, J. B. Green, "Understanding the transition between conventional spark-ignited combustion and HCCI in a gasoline engine", 31st International Symposium on Combustion (Heidelberg, Germany; August 2006).

4. C. S. Daw, "Experimental observations of bifurcations in the transition from conventional to HCCI combustion in a spark ignited engine", Dynamics Days 2006 (Bethesda, MD, USA; January 2006).

5. R. M. Wagner, "Diagnosing Combustion Instabilities Associated with HCCI Engine Operation", Engineering the Automotive Future at the University of Alabama (Tuscaloosa, AL; January 2006).

6. R. M. Wagner, "Understanding the transition between conventional spark-ignited combustion and HCCI in a gasoline engine", 2006 AEC Working Group Meeting at Sandia National Laboratories (Livermore, CA; February 2006).

7. K. D. Edwards, "Understanding and controlling the transition between conventional spark-ignited combustion and HCCI", 2006 DOE National Laboratory ACE Merit Review & Peer Evaluation at Argonne National Laboratory (Argonne, IL; May 2006).

8. R. M. Wagner, "Hybrid SI-HCCI Combustion Modes for Low Emissions in Stationary Power Applications", 3rd Annual ARES Meeting (Argonne, IL; June 2006).

9. R. M. Wagner, "Identification of hybrid combustion states for improved utilization of 'near-flameless' combustion in engine", poster presentation 31st International Symposium on Combustion (Heidelberg, Germany; August 2006).

10. R. M. Wagner, "Hybrid SI-HCCI combustion modes and the potential for control", 2006 SAE HCCI Symposium (San Ramon, CA; September 2006).

Special Recognitions & Awards/Patents Issued

"A method for diagnosing and controlling combustion instabilities in internal combustion engines operating in or transitioning to homogeneous charge compression ignition modes", IDEAS 05-156, patent pending.

II.A.12 Development of High Efficiency Clean Combustion Engine Designs for Spark-Ignition and Compression-Ignition Internal Combustion Engines

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NETL Project Manager: Carl Maronde

Subcontractor:
Sturman Industries, Woodland Park, CO

Objectives

- Develop and demonstrate prototype gasoline and diesel engine hardware which enables operation of homogeneous charge compression ignition (HCCI) combustion for improved fuel efficiency and emissions performance.
- Understand and reduce the risks and roadblocks associated with this new combustion system by designing and demonstrating hardware solutions.
- Demonstrate enabling system on a 2.0-2.4L L4 gasoline engine in a mid-size car.
- Demonstrate fully flexible system on a 2.0-2.4L L4 gasoline engine in a mid-size car.
- Demonstrate simple variable valve actuation system on a 4.5L DOHC V8 engine in a mid-size sport utility vehicle.
- Demonstrate fully flexible system on a single-cylinder diesel engine.
- Demonstrate fully flexible system on a 4.5L DOHC V8 engine in a mid-size sport utility vehicle.

Accomplishments

Gasoline Systems

- Analysis and bench testing of critical subsystems for the enabling system indicated that subsystem performance (sensors, actuators) was sufficient to meet project goals.
- Completed design, procurement, and build of enabling system engine builds, and successful operation of all subsystem functions was achieved on motored and fired engine builds.
- Development and failure mode analysis of variable valvetrain hardware for the enabling system continued with limited success in achieving desired robustness; this is an area of continued focus.
- Mule vehicle build for enabling system nearly completed.
- Completed architecture selection and design of single valve test fixture for fully-flexible system.
- Completed sensitivity analysis of important contributors to variation of performance of fully-flexible system.

Diesel Systems

- Completed commissioning and initial bench testing of the full variable valve actuation (FVVA) system.
- Developed modification to solve a fuel feeding issue with the FVVA system.
- Installed FVVA system on single-cylinder diesel engine.
- Developed diagnostic for high frequency, high amplitude noise with the FVVA system.
- Completed FVVA system demonstration on single-cylinder diesel engine.
- Installed simple, variable intake cam timing (VCT) system on a 4.5L DOHC V8 engine which is running on an engine dynamometer.
- Completed preliminary evaluation of the VCT system's performance, and its impact on engine emissions during steady-state, engine dynamometer conditions.

Future Directions

- Multi-Cylinder/Vehicle Evaluation of Simple VCT Mechanism
  - Resolve robustness issues with enabling system valvetrain hardware.
  - Demonstrate operation of multi-cylinder hardware.
  - Integrate the VCT controls into the electronic control unit (ECU) for transient testing.
  - Assess potential of simple VCT system to meet Bin 5 emissions requirements without NOx aftertreatment.
  - Assess the efficiency and cost effectiveness of simple VCT system based on vehicle development and testing including a performance and drive quality assessment.

- Single-Cylinder FVVA Development and Assessment
  - Build and test fully-flexible single valve test fixture.
  - Assess the effectiveness and cost of a FVVA system based on single cylinder test results.
  - Assess potential of a FVVA system to meet Bin 5 emissions requirements. without NOx aftertreatment based on single cylinder combustion measurements.
- Multi-Cylinder/Vehicle FVVA Buildup and Testing
  - Complete design, procurement, and build of fully-flexible multi-cylinder hardware.
  - Demonstrate operation of enabling system on a dynamometer and in a vehicle.
  - Demonstrate sufficient combustion mode switching performance using enabling system on bench test and in vehicle.
  - Assess potential of FVVA system to meet Bin 5 emissions requirements without NOx aftertreatment at the dynamometer and vehicle level including a performance and drive quality assessment.

Introduction

The objective of the gasoline portion of this project is to demonstrate operation of gasoline HCCI engine designs using both an "enabling" valvetrain system and a fully-flexible valvetrain system. By executing design and development of hardware systems, the risks and roadblocks associated with gasoline HCCI engines will be better understood, and potential solutions may be identified. Reduction of risks and elimination of roadblocks are key aspects of understanding the cost-effectiveness and production feasibility of gasoline HCCI engine designs.

The objective of the diesel portion of this project is to demonstrate operation of diesel HCCI engines using both a simple and a fully-flexible valvetrain system design. The performance objectives are to improve fuel efficiency for diesel engines while meeting the Tier 2 Bin 5 emission specifications without needing NOx aftertreatment. The efficiency and cost effectiveness of the simple and the fully-flexible variable valve actuation systems will be assessed based on their demonstrated performance.

Approach

The gasoline and diesel portions of this project include feasibility analysis, computer simulation work to guide concept selection and designs, overall engine design, engine component design and fabrication, subsystem bench testing, engine build and development testing, and vehicle build and development testing.

Results

Gasoline Systems

Simulation analysis of subsystems contributing to both the enabling and fully-flexible valvetrain systems was completed. Figure 1 shows an example result from system simulation analysis of the enabling system, including response of engine control signal for valvetrain switching, controlled engine oil pressure, cam phaser, and valve lift events. Based on the simulation analysis, the expected response capabilities of the individual subsystems were judged to be acceptable for the project demonstration purposes.

A photograph of the completed engine build using the "enabling" valvetrain system is shown in Figure 2. Initial testing of the complete system has indicated that all subsystems are functional. Integration of subsystem-to-subsystem functions is ongoing. A particularly challenging area has been a lack of robustness of the prototype switching valvetrain hardware, and considerable effort has gone into failure mode identification, development of corrective actions, and implementation of corrective actions. Currently the

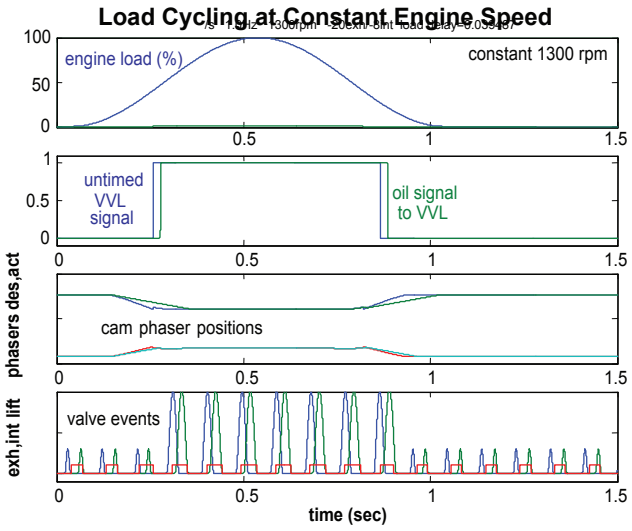


FIGURE 1. System Simulation Analysis of Response of Enabling Valvetrain System to a Load Change at Constant Engine Speed

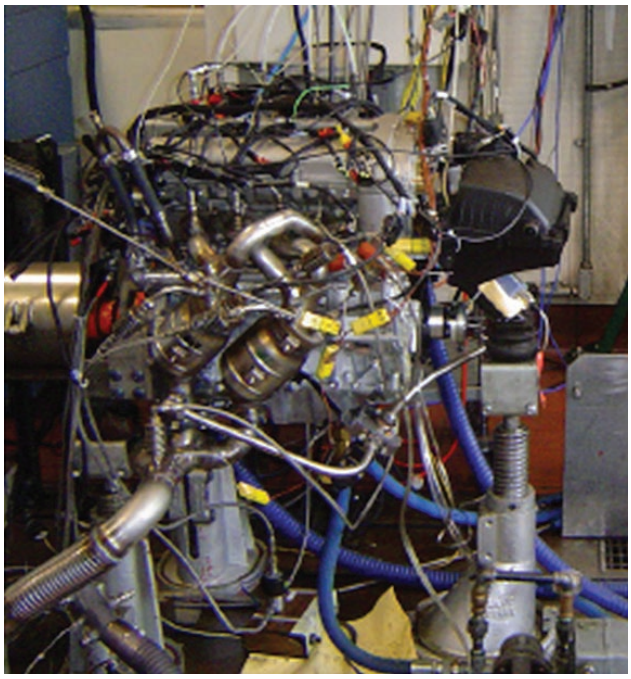


FIGURE 2. Engine with Enabling Valvetrain System Installed on Dynamometer

corrective actions that have been implemented have resulted in component performance that is sufficient for engine development to continue. Further corrective actions are being implemented, however.

A mule vehicle build has been nearly completed. The purpose of the mule build is to identify and correct vehicle mechanical and controls system issues prior to installation of the engine into the demonstration vehicle (which is a different vehicle). First fire of the mule vehicle has occurred, but currently all subsystem functions are not active.

The architecture selection and initial single valve fixture design for the fully-flexible valvetrain system has been completed. In support of the architecture selection and single valve fixture design, a significant amount of system simulation analysis was performed. Simulation analysis included actuator and component sizing studies, sensitivity analyses of parameters expected to contribute to cycle-to-cycle and cylinder-to-cylinder variation, and studies of valve motion control performance. With release of the single valve fixture designs to fabrication, design efforts have recently begun on the multi-cylinder valvetrain layout and hydraulic supply system layout.

Diesel Systems

Engine level development of the FVVA system was performed on a single-cylinder diesel engine. Hardware for the FVVA system was tested by the supplier and delivered to GM. The system was installed on a single-cylinder diesel engine for bench testing as shown in Figure 3. The development process has needed to address a variety of typical debug and diagnostic issues. For example, a system modification was required to resolve a fuel feeding problem. In another case, a diagnostic was developed for an issue with high frequency, high amplitude noise. These development efforts have culminated in a working demonstration of the FVVA system.

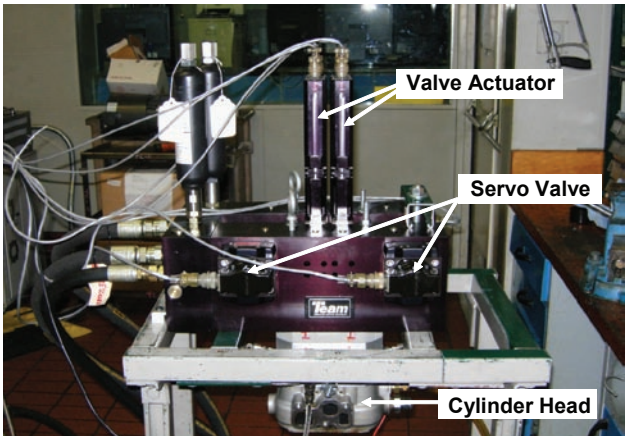


FIGURE 3. Bench Setup for Single-Cylinder Diesel Engine with FVVA System

Development efforts at the vehicle level have focused on a simple VCT valve actuation system. The initially selected simple VCT system was installed on a dynamometer-mounted 4.5L DOHC V8 diesel engine. A baseline calibration without employing the VCT system was developed. The running engine accumulated over 450 hours in the test cell without any major mechanical failures. This allowed a preliminary evaluation of the VCT system's performance and engine emissions during steady-state conditions. Several issues have been identified based on these test results and are in the process of being addressed. For example, the effects of inadequate high pressure stage turbo-charging resulted in lower than expected trapped mass and EGR rate. The turbocharger was returned to the supplier for analysis, and the cause is still being investigated. The engine is being disassembled at a GM facility for inspection and analysis.

Conclusion

Based on the progress made on the "enabling" design for the gasoline HCCI engine, a successful demonstration of the flexible valve actuation mechanisms on the diesel engine is expected. For the diesel HCCI engine, significant progress has been made on both the simple and the fully-flexible designs. Multi-cylinder testing of the VCT valve actuation system is underway and initial testing of the single-cylinder engine

equipped with the fully flexible valve actuation system has begun. This has allowed issues to be identified and evaluations of preliminary performance to be made. Both systems should continue to be developed, so that their potential performance, efficiency, and cost effectiveness can be properly assessed. The major focus of the upcoming work will be to understand the emissions benefits that are achievable for variable valve actuation mechanisms on the diesel engine.

FY 2006 Publications/Presentations

1. Patton, K., and Marriott, C., "Engine Design Concepts to Enable Advanced Gasoline Combustion Systems," presented at 2006 Society of Automotive Engineers Government/ Industry Meeting panel discussion on Bringing Efficient, Clean Engine Technology to the US Vehicle Market – Part I, May 9, 2006, Washington, D.C.

II.A.13 KIVA-4 Development

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Objectives

- Validate parallelization of KIVA-4 in different geometries.
- Publish a description of KIVA-4's numerical algorithms and results in a peer-reviewed journal.
- Test KIVA-4 with complex 3-D engines.
- Collaborate in the development of adaptive mesh refinement capability in KIVA-4.

Accomplishments

- The parallelization of KIVA-4 was tested in moving piston geometries and 3-D engines with valves. A parallel run with four processors reduced the computational time by 3.2 using a moving square bowl grid. A parallel run with two processors reduced the computational time by 1.6 using a 2-valve engine.
- KIVA-4 was tested against several analytical solutions. These results along with KIVA-4's numerical algorithms have been published in the Journal of Computational Physics.
- Currently KIVA-4 has been tested in six different 3-D engine geometries. An algorithm for improving the meshing in ports has also been developed.
- A preliminary adaptive mesh capability was added to KIVA-4.
- The University of Wisconsin tested the algebraic stress models against the experimental data of Paul Miles from Sandia National Laboratory with the help of LANL's initial implementation.

Future Directions

- Integrate advanced combustion models into KIVA-4.
- Implement grid converters to convert grid formats (ICEM, Cubit, TrueGrid) to KIVA-4 format, so established grid-generation software can be used to create KIVA-4 grids.
- Develop a collocated version of KIVA-4 where all variables (pressure, temperature, density and velocity) are located at the cell-center. This implementation will improve the accuracy of KIVA-4's numerics in unstructured grids.

Introduction

The KIVA codes were designed to simulate internal combustion engines. Our development of KIVA-4 has retained all the features of previous versions of KIVA and in addition allowed engine simulations to be performed on unstructured grids. Unstructured grids are a larger class of grids that are generally easier to generate than structured grids. Unstructured meshes can use a variety of element types (hexahedra, prisms, tetrahedra and pyramids) to fill up the interior of a computational domain. We have begun to develop converters to convert established grid generator formats to a KIVA-4 format. This will enable grid generation software to produce structured and unstructured grids efficiently for KIVA-4 simulations.

Recently we also developed a parallel version of KIVA-4 which allows computations to be performed on multiple processors simultaneously. Parallel simulations will allow engine simulations to be completed many times faster. The flexibility of using grid generators and the capability of computing in parallel are attractive features which will enhance KIVA-4 and make it more attractive as an engine simulation tool, enabling users to design more fuel efficient engines which generate fewer emissions. KIVA-4 is an open source code and thus it enables universities and users to interact directly with the code and conduct fundamental research and submodel development.

Approach

We have focused our efforts on continued development of KIVA-4. These efforts include expanding the class of geometries the parallel version of KIVA-4 can accommodate.

We also devoted time to describing KIVA-4's numerical algorithms and performing tests against analytical solutions with structured and unstructured grids in a paper which has appeared in the Journal of Computational Physics.

Realizing that KIVA-4 will be exercised primarily in 3-D engine geometries, we have expanded the suite of 3-D geometries simulated by KIVA-4. We have

converted engine meshes from KIVA-3V and tested them with KIVA-4.

Results

The parallel version of KIVA-4 was extended to moving boundaries and spray. We have enabled the snappers in KIVA-4 to work in the parallel environment. This has allowed parallel KIVA-4 to simulate moving geometries efficiently.

The KIVA snappers allow layers of cells to be added or deleted as the piston moves up or down. To accommodate the snappers, all relevant information is gathered to one processor where the snapping procedure is performed. Information is then scattered back to all processors.

We also have enabled KIVA-4 to accommodate spray in its parallel computations. Our strategy is to find the cell the spray particle resides in and use the processor that owns that cell to perform the computations relevant to the spray particle.

We ran parallel simulations with spray with a square bowl grid and a vertical 2-valve engine. A parallel run with 4 processors reduced the computational time by 3.2 using the square bowl grid. A parallel run with two processors reduced the computational time by 1.6 using the 2-valve engine. We also have tested a parallel implementation with periodic boundaries.

KIVA-4 was tested with additional 3-D engines. Figures 1 and 2 show 180° engine meshes that were run with KIVA-4. The mesh in Figure 2 was provided by Jyh-Yuan Chen of the University of California at Berkeley. Figures 3 and 4 show a 4-valve engine that has been simulated with KIVA-4. Figure 4 shows how the meshing around the ports has been improved compared to the original mesh in Figure 3. Figure 5 shows a 3-valve engine mesh run with KIVA-4. An effort has

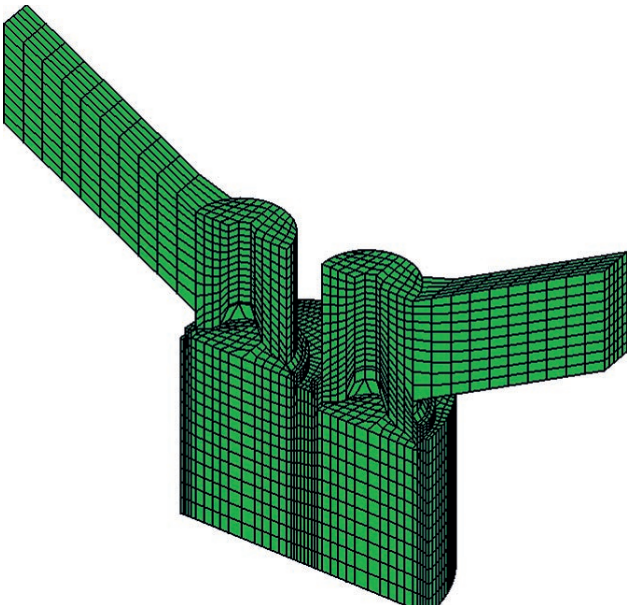


FIGURE 2. A 180° Mesh Simulated with KIVA-4 (provided by Jyh-Yuan Chen of the University of California at Berkeley)

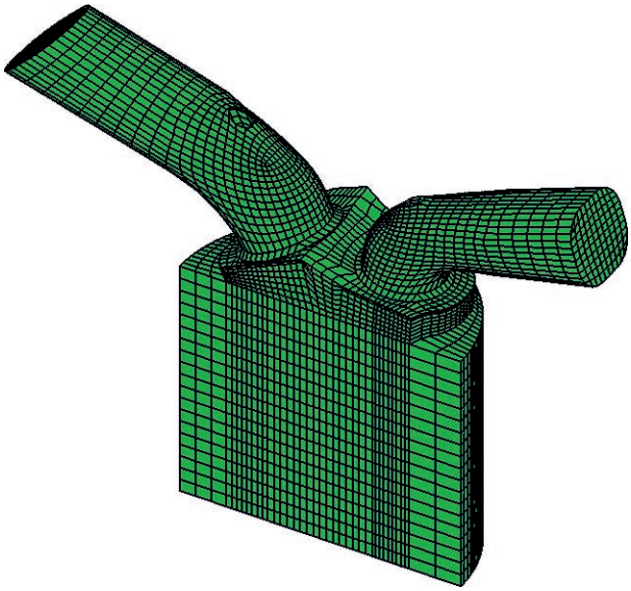


FIGURE 1. A 180° Mesh Simulated with KIVA-4

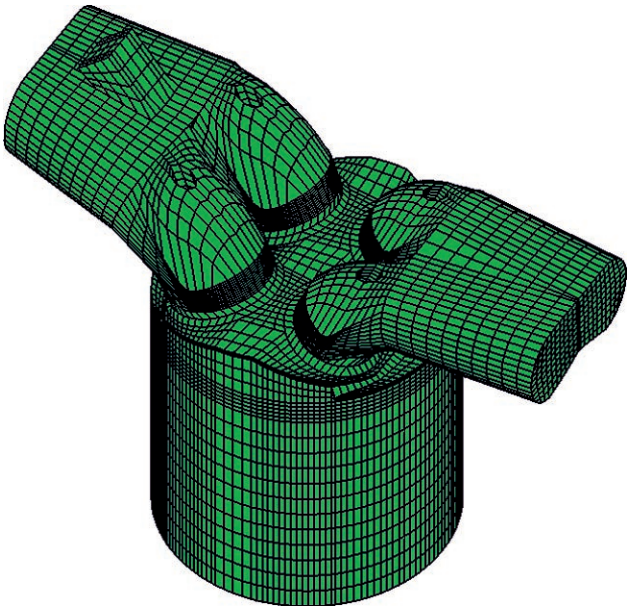


FIGURE 3. A 4-Valve Mesh Simulated with KIVA-4 with Poor Mesh Quality Around Ports

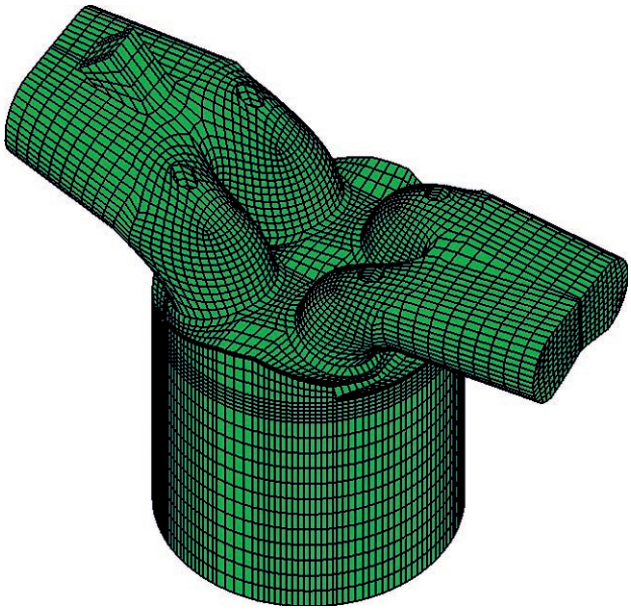


FIGURE 4. The same 4-valve mesh shown in Figure 3 with improved mesh quality around the ports which has been simulated with KIVA-4.

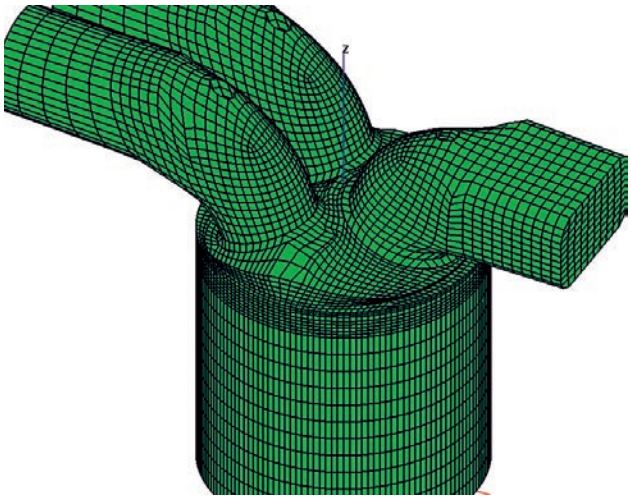


FIGURE 5. A 3-Valve Mesh Simulated with KIVA-4.

also been made to improve the rezoning process which manages the movement of grid vertices.

During the summer of 2006, a graduate student from Iowa State, Qingluan Xue, visited Los Alamos National Laboratory with funding from Ford Motor Company. During the summer, adaptive mesh refinement capability was added to KIVA-4. Adaptive mesh refinement allows one to subdivide a cell into smaller cells without subdividing any neighboring cells.

During the spring of 2006, Mike Bergin, a graduate student of the University of Wisconsin tested new algebraic stress models with KIVA-3V against experimental data from Sandia National Laboratory. The algebraic stress model was initially implemented at LANL.

Conclusions

KIVA-4 has been parallelized to run with both moving and non-moving meshes and spray. The numerical algorithms in KIVA-4 and numerical results have appeared in the Journal of Computational Physics. The test suite of problems KIVA-4 uses for validation has been expanded to additional 3-D engine geometries. Collaborations with Ford Motor Company, Iowa State and the University of Wisconsin continue.

FY 2006 Publications

1. D.J. Torres and M.F. Trujillo, KIVA-4: An Unstructured ALE Code for Compressible Gas Flow with Sprays, Journal of Computational Physics, 219 (2006), 943-975.

2. M.F. Trujillo and D.J. Torres, Droplet Vaporization in a Supercritical Environment, ILASS Americas 19th Annual Conference on Liquid Atomization and Spray Systems, May 2006.

3. D. J. Torres, Parallel KIVA-4, International Multidimensional Engine Modeling User's Group Meeting Proceedings at SAE Congress, April 2006.

FY 2006 Presentations

1. D. J. Torres, "KIVA-4 Development", Advanced Engine Combustion Working Group Meeting, Detroit, June 2006.

2. D. J. Torres, "Parallel KIVA-4", DOE National Laboratory Advanced Combustion Engine R&D, Merit Review of Advanced Combustion, Emissions Control and Fuels Research, Argonne, IL, May 2006.

3. D.J. Torres, "Parallel KIVA-4", International Multidimensional Engine Modeling User's Group Meeting at SAE Congress, Detroit, April 2006.

4. D. J. Torres, "Parallel KIVA-4", Advanced Engine Combustion Working Group Meeting, Livermore, CA, February 2006.

II.A.14 Chemical Kinetic Modeling of Combustion of Automotive Fuels

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Objectives

- Develop detailed chemical kinetic reaction models for components of fuels, including olefins and cycloalkanes used in diesel, spark-ignition and homogeneous charge compression ignition (HCCI) engines.
- Develop surrogate mixtures of hydrocarbon components to represent real fuels and lead to efficient reduced combustion models.
- Characterize the role of fuel composition on production of emissions from practical automotive engines.

Accomplishments

- Completed models for chemical kinetics of combustion of three major fuel components, methyl cyclohexane, and di-isobutylene, and assembled model for cyclohexane.
- Continued development of surrogate mixtures to describe HCCI ignition.

Future Directions

- Extend model capabilities to additional classes of fuel components, including biodiesel components and larger hydrocarbon components.
- Validate model for chemical kinetics of combustion for cyclohexane. Use new reaction rate rules for cyclohexane to improve methyl cyclohexane model.
- Continue development of increasingly complex surrogate fuel mixtures.
- Investigate the effect of fuel molecular structure on sooting under diesel engine conditions.
- Increase collaborations with programs outside Lawrence Livermore National Laboratory (LLNL) dealing with automotive fuel issues.

Introduction

Automotive hydrocarbon fuels consist of complex mixtures of hundreds or even thousands of different components. These components can be grouped into a number of structurally distinct classes, consisting of n-paraffins, branched paraffins, cyclic and branched cyclic paraffins, olefins, oxygenates, and aromatics. The fractional amounts of these mixtures are quite different in gasoline, diesel fuel and oil-sand derived fuels, which contributes to the very different combustion characteristics of each of these types of combustion systems.

To support large-scale computer simulations of each kind of engine, it is necessary to provide reliable chemical kinetic models for each of these fuel classes. 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 n-paraffins such as propane, n-heptane and even n-octane have been developed, but detailed models do not yet exist for the much larger versions such as n-hexadecane, characteristic of diesel fuels. 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, but these substitutes, or surrogates, will also then be reproducible in both experiments and modeling studies. Detailed kinetic models for groups of fuels can then be simplified as needed for inclusion in multidimensional computational fluid dynamics (CFD) models or used in full detail for purely kinetic modeling.

Approach

Chemical kinetic modeling has been developed uniquely at LLNL to investigate combustion of hydrocarbon fuels in practical combustion systems such as diesel and HCCI engines. The basic approach is to integrate chemical rate equations for chemical systems of interest, within boundary conditions related to the specific system of importance. This approach has been used extensively for diesel and HCCI engine combustion, providing better understanding of ignition, soot production, and NOx emissions from these engines in fundamental chemical terms.

The underlying concept for diesel engines is that ignition takes place at very fuel-rich conditions, producing a mixture of chemical species concentrations that are high in those species such as acetylene, ethene, propene and others which are well known to lead to soot production. Some changes in combustion conditions reduce the post-ignition levels of these soot precursors and reduce soot production, while other changes lead to increased soot emissions. The LLNL program computes this rich ignition using kinetic modeling, leading to predictions of the effect such changes might have on soot production and emissions.

Ignition under HCCI engine conditions is closely related to that in diesel engines, since both are initiated by compression ignition of the fuel/air mixtures. In very fuel-lean HCCI ignition, the premixing of fuel and air in the gaseous state results in no soot and extremely low NOx production. Kinetic modeling has proven to be exceedingly valuable in predicting not only the time of ignition in HCCI engines, but also the duration of burn and the emissions of unburned hydrocarbons, CO, NOx and soot.

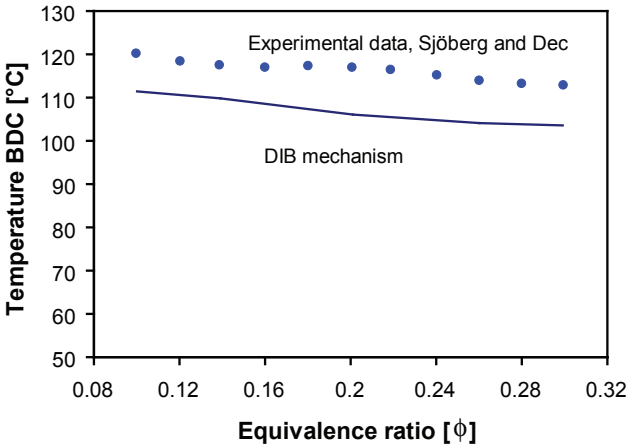


FIGURE 1. The temperature required at bottom dead center to maintain ignition phasing at top dead center in an HCCI engine at Sandia. (Ignition phasing is determined by the 50 percent burn point.) The equivalence ratio is varied by changing the amount of fuel injected into the engine. The fuel is diisobutylene. The points are the experiments and the curve is the result of the model. Engine speed is 1200 rpm and the intake pressure is 100 kPa.

Results

During the last, year we completed chemical mechanisms for important components to include in surrogate models for gasoline, diesel and oil-sand derived fuels. These components are diisobutylene and methylcyclohexane. First, a diisobutylene mechanism was developed to represent olefins in gasoline. In our work on diisobutylene, we discovered key reaction routes that affect the oxidation of large olefins. These routes involve the consumption of resonantly stabilized radicals that are produced by large olefins. These reaction routes accelerate the ignition of diisobutylene and are an important inclusion in the mechanism to enable proper prediction ignition delay times under engine conditions. In collaboration with Magnus Sjöberg and John Dec at Sandia, we used our newly developed mechanism for diisobutylene to model the HCCI engine experiments. We found the diisobutylene model simulated well the ignition phasing in the HCCI engine as a function of equivalence ratio (Figure 1). We published our work on the development of a diisobutylene mechanism in the Proceedings of the Combustion Institute.

Mechanisms for methylcyclohexane and cyclohexane were developed to represent cycloalkanes in gasoline, diesel and oil-sand derived fuels. For methylcyclohexane (MCH), we completed a paper documenting our development of a mechanism for MCH and our mechanism validation by comparisons to experiments in a rapid compression machine (Figure 2). In the MCH work, we were able to establish new reaction rate rules that will assist us in developing

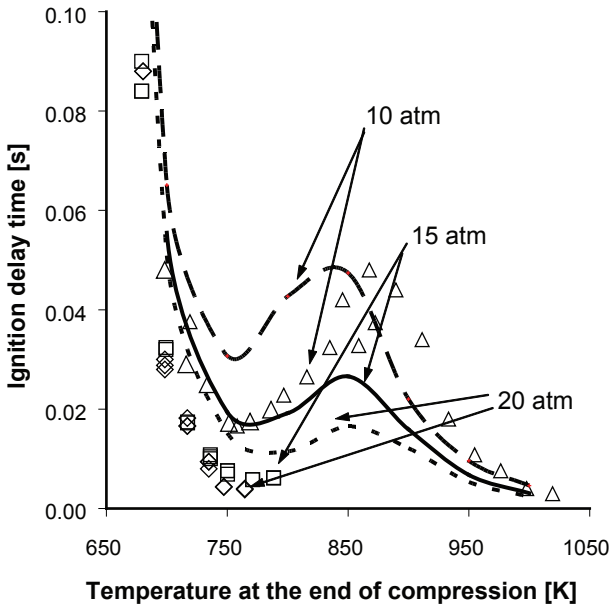


FIGURE 2. Experimental (points) and model-predicted ignition-delay times (curves) at 10, 15 and 20 atm for methylcyclohexane in a rapid compression machine. The experiments were performed at the National University of Ireland in Galway.

further mechanisms for higher molecular weight cycloalkanes. These rules relate particularly to rate constants for reactions responsible for low temperature heat release. It is critical to get these rate constants correct for modeling of combustion in HCCI engines. We collaborated with Magnus Sjöberg and John Dec at Sandia and used our MCH mechanism to model their

experiments in an HCCI engine (Figure 3). We used our new MCH mechanism to simulate the ignition phasing of MCH in an HCCI engine as a function of equivalence ratio (Figure 3). The agreement between the predictions and the experiment are quite good. The paper on MCH mechanism development and validation will be published in the Proceedings of the Combustion Institute.

This year, we began assembling and testing a mechanism for cyclohexane to use to represent cycloalkanes in gasoline, diesel and oil-sand derived fuels. The mechanism testing will be completed in FY 2007. We compared results from our detailed chemical kinetic model to experimental results in a rapid compression machine in the literature (Figure 4). We found that we could simulate both the ignition delay under engine-like conditions and we could also simulate the combustion products produced (Figure 5). This work will be written up for a journal publication in FY 2007. Refinements in reaction rate rules determined in this work will be applied later to cycloalkanes of higher molecular weight needed in surrogate mechanisms for diesel and oil-sand derived fuels (Figure 6).

During this year, we wrote a landmark paper on the effect of oxygenates on sooting tendencies under diesel engine conditions. This paper represented a culmination of our DOE supported work on oxygenated fuels over the last 10 years. We used our kinetic model to show how different oxygenates, ester structures in particular, can have different soot-suppression efficiencies due to differences in the molecular structure of the oxygenated species.

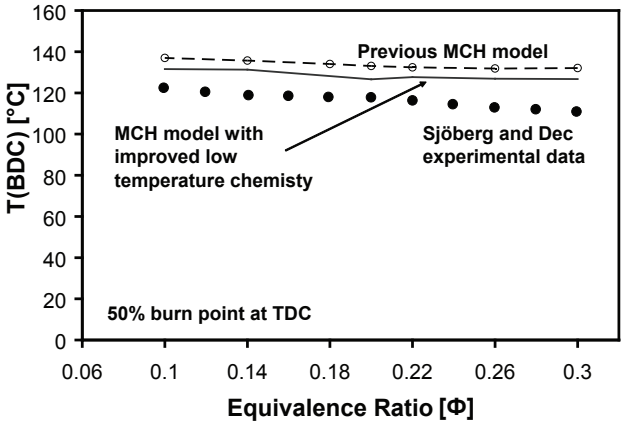


FIGURE 3. The temperature required at bottom dead center to maintain ignition phasing at top dead center in an HCCI engine at Sandia. (Ignition phasing is determined by the 50 percent burn point.) The equivalence ratio is varied by changing the amount of fuel injected into the engine. The fuel is MCH. The points are the experimental results. The curves show the simulated results for a previous MCH model (dotted curve) and an improved MCH model (solid curve).

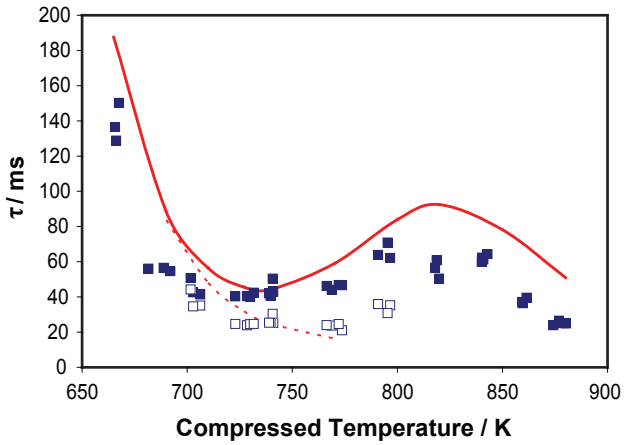


FIGURE 4. Experimental (points) and model predicted ignition delay times (red solid curve) at 7-9 atm for cyclohexane in a rapid compression machine. The experiments were performed at University of Sciences and Technology, Lille, France. Open symbols and the dashed curve correspond to cool flame ignition measurements and predictions, respectively.

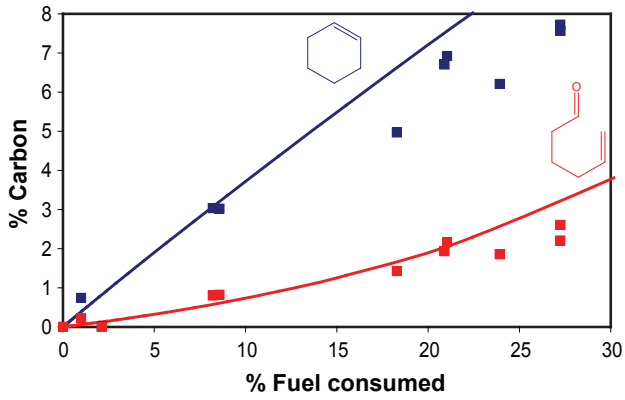


FIGURE 5. Major intermediate products produced in the oxidation of cyclohexane in the rapid compression machine. Cyclohexene (navy blue, experimental (points), model (curve)) and hex-5-enal (red, experimental (points), model (curve)). The percentage of carbon in the fuel that is contained in the intermediate product is plotted as a function of fuel consumed. The experiments were performed at University of Sciences and Technology, Lille, France.

Conclusions

Kinetic modeling provides a unique tool to analyze combustion properties of diesel, spark-ignition and HCCI engines. A kinetic model can be very cost-effective as an alternative to extended experimental analyses and as guidance for more efficient experimentation, and computations can also provide a fundamental explanation of the reasons for the observed results. LLNL kinetic models are providing this valuable capability for engine research at many university and

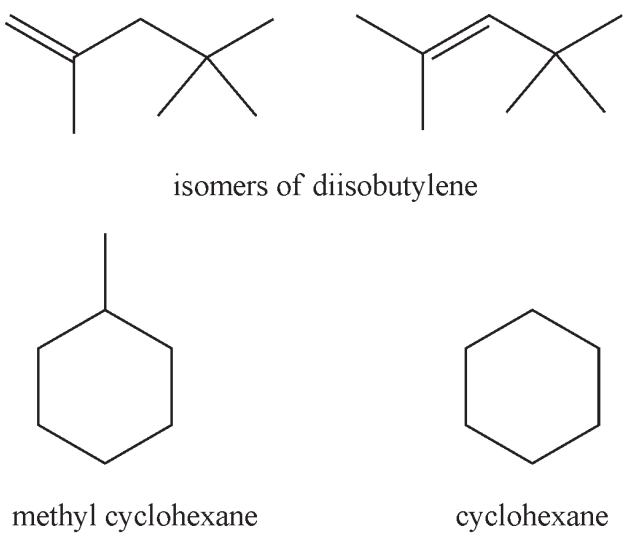


FIGURE 6. Carbon skeletal structures of fuels for which detailed chemical kinetic mechanisms have been developed: diisobutylene, methylcyclohexane and cyclohexane.

industrial facilities in the United States and are an essential tool in engine research.

FY 2006 Publications/Presentations

1. W. J. Pitz, C. V. Naik, T. Ní Mhaoldúin, C. K. Westbrook, H. J. Curran, J. P. Orme, and J. M. Simmie, "Modeling and Experimental Investigation of Methylcyclohexane Ignition in a Rapid Compression Machine", Proceedings of the Combustion Institute, Volume 31, In press, 2007.

2. Metcalfe, W. K., Pitz, W. J., Curran, H. J., Simmie, J. M., and Westbrook, C. K. "The Development of a Detailed Chemical Kinetic Mechanism for Diisobutylene and Comparison to Shock Tube Ignition Times", Proceedings of the Combustion Institute, Volume 31, In press, 2007.

3. Naik, C.V., Pitz, W.J., Sjöberg, M., Dec, J.E., Orme, J., Curran, H. J., Simmie, J. M., and Westbrook, C.K., "Detailed Chemical Kinetic Modeling of Surrogate Fuels for Gasoline and Application to an HCCI Engine", SAE 2005 Transactions of Fuels and Lubricants, Presented at the 2005 Fall Powertrain and Fluid Systems Conference & Exhibition, San Antonio, Texas. SAE paper 2005-01-3742, 2005.

4. Westbrook, C. K., Pitz, W.J., and Curran, H. J., "A Chemical Kinetic Modeling Study of the Effects of Oxygenated Hydrocarbons on Soot Emissions from Diesel Engines." Journal of Physical Chemistry A, 110, 6912-6922, 2006.

5. J. P. Orme, H. J. Curran, J. M. Simmie, "An Experimental and Modelling Study of Methyl Cyclohexane Pyrolysis and Oxidation", J. Phys. Chem. A, 110:114-131 (2006).

6. Pitz, W. J., Cernansky, N. P., Dryer, F. L., Egolfopoulos, F. N., Farrell, J. T., Friend, D. G., and Pitsch, H., "Development of an Experimental Database and Chemical Kinetic Models for Surrogate Gasoline Fuels", submitted, 2007 SAE World Congress, Detroit, MI.

7. Saylam, A., Ribaucour, M., Pitz, W. J., and Minetti, R., "Reduction of Large Detailed Chemical Kinetic Mechanisms for Autoignition Using Joint Analyses of Reaction Rates and Sensitivities", International Journal of Chemical Kinetics, submitted, 2006.

Presentations

1. W. J. Pitz, C. V. Naik, T. Ní Mhaoldúin, C. K. Westbrook, H. J. Curran, J. P. Orme, and J. M. Simmie, "Modeling and Experimental Investigation of Methylcyclohexane Ignition in a Rapid Compression Machine", 31st International Symposium on Combustion, Heidelberg, Germany, August 8, 2006.

2. Metcalfe, W. K., Pitz, W. J., Curran, H. J., Simmie, J. M., and Westbrook, C. K. "The Development of a Detailed Chemical Kinetic Mechanism for Diisobutylene and Comparison to Shock Tube Ignition Times", 31st International Symposium on Combustion, Heidelberg, Germany, August 8, 2006.

3. Naik, C.V., Pitz, W.J., Sjöberg, M., Dec, J.E., Orme, J., Curran, H. J., Simmie, J. M., and Westbrook, C.K., "Detailed Chemical Kinetic Modeling of Surrogate Fuels for Gasoline and Application to an HCCI Engine", 2005 Fall Powertrain and Fluid Systems Conference & Exhibition, San Antonio, Texas. (SAE Oral Presentation Award).

4. C. K. Westbrook and W. J. Pitz, "Estimation Strategies for Chemical Kinetic Reaction Rates", 11th International Conference on Numerical Combustion, Granada, Spain, April 23-26, 2006

Special Recognitions & Awards/Patents Issued

1. SAE Oral Presentation Award for SAE (presentation 3 above).

II.A.15 Achieving and Demonstrating FreedomCAR Engine Fuel Efficiency Goals

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DOE Technology Development Manager:
Gurpreet Singh

Objectives

- Achieve and demonstrate peak brake thermal efficiency (BTE) of 41% in FY 2006, 42% in FY 2007, and 45% in FY 2010 with associated emissions levels as specified in the Office of FreedomCAR Research and Development Plan.
- Provide valuable insight into the development, implementation, and demonstration of technologies for improved BTE.

Accomplishments

- Achieved and demonstrated 2006 FreedomCAR goal of 41% peak BTE on a light-duty diesel engine.
- Demonstrated potential of advanced combustion operation for achieving Tier 2 Bin 5 emissions regulations.
- Acquired more modern engine platform from General Motors (GM) and are in the process of installing and developing the control system.

Future Directions

- Improve leveraging with existing ORNL activities. Complementary ORNL activities include studies of advanced combustion modes, stretch efficiency concepts, and aftertreatment integration.
- Explore advanced combustion approaches for achieving improved efficiency and reduced emissions.
- Investigate potential of waste heat recovery (WHR) strategies.
- Complete transition to GM 1.9-L engine for improved collaboration with universities and other national laboratories.

Introduction

Modern light-duty diesel engines have peak BTEs in the range 38-40% for high-load operation and considerably lower efficiencies for part-load operation. The FreedomCAR roadmap has established several goals over the next several years with a 45% peak BTE 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 project leverages several ongoing activities at ORNL involving exploration of new combustion regimes, researching novel approaches to stretch engine efficiency, as well as NOx mitigation technologies. The underpinning philosophy of the effort is that improving efficiency is best approached by thoroughly understanding the mechanisms and magnitudes of the various losses in engines with respect to converting fuel energy to work. Analyses of energy balances (First Law of Thermodynamics) and availability management (Second Law) are both instructive and necessary to identify and assess opportunities for improvements.

The following methodology will be used in this activity:

1. Establish baseline for modern light-duty diesel engines.
2. Acquire and/or develop models to characterize loss mechanisms.
3. Conceive methods to mitigate losses.
4. Evaluate methods (paths) with system models.
5. Integrate technologies and methods into engine experiments to characterize effects on BTE and emissions.

Technologies for improving efficiency and emissions in light-duty diesel engines are being investigated at ORNL on a highly modified Mercedes 1.7-L common rail four-cylinder diesel engine. This engine is equipped with a full-pass engine control system, allowing complete control of all engine parameters including exhaust gas recirculation (EGR) and fuel injection parameters (timing, duration, number). A more modern engine platform is currently being installed at ORNL and will be used for this activity as well as the leveraged activities in subsequent years.

Results

Significant improvements in engine efficiency will require considering the engine and aftertreatment technologies as a system. To this end, this activity will continue to leverage several ongoing activities at ORNL related to advanced combustion modes, aftertreatment technology, and novel approaches to engine efficiency. Several potential pathways for improving engine efficiency while making progress toward Tier 2 Bin 5 emissions levels were investigated in FY 2006. These experiments led to meeting the FY 2006 milestone of achieving and demonstrating 41% BTE in a light duty diesel engine.

Enabling technologies investigated to accomplish 41% BTE include improved thermal management of air, improved turbocharger efficiency, more aggressive combustion strategies, and reduced friction. The combination of these enablers resulted in an increase in BTE by 2% for this engine. Efficiency results are shown in Figure 1 as a function of intake charge temperature. More details on these technologies and their impact are summarized in the following.

Thermal Air Management. Effect of intake temperature was investigated and found to be a critical parameter for improving BTE. Intake temperature <30°C was assumed plausible for these experiments.

Turbocharger Technology. A variable geometry turbocharger was installed on a re-designed exhaust manifold. More flexible and improved turbocharger technology found to be a critical parameter for improving BTE.

Combustion. More aggressive injection strategies were investigated for improving BTE. Maximum peak pressure rise was maintained <10 bar/deg.

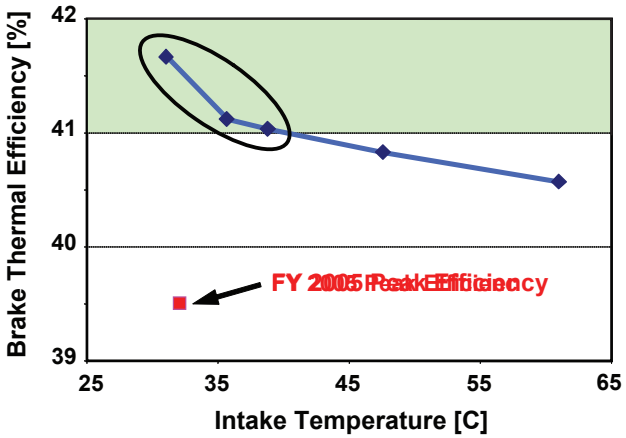


FIGURE 1. BTE as a function of intake charge temperature at 2,000 rpm, 100% load (14.7 bar BMEP). Also shown for reference is the peak BTE achieve in FY 2005.

Friction. Low-viscosity premium lubricating oil was used in an attempt to reduce friction. The effect of premium lubricating oil on BTE was very small and difficult to quantify.

Meeting or exceeding future BTE objectives will most likely require some form of exhaust WHR. We are in the process of developing thermal electric and thermodynamic cycle simulations for inclusion in our full cycle engine models to provide guidance in matching WHR technologies to our engine platform. To further bound the potential of exhaust WHR, first and second law thermodynamic analyses have been performed for the peak BTE condition of 2,000 rpm, 14.7 bar brake mean effective pressure (BMEP). The results of these analyses are shown in Figure 2 and indicate approximately 27% of the fuel energy is in the exhaust mass and approximately 7% of the fuel energy

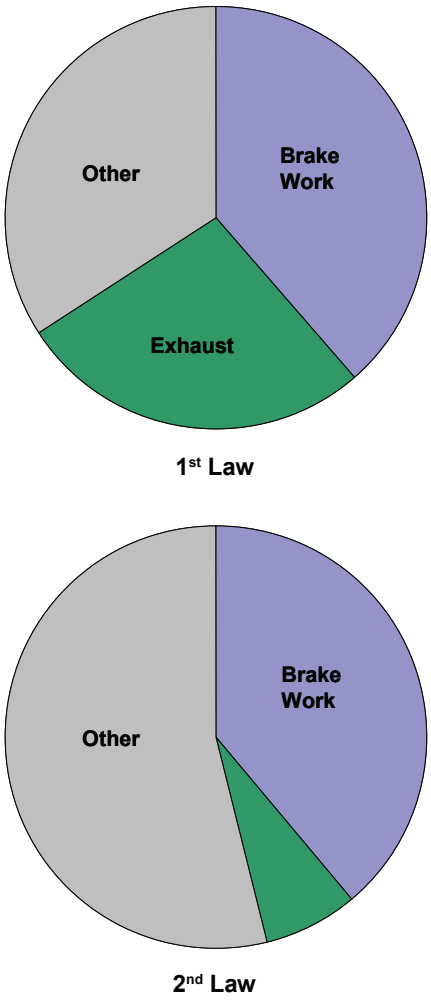


FIGURE 2. First and Second Law analysis of peak BTE conditions to provide better understanding of efficiency opportunities. Note that the first law analysis is based on HHV to be consistent with the second law analysis whereas the BTE calculation is based on LHV as is the convention.

is available from the exhaust for potential use. While a more detailed accounting of the fuel energy is possible with additional measurements, the energy in the exhaust gases is the focus for the near-term. More detailed accounting will occur with improved instrumentation during the next year. For clarification purposes, please note that the first law analysis is based on fuel higher heating value (HHV) to have a consistent reference state with the second law analysis, whereas the BTE calculation follows convention and is based on lower heating value (LHV). Another important factor which may dictate the most effective form of WHR is exhaust temperature. Exhaust temperature has been mapped across the speed-load range of the engine and is being used in the sizing and design of a WHR system.

Advanced combustion strategies were used as the primary method of achieving reduced emissions in FY 2006. Four speed-load conditions and weighting factors were used to estimate the magnitude of drive cycle emissions for advanced combustion or HECC (High Efficiency Clean Combustion) operation. These modes and weighting factors were developed by an industry working group and are discussed in the literature [1, 2]. The composite emissions estimates for HECC operation are shown in Figure 3 and compared to U.S. Tier 2 Bin 5 regulatory standards in Table 1. Recall that these emissions estimates are based on steady-state data from a fully warm engine and do not include important effects associated with cold-start and transient load-speed operation. Examination of Table 1 indicates some form of aftertreatment will most likely still be required for the form of HECC used in this activity. While significant in-cylinder NOx reduction was achieved and dramatically reduces the NOx aftertreatment requirement, HC and CO emissions were increased in the process, resulting in the need for increased aftertreatment oxidation as compared to conventional operation. Also note that a diesel particulate filter (DPF) was used in the low-pressure EGR system and is necessary to meet the engine-out HECC emissions values shown in Table 1.

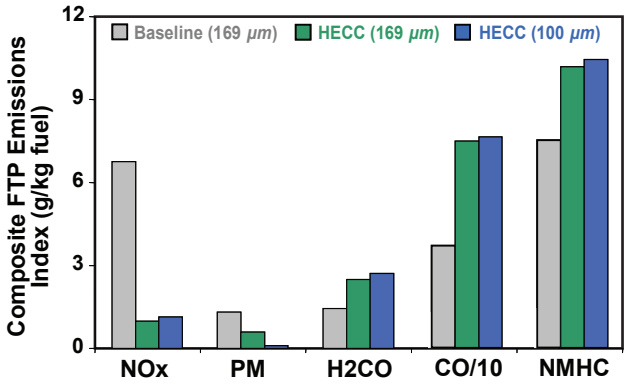


FIGURE 3. Composite emissions indices based on steady-state modal conditions representative of the FTP drive-cycle.

In the future, simultaneous improvements in efficiency and emissions will most likely involve a combination of advanced combustion operation working synergistically with the appropriate aftertreatment technologies. The reader is encouraged to reference the publications/ presentations list for more information.

TABLE 1. U.S. Tier 2 Bin 5 Emissions Standards, HECC FTP Drive-Cycle Emissions Estimates, and Required Aftertreatment Effectiveness Estimates

Pollutant	Tier 2 Bin 5 g/mi	HECC g/mi	Required Aftertreatment Effectiveness
NOx	0.07	0.075	7%
NMHC	0.09	0.694	87%
CO	4.2	5.08	17%
H_2CO	0.018	0.181	90%
PM	0.01	0.007	Required for Low-Pressure EGR

Selection of the base engine platform is important in order to best represent the most recent engine technologies. ORNL is in the process of installing a state-of-the-art GM 1.9-L diesel engine and developing full control authority similar to that on our Mercedes 1.7-L diesel engines. This research platform is also being used at Sandia National Laboratory (optical single-cylinder engine) and the University of Wisconsin (metal single- and multi-cylinder engines). Collaboration among these institutions is expected to be beneficial in identifying new pathways for meeting the FreedomCAR efficiency and emissions goals. The GM 1.9-L engine will be phased in over the next fiscal year.

Conclusions

This activity has shown progress toward the development, implementation, and demonstration of technologies for improved BTE. Specific observations are as follows:

- Demonstrated 2006 FreedomCAR goal of 41% peak BTE on a light-duty diesel engine. An increase in BTE by 2% was achieved with improved thermal air management, more efficient turbocharger technology, and more aggressive combustion strategies.
- Characterized fuel energy in the exhaust gases as well as the potential for use.
- Demonstrated the potential of advanced combustion strategies for achieving Tier 2 Bin 5 emissions levels.
- Acquired new engine platform which is more representative of the state-of-the-art and which will lead to improved collaboration with universities, laboratories, and industry.

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2. Gonzalez, M., Clark, W., Wolf., L., Garbak, J., Wright, K., Natarajan, M., Yost., D., Frame, E., Kenney, T., Ball, J., Wallace, J., Hilden, D., and Eng, K., "Impact of Engine Operating Conditions on Low-NOX Emissions in a Light-Duty CIDI Engine Using Advanced Fuels," SAE Paper Number 2002-01-2884. Society of Automotive Engineers, Warrendale, 2002.

FY 2006 Publications/Presentations

C. Scott Sluder, R. M. Wagner, "An Estimate of Diesel High-Efficiency Clean Combustion Impacts on FTP-75 Aftertreatment Requirements", SAE 2006-01-3311 (Toronto, Ontario, Canada; October 2006).

II.A.16 Free-Piston Engine Research

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Objectives

- Continue to model stability of electrically coupled opposed free pistons.
- Further improve computational fluid dynamics (CFD) model for opposed piston uniflow scavenging.
- Establish collaboration with other research institutions and industry partners and secure funding for prototype construction.

Accomplishments

- Established collaborative modeling research with University of Michigan (funded by General Motors) and General Motors to simulate full hybrid vehicle platform powered by a free-piston engine.
- Initiated Flux2D modeling of opposed piston coupling and in process of developing real time Mathematica-based comparison model with Ron Moses (Los Alamos National Laboratory, LANL).

Future Directions

- Complete and compare Flux2D and real-time Mathematica models to optimize coupling of current linear alternators (from Magnequench International, Inc).
- Complete optimization of uniflow opposed piston scavenging with port fuel injection.
- Optimize linear alternator/power conditioning system for battery charging in collaboration with General Motors.
- Initiate design, fabrication, and construction of two-stroke opposed piston prototype utilizing optimized coupling of Magnequech alternators as a proof-of-concept tool.

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. Unfortunately, current crankshaft spark ignition internal combustion engines with optimized power outputs of 30 KW have thermal efficiencies of less that 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 CFD 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 project goal is to combine the developed components into a research prototype for demonstration of fuel conversion efficiency.

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 (the goal of this project) for performance demonstration, understanding of the pieces in the device will allow proper allocation of each component to the combined performance of the assembly.

This year, due to late funding of this effort and the departure of post doctoral appointee Hans Aichlmayr, much of the work reported was conducted with consultants to Sandia. Collaboration with many of the partners is in the early stages.

Results

The most important result of the past year has been the increased confidence in the viability of the opposed dual piston concept over the double-ended single piston concept. The opposed piston design has several nice features:

- Long stroke/bore ratio – 5 or more – resulting in a lower surface area to volume ratio at combustion than the single piston design (minimizes heat loss at combustion)

- Ideal candidate for uniflow scavenging – no valve actuation required
- Perfect balance

Figure 1 shows a proposed setup for the opposed piston design. In 2002, an eight member European Union Consortium started a $3 million project to design and build a free-piston engine. The result in 2005 was a single piston double-ended prototype, shown in Figure 2, very similar to Sandia's initial free piston design.

Over the past year collaborative efforts have been initiated. General Motors has begun sponsoring modeling at the University of Michigan. The focus there will be the application of a free-piston engine in a full hybrid vehicle platform. This is a system-level study that will greatly help in understanding how the complex electrical output from the linear alternator can be utilized. Sandia is collaborating with both the University of Michigan and General Motors.

Simultaneously, Sandia has renewed its software license for Flux2D, an electromagnetic FEA package, and has begun to model the opposed piston electrical coupling and output. This will be concurrent with the ongoing work by Ron Moses (LANL) to determine the maximum piston coupling possible with the current linear alternator supplied by Magnequench International shown in Figure 3. This linear alternator has a magnet configuration that produces single phase output with power switching of the coils to follow the piston position, thus removing undriven coils from the electrical circuit. If advantageous the alternator can be reconfigured as a three-phase device by replacing the permanent magnets with new magnets of lengths varied to achieve the three-phase configuration. The three-phase geometry has advantages such as ease of starting, lower cogging force, etc. Previous modeling conducted by Ron Moses with a Mathematica-based model has shown that the single-phase configuration has higher stability. However, both single and three-phase setups are stable enough to show the coupling concept of an opposed piston design should be further investigated.

With Sandia's ongoing effort utilizing Flux2D combined with an improved, real-time coupling model with more accurate combustion and transport models from Ron Moses, an iterative optimization of the current Magnequench linear alternator can be achieved by utilizing feedback from the system-level modeling being constructed at the University of Michigan. Once the optimal design has been achieved, design and fabrication of the continuous operation research engine components can begin.

One of the greatest challenges of the coming year is staffing the project with a Post Doctoral Appointee. As of November 2006 a promising candidate is going through the Sandia approval process and hopefully will be approved shortly. A PhD student from the University of Michigan (Jerry Fuschetto, a student of Prof. Assanis) came onboard at Sandia in October 2006.

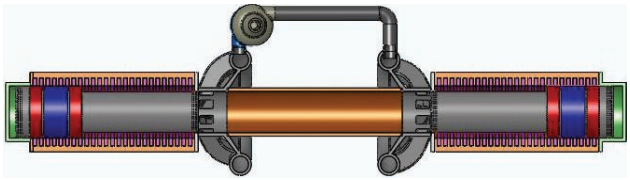


FIGURE 1. Proposed Layout of Sandia's Opposed Piston, Uniflow Scavenged Engine

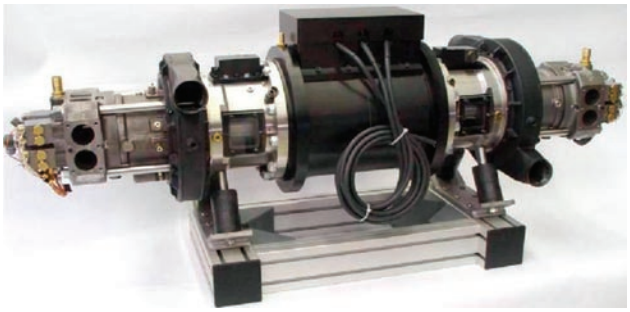


FIGURE 2. The European Union's Free Piston Energy Converter Prototype Engine

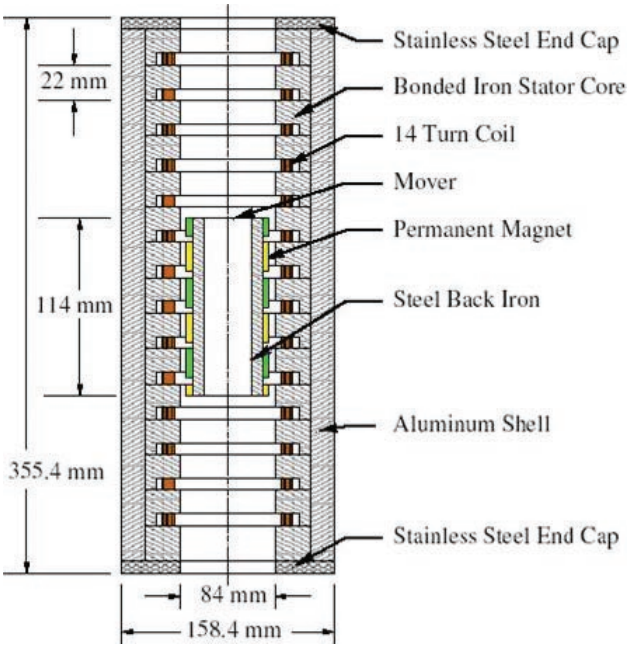


FIGURE 3. Layout of Magnequench International's Linear Alternator In Single-Phase Configuration

Previous and new industrial collaborators are being involved in the prototype design. Sandia continues to

expand the concept to other applications. The goal is an operational research prototype by the end of FY2008.

Conclusions

- Linear alternator characterization is on schedule to be completed early this FY.
- Scavenging system design is progressing and will finish early in FY2007.
- Opposed piston design continues to have attractive features for prototype.
- Prototype design, fabrication, and characterization are on track to begin this FY.

II.A.17 In-Cylinder Hydrogen Combustion Visualization in a Non-Optical Engine

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Objectives

- Evaluate the performance of hydrogen powered engines, both port fuel injected (PFI) and direct injected (DI), by utilizing endoscope imaging.
- Explore combustion anomalies such as knock and pre-ignition specifically pertaining to hydrogen operation.
- Demonstrate the potential of endoscope imaging to provide combustion information at high speed, high load engine operation.
- Utilize spectroscopy to obtain combustion gas temperature measurements in-cylinder.
- Complement the data and engine operating conditions utilized by the Combustion Research Facility at Sandia National Laboratories to provide a more complete view of hydrogen engine combustion.

Accomplishments

- Operated the engine under full-speed and full-load conditions while obtaining endoscope images. Full emissions and performance results were obtained concurrently with the endoscope results.
- OH* chemiluminescence images were obtained using ultraviolet (UV) imaging that show the progression of the combustion event. A correlation between heat release and OH* intensity was obtained.
- Images were obtained at over 2,000 RPM and over 6 bar indicated mean effective pressure (IMEP) for PFI, single injection DI and double injection DI.
- Gas temperature measurements were obtained in-cylinder, as a function of crank-angle.

Future Directions

- Further characterize the multiple injection DI strategy to improve performance while minimizing emissions.
- Conduct experiments that vary important parameters, such as DI injection pressure and multiple injections, and measure their influence upon combustion anomalies.
- Evaluate the capability of this engine to meet emissions standards with minimal to no NOx after-treatment by studying the detailed mechanisms of combustion – especially at high speed and high load.

Introduction

This work began as an effort to provide complementary information to the work conducted using fully optical engines at Sandia National Laboratories. Fully optical engines provide tremendous optical access – laser based diagnostics along with a very large field of view and high optical quality – but are limited in the range of engine conditions that can be run. Optical engines usually need to be skip-fired (a few fired combustion events followed by several un-fired events) to minimize heat damage – meaning that emissions measurements are usually not meaningful. To maintain optical quality, they tend to operate un-lubricated – which requires special piston rings. Finally, the rates of pressure rise need to be modest to insure that the quartz pistons and liners do not get damaged. These restrictions impose stringent limitations regarding the engine conditions that can be run – low speed and modest load.

Most engine manufacturers require information regarding high speed and high load conditions to insure their customer demands are satisfied. Endoscope imaging provides the opportunity to operate the engine at high speeds and loads while simultaneously acquiring many other measurements – such as cylinder pressure measurement, emissions measurements, etc. This is due to the low level of intrusion required for endoscope imaging. A 12-mm tube machined into the cylinder head is all that is required. The technique is dependent upon naturally occurring radiation in combustion – soot luminosity, chemiluminescence, etc. and therefore lasers cannot be used – but the engine can be run in its full operating range. Hydrogen powered engines offer the opportunity to operate the engine without a throttle and

without after-treatment. However, the need to retain high power density and high efficiency while reducing NOx emissions is a significant challenge. This challenge is being addressed by the ability to use hydrogen in multiple injection DI operation.

Approach

The endoscope imaging system was installed in an automotive style engine, a Ford 0.5 liter naturally aspirated, direct or port injected hydrogen engine. This engine provided the lowest cost opportunity to explore the capabilities of endoscope hydrogen combustion imaging. The engine was controlled by an external system made by Motec to control spark timing, injection timing and injection duration. This provided the opportunity to vary and control almost all engine operating parameters. The endoscope system provided the ability to view most of the combustion chamber and to acquire images of OH* chemiluminescence.

The gas temperature measurement technique was utilized by taking advantage of the existing endoscope access port and inserting an appropriately sized fiber optic line to gain spectroscopic access to the combustion chamber. The fiber then transmitted the light to the spectrograph, using the intensified charged-coupled device (ICCD) camera as the pixel array for light intensity measurement. Several gratings were used in assessing the performance of the optical equipment – very fine gratings provide maximum resolution, but with minimal signal transmission due to the large amount of light scattering. Coarse gratings provide less resolution, but greatly improved signal transmission due to reduced light scattering. An important parameter is to use the most highly resolved grating that still allows for an acceptable amount of signal transmission to the pixel array. These parameters are then entered into the simulation code to allow for accurate simulation of the OH* spectral signature for comparison to the experimental distribution. A least-squares fit was then applied to perform the gas temperature calculation.

The engine was operated at a few primary conditions to verify the optical techniques applied – 2,000 RPM, 70% and 100% load, and 3,000 RPM 75% load. The primary variables for base-lining the engine were spark timing (moving from the knock limit to the pre-ignition limit) and in DI operation, injection timing. For double injection DI, the variables also included percentage of fuel per injection and dwell time between injections. Ten repeat conditions were conducted to insure statistical reliability of the data and the endoscope data was acquired in conjunction with traditional measurements to insure proper operation of the engine.

Results

In Figure 1, the images show an example of comparing the PFI approach with DI. The light intensity is the rough equivalence to NOx production – *i.e.* more light intensity equals more NOx. It can be clearly seen that the light intensity for the DI case is significantly lower than for the equivalent PFI case. Figure 1 clearly demonstrates the opportunity to utilize late injection DI as a strategy (under specified conditions) to keep power density and efficiency high, while reducing NOx emissions.

In Figure 2, an experimental and simulated spectral profile of OH* molecule (created by hydrogen combustion) are shown. The spectral profile displays the quantum mechanisms that the OH* molecule uses to store thermal energy. A simulated spectral profile is

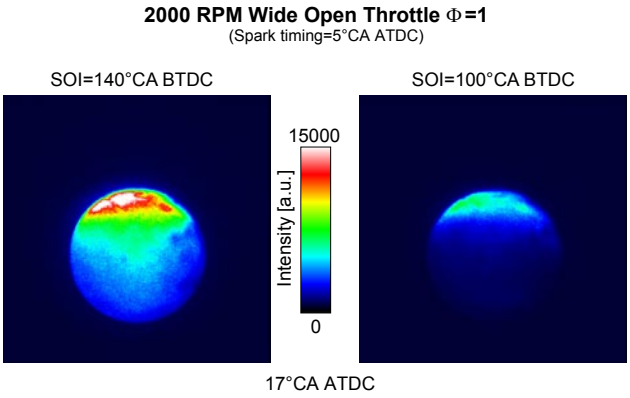


FIGURE 1. Comparison of OH* Intensity at 2,000 RPM and 100% Load for PFI (left) and DI (right) Operation

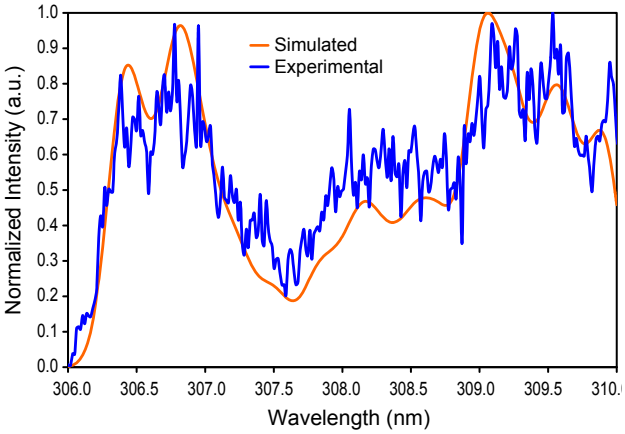


FIGURE 2. Simulated and Experimental Spectral Profiles of OH* Light Intensity during Hydrogen Combustion at 2900K

created by initially guessing the OH* temperature and this simulated profile is compared to the experimental profile actually measured. The simulated profile is then iterated as a function of temperature until the difference between the simulated and experimental profiles are minimized by using a least-square statistical fit. For the example in Figure 2, the calculated temperature was 2,900K, which is a very reasonable value. This calculated temperature algorithm is then performed at each successive moment in time during the combustion event, allowing for the creating of a thermal profile of the combustion event as a function of time. This thermal profile can be seen in Figure 3. A set of 10 measurements was made at each point in time, allowing for the creation of error bars in the measurement, as also seen in Figure 3.

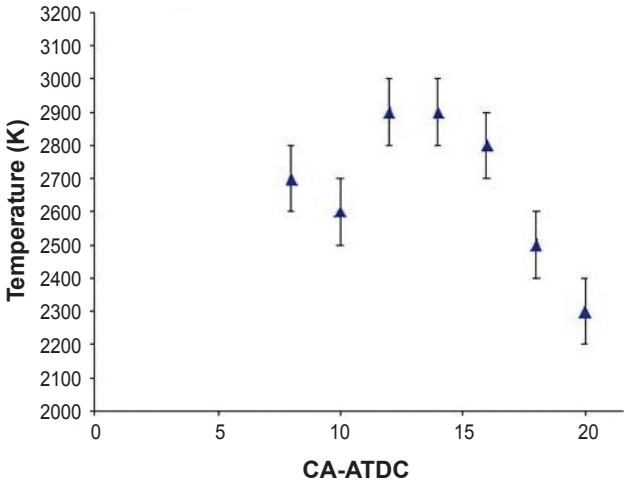


FIGURE 3. Thermal Profile of Hydrogen Combustion as a Function of Engine Crank-Angle Position (Time) for Engine Conditions of 2,000 RPM and 70% Load

Conclusions

- Endoscope imaging provides 2-D information that captures increased detail about engine combustion over 0-D techniques.
- Combustion gas temperature measurements can be made with real engines, operated under the full range of conditions when using endoscope imaging.
- Other diagnostic techniques can be used in conjunction with endoscope imaging, such as cylinder pressure, emissions measurement, and others.
- Detailed OH* chemiluminescence measurements can be linked to pressure and heat release information, providing insight into the mechanisms behind engine combustion changes.

FY 2006 Publications/Presentations

1. ASME paper ICEFS006-1398, "Study of Combustion Anomalies of H_2ICE with External Mixture Formation", S. A. Ciatti, T. Wallner, H. K. Ng, W. F. Stockhausen, B. Boyer – Aachen, Germany, May 2006.

2. Global Powertrain Conference - invited presentation, "Combustion Imaging in Alternative Fuel Engines", Novi, MI, September 2006.

3. International Conference on Hydrogen I.C. Engines, "Endoscopic Investigations in a Hydrogen Internal Combustion Engine", Wallner, T., Ciatti, S. A., Stockhausen, W. F., Boyer, B., Graz, Austria, September 2006.

II.A.18 OH* Chemiluminescence Measurements in a Direct-Injection Hydrogen Engine

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Objectives

- Develop the science base needed by engine companies to develop hydrogen internal combustion engines (H_2ICEs) that meet DOE's near term goals:
  - peak brake thermal efficiency (BTE) ≥45%,
  - Tier2/Bin5 emissions or better (NOx ≤0.07g/mile),
  - power densities greater than present-day gasoline engines.
- Provide validation data to support modeling efforts at SNL using the large eddy simulation (LES) technique.

Accomplishments

- Measured flame front propagation speeds for hydrogen injection prior to intake valve closure at various equivalence ratios.
  - validation data to be used for the LES numerical simulations
- Used OH* chemiluminescence imaging to evaluate combustion and global trends related to in-cylinder mixture formation in a direct-injection hydrogen engine.
- Found an empirical correlation between OH* chemiluminescence emission intensity and equivalence ratio that is used to obtain a semi-quantitative measure of the maximum in-cylinder equivalence ratio.
- Begun assembly of the laser-based optical diagnostic experimental setups.

Future Directions

- Use planar laser induced fluorescence (PLIF) to obtain a spatially resolved quantitative measure of in-cylinder equivalence ratio.
- Use particle image velocimetery (PIV) to investigate in-cylinder mixing and for LES validation data.
- Implement an emissions bench to measure engine-out NOx and H_2 emissions.

Introduction

Hydrogen-fueled internal combustion engine (H_2ICE) development efforts are focused to achieve an advanced hydrogen engine with a peak brake thermal efficiency greater than 45%, near-zero emissions, and a power density that exceeds gasoline engines. With respect to these efforts, the direct-injection (DI) H_2ICE is one of the most attractive H_2ICE options [1-4]. Compared to a port-fuel-injected (PFI) H_2ICE, a DI-H_2ICE avoids the power density loss associated with the displacement of air by lighter hydrogen because fuel is injected after the intake valve has closed. In addition, the problems of pre-ignition associated with PFI-H_2ICEs can be mitigated in a DI-H_2ICE by timing injection to both minimize the residence time that a combustible mixture is exposed to in-cylinder hot-spots and to allow for improved mixing of the trapped residual gas with the intake air. Lastly, in-cylinder injection offers multiple degrees of freedom available for controlling emissions and optimizing engine operation and efficiency.

The challenge with DI-H_2ICE operation is that in-cylinder injection affords only a short time for hydrogen-air mixing. For early injection, coincident with intake valve closure (IVC), maximum mixing times range from approximately 20-4 ms across the speed range 1000-5000 rpm, respectively. In practice, to reduce the compression work of the engine [2] and to mitigate pre-ignition, start of injection (SOI) is retarded with respect to IVC, and mixing times are further reduced. Since mixture distribution at the onset of combustion is critical to engine performance and emissions, a fundamental understanding of the mixture formation processes is necessary to optimize DI-H_2ICE operation to meet DOE's near term goals [5].

Approach

Owed to the complexities of the turbulent mixing processes that mix hydrogen and air in a direct-injection hydrogen engine, a comprehensive evaluation of the in-cylinder mixture formation process is a difficult task. Therefore, a systematic experimental approach is used that begins with OH* chemiluminescence imaging. In the first part of this work, images of the chemiluminescence emission from excited-state OH (OH*) are used to measure flame propagation characteristics and cycle-to-cycle variability, and to qualitatively evaluate mixture distribution. The ability to evaluate mixture distribution from the OH* chemiluminescence images is possible since OH* chemiluminescence emission is long known to be correlated with equivalence ratio [6]. In the second part of this work an empirical relationship between the OH* chemiluminescence intensity, cylinder pressure, and equivalence ratio is determined. This empirical relationship is then used to extract a semi-quantitative measure of the maximum line-of-sight averaged equivalence ratio from the OH* chemiluminescence images.

The test engine is an automotive-sized, single-cylinder, optical research engine. The engine head is a pent-roof type, with two intake and two exhaust valves, a central-spark plug, and a side injector located between the two intake valves and orientated at an angle of 40º to the horizontal. The experimental prototype injector used in the experiments has a six-orifice nozzle and an included cone angle of 90º. Each orifice diameter is 0.56 mm and the hole-pattern is symmetric about the injector axis. Hydrogen pressure to the injector is maintained above a critical pressure to establish choked flow conditions at the orifice throughout the injection event. The experiments include measurements for engine operation with hydrogen injection in-cylinder either prior to or after IVC. For pre-IVC injection start-of-injection (SOI) is at -270 CAD. Pre-IVC injection is investigated to establish a baseline comparison for post-IVC injection. For post-IVC injection SOI is varied between -112 and -40 CAD. The former CAD corresponds to IVC and the latter is limited by flame stability considerations. The global equivalence ratio is maintained near $\phi \approx 0.55$, chosen because it is near the equivalence ratio where NOx rapidly increases [2,7], such that, mixture distribution is critical for this operating point.

Results

Sample OH* chemiluminescence images of a single cycle and the ensemble average of 20 single cycles for an equivalence ratio of 0.51 acquired at 0 CAD (11 CAD after spark) are shown in Figure 1(a) and (b), respectively. Images for an equivalence ratio of 0.82 acquired at 8 CAD (6 CAD after spark) are shown in Figure 1(c) and (d). The difference in the OH* chemiluminescence intensity levels between the two equivalence ratios illustrates the strong dependence of OH* chemiluminescence emission on equivalence ratio. Since OH* exists both at the flame front and in the burned gas region, its distribution thickness is wide compared to the flame thickness. In general, approaching the reaction zone along a line from the unburned-gas region, the OH* chemiluminescence intensity increases exponentially at the edges of the flame front, peaks at the location of maximum heat release, followed by a stretched exponential decay in the burned gas region. Consequently, to obtain a measure of flame propagation characteristics from the OH* chemiluminescence images, a threshold must be applied to the images to isolate the flame front. The threshold procedure used here is to use a threshold value that corresponds to 66.7% of the intensity at the peak of the exponential rise that occurs at the edge of the flame front.

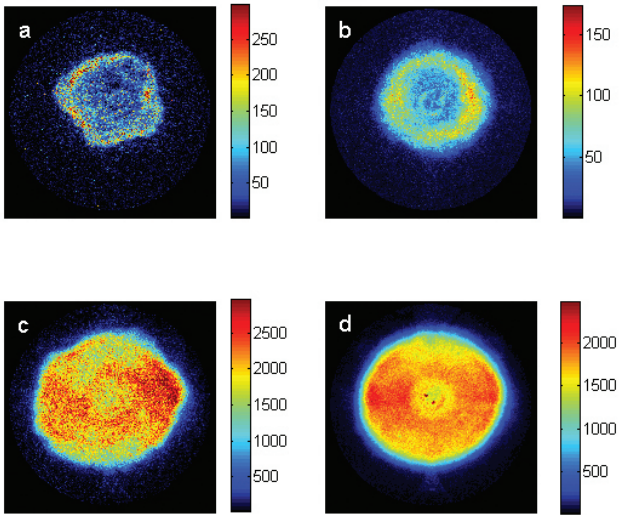


FIGURE 1. Sample OH* chemiluminescence images with pre-IVC injection for $\phi = 0.51$ acquired at 0 CAD (11 CAD after spark) for (a) a representative single cycle and (b) ensemble averaged over 20 single cycles and for $\phi = 0.82$ acquired at 8 CAD (6 CAD after spark) for (c) a representative single cycle and (d) ensemble averaged over 20 single cycles. The color bar corresponds to OH* chemiluminescence intensity in detector counts.

A measure of the average flame radius, r_f, at a given CAD is determined by fitting a bounding box to the threshold ensemble-averaged image. The average flame radius is defined as one-half the square-root of the area of the bounding box (*i.e.*, $r_f = \sqrt{A}/2$). The maximum flame radius that could be measured is limited by the size of the quartz window (*i.e.*, $r_{fmax} = 32.5$ mm) and the minimum is limited by the dwell between spark discharge and the first image. For each equivalence

ratio, the corresponding mean flame front expansion speed, u_f, determined from the time rate of change of r_f,

$$u_f = \frac{dr_f}{dCAD} \cdot \frac{dCAD}{dt} \quad (1)$$

is approximately constant over the CAD duration measured. Figure 2 shows the mean flame front expansion speeds plotted against equivalence ratio. The laminar flame velocity versus equivalence ratio for a hydrogen-air mixture at room temperature and atmospheric pressure [8] is plotted for reference. The flame propagations speeds measured here serve as excellent validation date for the LES simulations.

Global trends related to the variation of in-cylinder mixture distribution with SOI are determined by comparing the OH* chemiluminescence images for post-IVC injection to pre-IVC injection obtained at similar equivalence ratio. The pre-IVC images closely approximate premixed operation and serve as a baseline for comparison. OH* chemiluminescence intensities that are higher (lower) than this baseline may indicate that combustion is at a higher (lower) equivalence ratio. In addition, the distribution of the OH* chemiluminescence emission serves as a metric for in-cylinder mixture distribution.

The ensemble-averaged OH* chemiluminescence images obtained at a CAD corresponding to 10% of the apparent heat release for SOI at -270, -112, -90 and -40 CAD are shown in Figure 3. Hydrogen injection pressure is 100 bar and the global equivalence ratio is approximately 0.55. The scaling-factor (SF) reported atop each image is a multiplicative factor based on the maximum intensity measured amongst the images. The pre-IVC injection image (*i.e.*, SOI at -270 CAD) shows a near symmetric distribution of intensity on an annulus centered about the spark plug, consistent with a center-spark-ignited near-homogeneous mixture. For SOI at -112 CAD (coincident with IVC) and -90 CAD, the images are similar to the pre-IVC image though the OH* chemiluminescence intensity is slightly higher (i.e., a lower SF) and the distribution is more asymmetric with higher intensities directly opposite the injector. For SOI at -40 CAD, the peak and distribution of intensity differs significantly from the pre-IVC image. The distribution is such that high intensities are observed on the left and rights sides of the image. The high intensities suggest that local regions are burning rich compared to the global equivalence ratio. These results illustrate the strong dependency of mixture preparation on SOI.

For the pre-IVC injection data-sets (many sets obtained for equivalence ratios ranging between 0.45 and 0.95), a measure of the mean OH* chemiluminescence intensity at a given CAD is obtained from the threshold ensemble-averaged image. These data are plotted in (I, P, ϕ) and a nonlinear least-squares regression is used to fit the data to the functional form,

$$I = AP^B \exp(CP^D\phi) \quad (2)$$

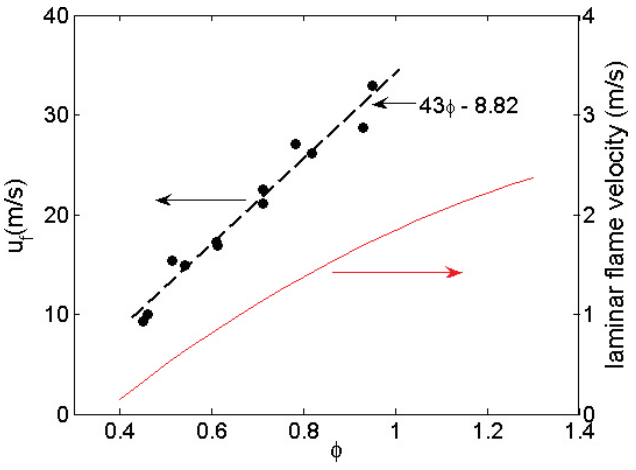


FIGURE 2. Flame front expansion speed (●) plotted against equivalence ratio. The dashed line is a least-squares linear fit to the data. The solid line is the laminar flame velocity versus equivalence ratio for a hydrogen-air mixture at room temperature and atmospheric pressure [8].

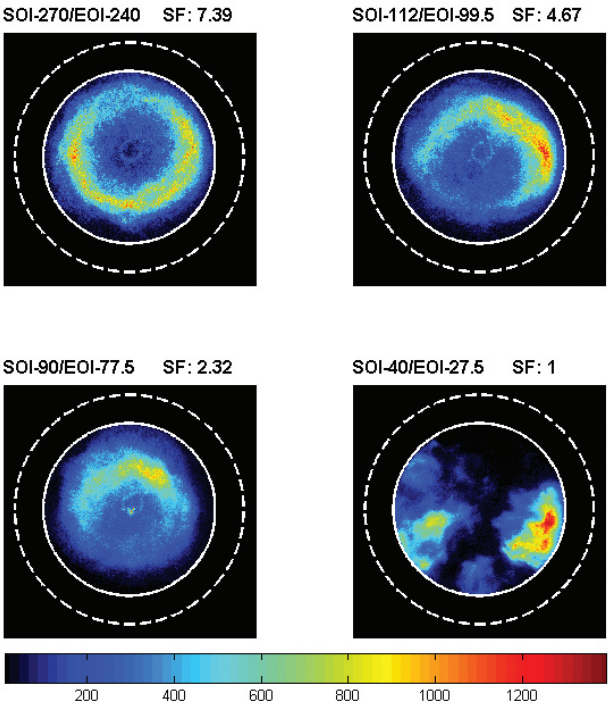


FIGURE 3. Ensemble-averaged OH* chemiluminescence images acquired at the CAD corresponding to the location of approximately 10% of the apparent heat release. Hydrogen injection pressure is 100 bar. The scaling-factor (SF) reported atop each image is a multiplicative factor based on the maximum intensity measured amongst the images.

where A = 4.915x10^2, B = -1.104, C = 7.566x10^{-1}, D = 3.882x10^{-1}, and the units of pressure are in kPa. The form of expression (2) was determined from piecing together fits to the data along lines of constant ϕ and constant P. Next, expression (2) is rearranged to yield,

$$\phi = \frac{\ln(I / AP^B)}{CP^D}. \quad (3)$$

The logarithmic dependence of the equivalence ratio on the OH* chemiluminescence intensity is favorable since the uncertainty in intensity has less effect on the uncertainty in the measure of the equivalence ratio. For example, using the measured OH* chemiluminescence intensity from the pre-IVC data-sets, the predicted equivalence ratio determined from expression (3) is within ±8% of the actual equivalence ratio despite the fact that the variation in the intensity on the front is typically ±20% (defined as ± one standard deviation).

By converting the measured OH* chemiluminescence intensity in the post-IVC images to equivalence ratio using expression (3), the maximum line-of-sight averaged equivalence ratio over the duration of combustion can be assessed. The maximum line-of-sight averaged equivalence ratio plotted as a function of SOI, for two injection pressures of 25 bar and 100 bar, are shown in Figure 4. The trends in the data show that the maximum equivalence ratio increases monotonically with retard of SOI from IVC, and are consistent with trends observed for variations in NOx with SOI. In particular, Eichlseder et al. [2] observed strong variations in NOx with variations in SOI, which they conjectured were due to increasing mixture inhomogeneities with retard of SOI from IVC. The results presented here directly support their hypothesis. In addition, knowledge of the expected bounds of the maximum in-cylinder equivalence ratio for a given SOI is extremely valuable for the calibration procedures used for the laser induced fluorescence (LIF) technique. The LIF technique is the next step in our systematic experimental approach to a comprehensive evaluation of the in-cylinder mixture formation process in a DI-H_2ICE.

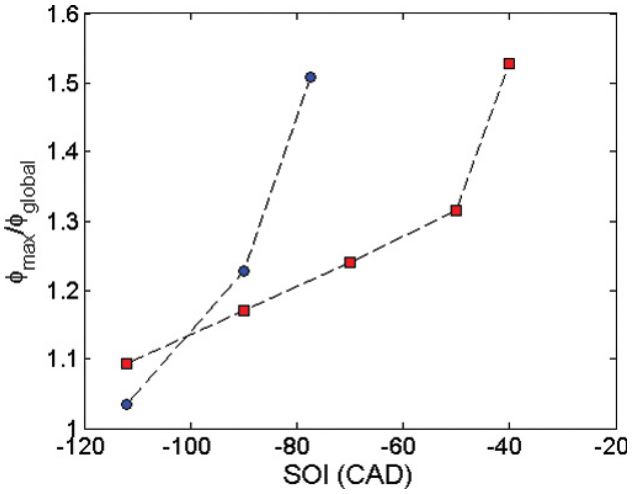


FIGURE 4. The maximum equivalence ratio measured for each SOI normalized by the global equivalence ratio for (●) Pinj = 2.5 MPa and (■) Pinj = 10 MPa.

Conclusions

- For pre-IVC injection, flame propagation speeds increase with increasing equivalence ratio and are significantly higher than the laminar flame velocity measured at the same equivalence ratio.
- SOI coincident with IVC produces a nearly homogeneous hydrogen-air mixture. However, with retard of SOI from IVC mixture inhomogeneities increase monotonically.
- An empirical correlation between OH chemiluminescence emission intensity and equivalence ratio was determined and used to obtain a semi-quantitative measure of the maximum in-cylinder equivalence ratio over the duration of combustion.
- A semi-quantitative measure of the maximum line-of-sight averaged equivalence ratio provides valuable information for interpretation of engine data, and an excellent starting point for the study of in-cylinder mixture formation processes in a DI-H_2ICEs using advanced laser-based diagnostics.

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II.A.19 Low-Temperature Combustion Using Pre-Mixed Charge Compression Ignition

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Roland Gravel

NETL Project Manager: Carl Maronde

Objectives

1. To design and develop advanced combustion systems capable of achieving U.S. Environmental Protection Agency (EPA) 2010 emission requirements while improving the brake thermal efficiency by 10% compared to current baselines.
2. To design and develop components and subsystems (fuel systems, air handling, controls, etc.) to enable construction and development of multi-cylinder engines capable of running steady-state and transient operating conditions.
3. 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 reducing petroleum imports by at least 5% via renewable fuel sources. To demonstrate the technology is compatible with B20 (biodiesel) to enable reduction of petroleum imports by at least 5%.
4. To mature the intended combustion technologies via rig and test development of heavy and light-duty multi-cylinder engines for demonstration of the robustness and commercial viability of the technology.

Accomplishments

- Fuel system specification for the ISB (6.7L) engine was completed, optimized for premixed charge compression ignition (PCCI) combustion utilizing the Cummins single-cylinder ISB research engine.
- Engine system simulations were completed to define air handling requirements to achieve desired in-cylinder conditions for PCCI combustion.
- Air handling equipment including turbomachinery, exhaust gas recirculation (EGR) components and required valves were designed and procured for multi-cylinder engine tests.
- Unique software was developed to support air handling and fuel system controls.
- Preliminary multi-cylinder steady-state engine tests were completed validating models and showing desired 10% improvement in fuel economy while meeting 2010 emission requirements.
- The ISB PCCI engine was tested successfully in a transient environment, showing compliance with 2010 emissions and 10% improvement in fuel economy relative to the baseline.
- Special fuel blends were developed by BP and tested at Oak Ridge National Laboratory and in the Cummins ISB single-cylinder research engine to determine effects of basic fuel parameters on PCCI combustion.
- ISX (15L) heavy-duty single-cylinder testing has been completed showing optimal injection nozzle specifications compatible with ultra-high injection pressure.
- Preliminary ISX steady-state multi-cylinder testing with optimized hardware has demonstrated 6% improvement in fuel economy relative to the baseline.

Future Directions

- Complete multi-cylinder demonstration of PCCI combustion with next generation turbochargers and controls.
- Finalize single-cylinder evaluation of high pressure injection on the ISX engine.
- Complete transient evaluation of ISX high pressure injection, advance air handling recipe.
- Conduct biodiesel fuel study of PCCI combustion utilizing the ISB single-cylinder engine.
- Conduct single-cylinder engine studies of advanced, multi-pulse injection systems.

Introduction

Cummins Inc. is working to develop and demonstrate advanced diesel engine technologies to improve diesel engine thermal efficiency while meeting future emissions requirements. These technologies include low-temperature combustion using premix charge, compression ignition. Reduced equivalence ratio, premix charge in combination with high EGR dilution is expected to result in low engine-out emission levels while maintaining high expansion ratios for excellent thermal efficiency. The various embodiments of this technology require developments in fuel systems, air handling systems and controls. Cummins is committed to demonstrate commercially viable solutions which meet these goals.

In addition to the engine technologies, Cummins is prepared to evaluate fuels, including biodiesel, for their applicability to these new combustion systems. Blend properties of existing diesel fuel stocks will be studied in addition to B20 biodiesel blends.

Approach

Cummins' approach to these project objectives continues to emphasize "Analysis-Led-Design" in nearly all aspects of the research. An emphasis is placed on modeling and simulation results to lead the way to feasible solutions.

Engine system solutions include air handling schemes, control system approaches, and fuel system combinations. Based on extensive model/simulation data, previous testing experience, or verifiable supplier's information, a best-choice solution set of system components is selected. A variety of laboratory tests are conducted to verify performance and to tune system functions. Model predictions are verified and models are refined as necessary. Often, different portions of the system are pre-tested independently to quantify their behavior and their data is analyzed in a model-based simulation before combined hardware testing is conducted. Concurrent to laboratory testing and tuning, a vehicle system demonstration is planned and prepared. 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 as well as resources.

Results

During FY 2006, Cummins Inc. advanced toward the Phase II project goals with a focus on combustion development and enabling technology development. The Phase I simulation predictions were verified in the combustion research single-cylinder test cells. Fuel system specifications were validated in the single-cylinder engine and applied to a multi-cylinder engine. The system simulations were used to specify unique turbomachinery and EGR equipment. This equipment was procured and combined with the combustion recipe in a multi-cylinder engine. Advanced controls were developed to manage the hardware. Finally, multi-cylinder engine tests were completed to verify system performance.

Major Accomplishments in 2006

Demonstration of 2010 transient emissions achieving >10% improvement in fuel efficiency relative to 2007 baseline for the Dodge pickup ISB engine

A unique engine configuration was developed enabling high efficiency PCCI combustion while maintaining emission and combustion noise limits. Phase I work had indicated solutions with high air/fuel (A/F) ratio and high EGR dilution as the keys to achieving these goals. System simulation using GT-Power software assisted with the definition of required air handling hardware to deliver the required charge conditions. This hardware was designed and developed with the assistance of Cummins Turbo Technologies. The control calibrations were then optimized to assess the system capabilities. Figure 1 shows the relative improvement in fuel economy demonstrated as a function of load and speed for the ISB. The green areas of the chart indicate improvement compared to baseline. On a duty cycle average basis, this represents more than 10% improvement when including after-treatment fuel cost avoidance by achieving low in-cylinder NOx control. Cummins continues to utilize the benefits of high-pressure, cooled, recirculated exhaust gas strategy to mitigate NOx emissions. This architecture has been thoroughly production-proven to be effective, efficient and robust.

A fuels design of experiments was created, with fuels blended, supplied, and tested

Cummins, Oak Ridge National Laboratory (ORNL) and BP collaborated to design a fundamental fuels property experiment for PCCI combustion. The fuel main effects selected included cetane, T90, T10 (distillation temperatures), and aromatics. BP engineers designed an appropriate experiment to allow for parameter determination with realistic, available blend stocks (based on a survey of available refinery streams). These fuels were delivered in drum quantity to Cummins

BSFC LB/HP-HR	Engine Speed (rpm)												
Brake Torque (lbf-ft)	800	900	1000	1100	1200	1300	1400	1500	1600	1700	1800	1900	2000
400						-0.003	-0.011	-0.003	-0.002	0.007	0.009	0.023	0.032
350						-0.025	-0.023	-0.015	-0.018	-0.008	0.012		
300							-0.028	-0.025	-0.021	-0.005	0.011		
275							-0.028	-0.024	-0.021	-0.010	0.006	0.020	0.026
250							-0.021	-0.022	-0.024	-0.021	0.005	0.018	0.032
225							-0.011	-0.019	-0.021	-0.017	0.001	0.013	0.034
200	0.000	0.000	0.000	0.000	-0.021	-0.018	-0.011	-0.009	-0.016	-0.016	0.009	0.017	0.026
175	0.000	0.000	0.000	0.000	-0.028	-0.019	-0.028	-0.017	-0.016	-0.020	0.014	0.015	0.022
150	-0.010	-0.031	-0.017	-0.026	-0.017	-0.019	-0.007	-0.027	-0.017	-0.004	0.003	0.009	0.025
125	-0.027	-0.030	-0.008	-0.019	-0.020	-0.014	-0.013	-0.027	-0.021	0.002	-0.002	0.015	0.012
100	-0.002	-0.020	-0.033	-0.025	-0.023	-0.024	-0.026	-0.027	-0.020	-0.019	-0.019	0.013	0.003
75	-0.024	-0.009	0.008	-0.025	0.004	-0.024	-0.019	-0.022	-0.029	-0.017	-0.029		
50	-0.014	0.011	-0.041	-0.036	-0.007	-0.034	-0.032	-0.049	-0.044	-0.041	-0.160		
25	-0.008												

FIGURE 1. Relative Fuel Consumption Improvement

for test on the ISB single-cylinder research engine. Each of 11 fuels is being tested with calibrations centered on the optimized PCCI calibration developed in the concurrent multi-cylinder test work. In addition, smaller quantities of fuel were delivered to ORNL for testing in their baseline, fumigated engine. This testing is complete at ORNL, but the analysis is on-going. This first round of fuels experimentation will be completed prior to the completion of Phase II.

Explored extremely high fuel injection pressures as a means of reducing NOx and particulate matter while improving fuel efficiency

During FY 2006 Cummins investigated the limits of fuel injection pressure and its influence on NOx and particulate matter (PM) emissions. A significant benefit to efficiency with simultaneous NOx and PM reduction was considered theoretically possible and test results verified the model predictions. It is theorized that with high velocity fuel jets (from high pressure injection) fuel parcel equivalence ratios are reduced substantially prior to the start of fast combustion reactions. This combustion method may yield a partial PCCI-type burn, but also increases turbulence for post fast-burn cleanup of soot particles (standard diffusion burn process). Optimized configurations partially developed during the previous Heavy-Duty Truck Program were developed and tested on a multi-cylinder engine. An initial calibration produced the NOx map as shown in Figure 2. Although not demonstrating full 0.2 g/hp-hr capability, initial results are promising and indicate future potential of this technology (Phase III and Phase IV work). These results were obtained while achieving an approximate 6% system improvement in fuel economy relative to the 2007 baseline (including after-treatment avoidance).

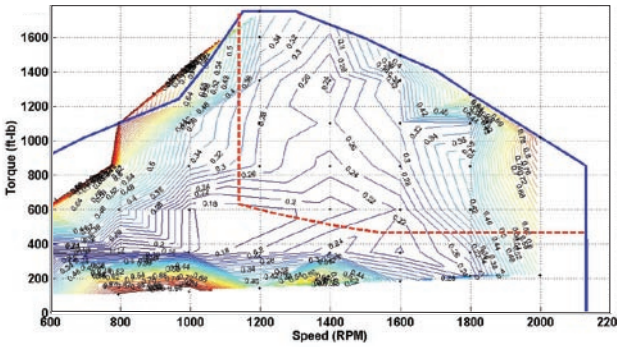


FIGURE 2. ISX High Pressure Injection bsNOx Map

Conclusions

During FY 2006, Cummins developed systems demonstrating PCCI combustion technology and their application for improving fuel economy while meeting stringent emission standards as evidenced by the following:

- Demonstration of a multi-cylinder ISB engine meeting 2010 transient emissions levels while improving fuel economy over 10% relative to baseline.
- Demonstration of an ISX multi-cylinder engine meeting steady-state emissions of 0.25 g/hp-hr NOx while improving fuel economy over 6% relative to the baseline.
- Explored fuel properties and their effects on PCCI combustion.

Our analysis led design commitment has consistently achieved project deliverables.

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II.A.20 High Efficiency Clean Combustion Advanced Combustion Report

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NETL Project Manager: Ralph Nine

Subcontractors:
- ExxonMobil (Paulsboro, NJ)
- Sandia National Laboratories (Livermore, CA)
- IAV Automotive (Detroit, MI)
- Alipro (Peoria, IL)

Objectives

The overall objective of this project is to develop clean combustion technologies that achieve the highest possible brake thermal efficiencies. The approach Caterpillar and its partners are using is a form of homogeneous charge compression ignition (HCCI). The Phase 2 effort is divided into seven areas with the following objectives:

- **Sandia Optical Experiments**: Utilize state-of-the-art optical diagnostics at Sandia National Laboratories to image the HCCI combustion process to gain a fundamental understanding of mixing and combustion.
- **Combustion CFD Model Development Activities**: Develop and validate combustion computational fluid dynamics (CFD) modeling tools so they are fully predictive and can be used to provide fundamental understanding of the mixing and combustion processes, design hardware and limit the amount of testing required.
- **Fuel Property Effects**: Collaborate with ExxonMobil to understand the effects of fuel property changes on fuel/air mixing, combustion, emissions and thermal efficiency in HCCI engines.
- **Cooling System and Heat Rejection Analysis**: Develop technologies to mitigate the increased air and water heat rejection increases associated with HCCI.
- **Advanced Controls Algorithm Development**: Develop required sensors and advanced controls techniques to successfully achieve transient operation on multi-cylinder HCCI engines.
- **Advanced Fuel System Concept Identification and Selection**: Develop state-of-the-art fuel injection technologies to enhance the mixing and combustion process for HCCI.
- **Combustion Development for Advanced Multi-cylinder HCCI Engines**: Develop and demonstrate the advanced multi-cylinder engine technologies necessary to achieve the overall project objectives.

Accomplishments

- Phase 2 optical diagnostic experiments complete on diesel and gasoline fuels.
- Single-cylinder engine fuels testing on low cetane fuels.
- Validated CFD HCCI model completed and in use for combustion development.
- New cooling system methodology developed for selective cooling.
- Preliminary controls architecture developed/ validated on multi-cylinder engine.
- Transient operation demonstrated on multi-cylinder engine with cylinder balancing and fuel trim strategies.
- Prototype fuel injection system developed and tested on single-cylinder engine demonstrating ultra-low smoke emissions.
- Advanced multi-cylinder engine with compression ratio flexibility developed and tested demonstrating benefits for emissions, efficiency and controls.

Future Directions

- Continue optical engine tests to further develop fundamental understanding.
- Refine and validate improved CFD submodels.
- Additional fuels effects testing to discern fuel property effects.
- Refinement of advanced cooling development process and validation with iron tests.
- Improvements to advanced fuel system capability and demonstration of benefits on multi-cylinder engines.
- Refinement of control strategies and implement on advanced multi-cylinder engines.

Introduction

Maintaining and improving fuel efficiency while meeting future emissions levels in the diesel on-road and off-road environments is an extremely difficult challenge. Caterpillar is currently engaged with several partners to address this challenge using a form of advanced low-temperature combustion. This project provides a fundamental understanding of the in-cylinder fuel/air mixing and combustion process through advanced optical diagnostics and computational fluid dynamics. We are also actively developing new fuel injection, controls, heat rejection reduction and engine technologies to enable this clean, efficient combustion. Finally, we are exploring the impact of different fuel types to understand the robustness of this combustion process to fuel variability. 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 powerplants.

Approach

In Task 1 we conducted fundamental optical diagnostic tests at Sandia National Laboratories on a Caterpillar 3171 single-cylinder engine to better understand the HCCI fuel/air mixing and combustion/emissions process in an advanced HCCI engine. The engine was prepared for evaluation of the Caterpillar HCCI method. This preparation included installation of a simulated exhaust gas recirculation (EGR) system, installation of exhaust emissions measurement equipment, modification of the fuel injection hardware and reconfiguring the base engine hardware to match the Caterpillar metal engine hardware. A baseline operating condition was established to match the metal engine data. A suite of optical techniques was then used to characterize the fuel-air mixing and combustion process for this baseline condition.

Task 2 involved model development activities to enhance current predictive capabilities in cycle simulation and 3-D combustion simulation tools. This task included the development and validation of reduced kinetic mechanisms for use in these CFD calculations to model ignition, combustion, and pollutant formation. The optical diagnostic results from Task 1 were to be used to validate and tune CFD models of the combustion process to enable future HCCI combustion development in a virtual environment. The goal is to accurately simulate all of the important processes in HCCI combustion. In particular, the goal is to represent the spray droplet size and spatial distribution, the fuel vapor distribution, wall film thickness and location, combustion, and emissions formation accurately as they happen in a diesel engine. With a more complete model of the HCCI process, modeling activities then focused on refinement of piston bowl and spray geometries to minimize hardware procurement.

Applied research in the area of fuels effects is the subject of Task 3. This work builds upon the collaboration between Caterpillar and ExxonMobil to better understand fuel property effects on HCCI combustion. Prior to shipment of any fuels, standard fuel property tests and detailed chemical characterization of each fuel were performed by ExxonMobil. Both diesel and gasoline fuels were studied in the Caterpillar metal engines and Sandia optical engine with close collaboration among all three organizations.

The cooling requirements for this HCCI engine are higher than normal combustion, and the heat rejection from such a system is a significant challenge to deal with in real world applications. Task 4 included a comprehensive modeling effort that was initiated to understand and suggest alternatives to mitigate this risk. Caterpillar codes Dynasty, 973, COOL1 and a commercial CFD code were used for this analysis. Conventional and alternative heat exchanger designs for clean gas induction coolers and inter/after coolers were evaluated including water-to-gas, gas-to-gas, separate circuit and primary surface heat exchangers.

Advanced controls work was completed on a multi-cylinder engine in Task 5. This work included developing a cylinder pressure based feedback control architecture, utilizing intake valve actuation to balance individual cylinders and using advanced strategies to limit pressure rise rate and engine stall on transient accelerations.

A prototype research fuel injection system was developed and validated on a fuel systems bench in Task 6. This piezo-based research common rail fuel system is capable of multiple fuel injections and >250 MPa injection pressure. An advanced multi-cylinder HCCI engine was also developed and tested. This engine has full variable compression ratio flexibility as well as variable valve timing flexibility. It has been used to demonstrate the performance, emissions and controls benefits as such an engine can potentially offer.

Results

Task 1- Sandia Optical Engine Tests: Many upgrades to the laboratory were completed in the first full year of the project. These included adding enhanced CO_2 capability for simulating EGR and purchasing or installing new emissions equipment to better characterize the gaseous and particulate emissions. A Karl Storz borescope and C-mount camera adaptor were procured. The borescope was used with a Phantom 7.3 high speed camera that was purchased through a DOE equipment grant. Timing control hardware is also in place to allow for high-speed imaging synchronized in time or with crankshaft position.

Shortly after work on this project commenced, it became evident that a peak cylinder pressure (PCP) capability of 20 MPa would be necessary to study high-load operating conditions of interest. This amounts to nearly doubling the PCP capability of the optical engine. Thus, all the combustion chamber components required re-evaluation for safe operation at 20 MPa PCP. Tests were done on drilled 3171 connecting rods on a reciprocator at Caterpillar to verify that the fatigue life of the current design was acceptable. Finite-element analysis (FEA) was done on a new design of the optical piston. FEA showed a number of highly stressed areas of the quartz piston window. The brittle nature of quartz means that the final piston design must all but eliminate tensile stress within the piston window; this often requires the use of complex shapes to ensure loads caused by PCP and piston motion result in mostly compressive stress within the piston window. Additional work yet remains to refine the new optical piston to achieve a design capable of 20 MPa PCP at 2,100 rpm.

Spray visualization for gasoline (G23) at 1,200 rpm, 300 kPa and 1,200 rpm, 400 kPa conditions was completed along with cycle integrated natural luminosity (CINL) imaging. These images were collected using a single camera gain within one order of magnitude of the varying camera gains used to acquire the diesel D14 CINL images in last year's report. The G23 CINL images do not show several bright spots of combustion luminosity which were observed for three of the four D14 load points. It was not expected to see such bright spots, since the G23 spray visualization showed the inner cone of fuel jets vaporizing before reaching the surface of the piston window. Figure 1 shows a set of averaged G23 CINL images for the three load points. In contrast to the diesel images which showed significant liquid impingement of the spray on the piston bowl (which resulted in high smoke emissions), these gasoline images show no evidence of liquid impingement and explain why the smoke emissions were negligible.

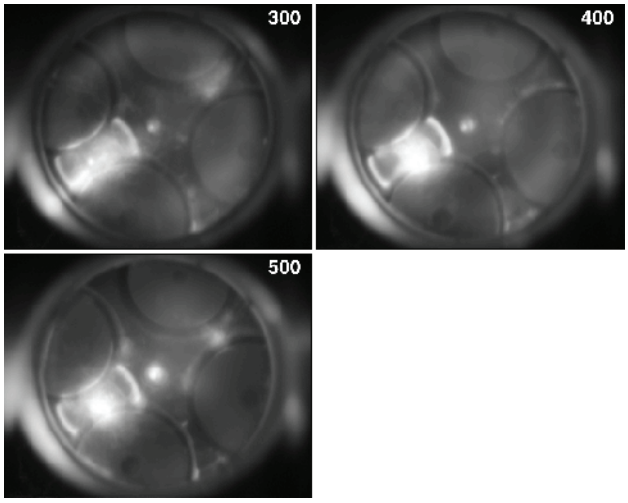


FIGURE 1. Gasoline (G23) Averaged CINL Images

Task 2 - Combustion CFD Model Development Activities: Significant improvements in the areas of liquid to gas momentum exchange, wall film treatment, and chemical kinetics have been made to the in-house CFD code, CAT3D. This has made it possible to apply the tool to gain a deeper understanding of the physical processes underlying HCCI combustion. Simulations of the Caterpillar metal and Sandia optical engine have provided valuable insights into the mixing and combustion processes. The CFD tool has been used to design piston bowls for the single and multi-cylinder engines and it was also used to evaluate the effects of glow plug and ion sensor location on cold-start behavior and signal-to-noise ratio, respectively. The results indicate that the CAT3D-simulations are able to capture effects of injection timing and sensor/glow plug location on the recorded ion signal. We have successfully linked regions of high temperature and large concentrations of O-radicals to regions of strong ion signals. In order to increase the accuracy of the analysis, detailed chemistry of ion formation would need to be incorporated into the n-heptane mechanism utilized to describe the heat release. This is a long-term goal, which would require significant development.

Task 3 - Fuel Property Effects Evaluation on Single-Cylinder Engine: Fuel effects testing is planned to be completed in the 4th quarter of 2006.

Task 4 - Cooling System and Heat Rejection Analysis: The goal of this work is to mitigate the increase in jacket water heat rejection (JWHR) with advanced combustion strategies in the cylinder liner and head by developing a process utilizing analytical tools which accurately predict heat transfer inside the engine. Once prediction capability is achieved, the cooling circuit passages can be designed to minimize heat transfer, while still maintaining structural life of the engine due to thermal cycling. The end-user benefit due to reduced heat rejection is a smaller frontal area cooling system and/or reduced fuel burned for cooling fan parasitic power. The premise is that the current structural development process utilizes coolant flow to keep the hottest areas of the engine (top land of liner and valve bridges) below material property design limits, and to achieve a desired structural life with combined assembly stresses plus thermal stress gradients. All excess jacket water pump flow is forced through the block and liner, resulting in overcooling of much of the iron and absorbing more jacket water heat than is necessary. Reduction in JWHR comes through reducing velocities of coolant in overcooled areas; hence the term "Precision Cooling". Success is only achieved by the integration of engine performance, jacket water coolant flow, and core engine cooling - including the prediction of boiling and structural analyses.

The method for developing predictive analysis tools for Precision Cooling JWHR has been to make the analytical prediction on a well defined baseline engine (Cat C15) as well as its external cooling system, run appropriate tests, and then correlate/tune the analysis models to match test results. This preliminary step has been completed. Once this capability is achieved, then design changes to the coolant passages of the engine can be made analytically with design iterations, possibly with optimization software, to minimize JWHR. The impact on structural life will also be predicted and compared with a baseline prediction. The reduction in heat load benefit can then be quantified by modeling in terms of external cooling system fan parasitic fuel consumption or a reduction in frontal area.

Task 5 - Advanced Controls Algorithm Development: A rapid prototyping system was developed for controls development using Matlab/Simulink software for model building and code generation. The rapid-prototyping hardware included a Caterpillar designed programmable field programmable gate array card enabling processing of speed-timing pulses from the crank/cam targets and generation of the output pulses needed for the various engine sub-systems such as fuel injection.

Demonstration of transient operation of an HCCI engine has been completed. This response depends on the maximum rate at which fuel can be added into the combustion chamber without causing undesirable operation (based on emissions and performance). For a HCCI engine the two parameters that limit the maximum fuel rate are rate of pressure rise and emissions. The rate of pressure rise primarily depends on the amount of EGR and the combustion-phasing angle. The emissions primarily depend on air/fuel ratio, amount of EGR, fuel injection pressure and the combustion-phasing angle. Hence, five different control inputs are identified that can affect the transient operation of the HCCI engine. These are compression ratio (CR), intake valve actuation (IVA, for the purpose of this report it is the crank angle at which intake valve is closed), EGR, fuel injection pressure and end of fuel injection angle (EOI). All of these parameters can be controlled in real time using our existing control architecture. Utilizing the variable compression ratio (VCR) engine shown in Figure 2, compression ratio is an additional control knob that was not available in our previous transient testing on the fixed compression ratio engine. Real time control of compression ratio (CR) is achieved using a feedback from position sensors on the hydraulic pistons that are used to change CR. In addition, oxygen sensors are installed in the intake and exhaust manifold to provide real time information on amount of EGR flowing into the cylinder. The oxygen sensors have a response time of ~150 ms, which is fast enough to provide real time EGR control. Intake valve closing angle is primarily

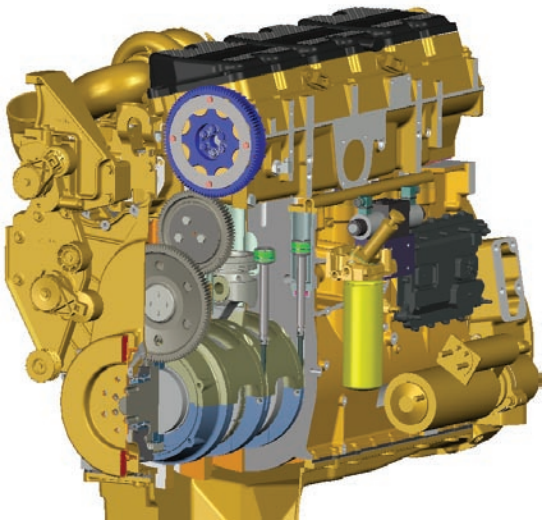


FIGURE 2. Variable Compression Ratio Engine

used for combustion phasing control. Solenoid control injectors are used to control the fuel injection pressure and injection angle in real time.

In order to best model the system, models must be developed that account for multiple inputs and non-linear behavior. Artificial neural networks have been chosen as one option to provide the level of accuracy and computational efficiency required. A neural networks based approach requires collecting a diverse set of output data (emissions and performance) for a widely varying range of input parameters. Hence, a map-based approach is followed to accommodate a different set of input maps for a widely varying range of input parameters. A key requirement in successfully capturing the system response in a data driven approach (like neural network-based modeling) is to collect output data for almost all possible input parameters combinations. Since it is not realistically possible to exploit all possible input combinations a large number of maps (~35) were generated to accommodate sufficient combinations of input parameters.

Transient operation of a multi-cylinder HCCI engine within two points in the engine operation condition was demonstrated. Various control maps were generated for different control inputs (IVA, EGR, CR, EOI and injection pressure) and these maps were loaded into engine control software to perform a specified speed-load transient. These transients provide understanding of the effects of different control parameters on performance parameters during transients. This understanding helped in developing better maps for different control parameters, which allowed transients to be performed with much higher speed load ramp values. The input-output data recorded during these transients are also utilized to develop the neural network-based

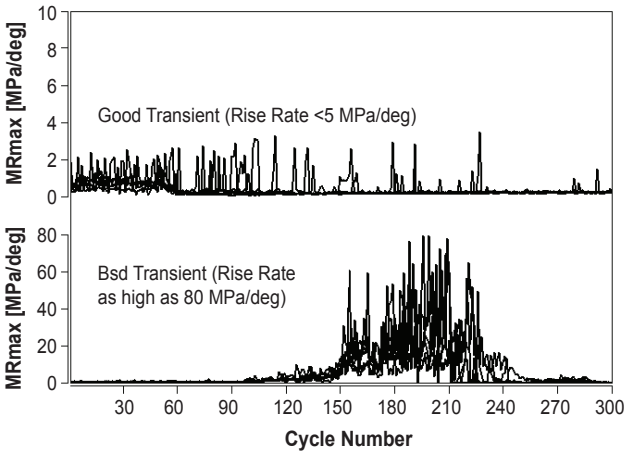


FIGURE 3. Comparison of Rise-Rates Achieved During Two Different Transients in MPa/deg

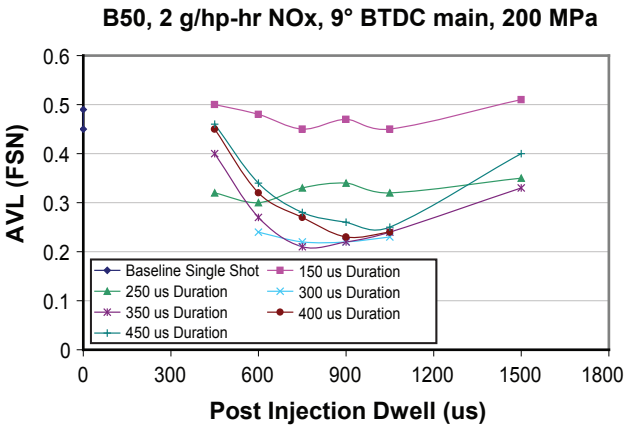


FIGURE 4. Effect of Post Injections on Smoke Reduction Using Advanced Fuel System

model for the engine. These models were used to perform multi-variable optimization on different input parameters and can be instrumental in developing optimum transient control strategies for the HCCI engines. Moreover, response time characterization of some control parameters is done to identify limitations of the current engine hardware. Examples of baseline and improved transient operation with regard to maximum rate of pressure rise are shown in Figure 3.

Task 6 - Advanced Fuel System Concept Identification and Selection: An advanced common rail fuel system was developed to enable low emissions and high efficiency combustion. The first version (Phase 1) features the ability to perform pilot injections of less than 5 mm^3 at rail pressures greater than 250 MPa with dwell between injections of less than 200 microseconds. The Phase 1, piezo actuated injector has been fully characterized on the single-cylinder test engine. Several discrete test programs have been successfully completed, which have demonstrated the benefits of the high injection pressure, and the multiple injection strategies, facilitated by this advanced injector. These initiatives included air/fuel ratio sensitivity to simulate a fuel/air ratio control limit during transient response, a lifted flame combustion strategy, ACERT™ early pre-mixed pilot, multiple injection strategies, and post injection optimization. Benefits of post injections on smoke reduction are shown in Figure 4.

Task 7 – Combustion Development for Advanced Multi-cylinder HCCI Engines: A new variable compression ratio engine was built and tested. The operational limits of the VCR HCCI engine were examined at two different engine loads. Specifically, the engine was run at all possible combinations of compression ratio, EGR fraction and IVA that yielded a combustion phasing of 2° ATDC. Intake temperature and fuel injection timing, which are the other two parameters that can affect combustion phasing in this particular engine, were held constant for those tests. Tests were conducted at 1,500 rpm, quarter (B25) and half load (B50) operating conditions. In general, the range of IVA, EGR and CR settings over which the engine could run with a near-top dead center combustion phasing was limited by either rise rates, combustion retard, air-fuel ratio, NOx emissions or VCR mechanism limitations. The first sweeps were for three different combustion phasings from a baseline operation of fixed compression ratio, EGR fraction and IVA setting which represented the best fuel consumption point at B25. The first sweep of combustion phasing was obtained by varying IVA from its baseline value while holding compression ratio and EGR constant. The second sweep was obtained by varying the compression ratio from its nominal setting while holding IVA and EGR constant, while the third sweep was obtained by varying EGR from its nominal setting while holding IVA and compression ratio constant. This set of data explored the effects of combustion phasing and highlighted the differences between the various methods by which the desired combustion phasing can be achieved. The second set of data consists of several EGR sweeps, each at a different combustion phasing value. This new data set illustrated how the limits of engine operation change for different values of combustion phasing. An understanding of this is required to get the complete picture of the interaction between CR, EGR, IVA and combustion phasing.

FY 2006 Publications/Presentations

1. Q1, Q2, Q3 Quarterly reports
2. Phase 1 Topical report
3. Presentation at 2006 DOE DEER Conference
4. Presentation at 2006 SAE HCCI Symposium
5. Paper submitted to 2007 SAE Congress

Special Recognitions & Awards/Patents Issued

Patents Applied for:

- Ignition Timing Control With Fast and Slow Control Loops (IVP and EGR).
- Mixed High and Low Pressure EGR in HCCI Engine.
- Strategy For Extending the HCCI Operation Range Using Low Cetane Number Diesel Fuel and Cylinder Deactivation.
- Recipe for High Load HCCI Operation.
- Power Balancing Cylinders in HCCI Engine.

II.A.21 Low Temperature Combustion Demonstrator for High Efficiency Clean Combustion

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

Objectives

- Complete initial subsystem evaluation including turbo, pistons, injectors and variable valve actuation (VVA) system.
- Procure fuel injection equipment (FIE) controller hardware. Make FIE hardware available to support subsystem testing. Complete fuel bench and injector calibration testing.
- Provide control system. Controller to operate engine exhaust gas recirculation (EGR), variable nozzle turbine (VNT) and FIE subsystems. The first objective is a device/communications checkout of the rapid prototyping system with the sensors and actuators associated with these subsystems.
  A second objective is to ensure that the controller and these subsystems are stable under steady-state engine operating conditions.
- Initial test of cylinder pressure based algorithms. They are to operate at the highest engine operating speed with cylinder pressure sampled on all engine cylinders at the highest running engine speed at least at every degree of crank angle rotation (every 4^{th} degree during exhaust/induction).

Accomplishments

Phase II of project consists of procurement and demonstration of functionality of individual components on the engine designed in Phase I. The engine, based on the ITEC 6.4L V8 platform, was redesigned to support a low-temperature or homogeneous charge compression ignition (HCCI) combustion mode for high efficiency and low emissions targeting 2010 federal emission standards using standard diesel fuel. The engine is designed to operate in HCCI mode up to 12.6 bar brake mean effective pressure (BMEP).

The key technologies implemented and function tested to date consists of engine build items:

- A custom charge air cooler (CAC) and intake heater bypass system.
- Three sets of new injector nozzles providing better atomization and mixing.
- Piston with a reduced compression ratio.
- An injector bench test unit and calibration procedure used to validate new injector drivers and map injector characteristics prior to engine installation.

Control system development items including:

- Stand alone processor, with crank angle based data acquisition was implemented with flexible control over custom injector drivers.
- Software was developed to provide combustion diagnostics based on cylinder pressure feedback control, allowing for control over start of combustion and torque.
- The control system has control over EGR, VNT and CAC/intake heater bypass.

With these systems HCCI combustion was demonstrated in a limited region of operation. Further development of this work is to be undertaken in Phase III.

The following items are in process to be completed:

- A two-stage turbocharger and EGR cooler system with a custom mixer. Parts have been received and are awaiting engine installation.
- An improved flow cylinder head was designed and is being procured with flush-mounted pressure transducers.
- A VVA system was designed and is currently being fabricated.

Future Directions

- Commission control system on engine. Engine controls will include FIE and VVA hardware with cylinder pressure feedback software. Controls are to run stable under steady-state conditions.
- Demonstration of 2010 emissions targets at target engine rating. Conduct engine testing under steady-state at target points.

Introduction

HCCI offers a new method of diesel combustion with the potential to reduce engine-out NOx and PM emissions to levels that will meet the 2010 limits without the use of aftertreatment devices [1]. The benefits of HCCI combustion have been well documented in the literature [2,3,4]. In general, the benefit of implementation of HCCI technology is lower emissions of NOx due to low temperature burn and improved fuel economy and lower PM emissions due to lean mixtures.

Approach

Implementation of HCCI combustion to a production engine poses several difficult challenges. HCCI combustion does not have a direct means of control such as spark timing for a spark ignition (SI) engine and injection timing for a compression ignition (CI) engine. HCCI auto-ignition occurs when the auto-ignition temperature is reached in-cylinder. This temperature is sensitive to in-cylinder and intake manifold conditions. Any mismatch can lead to either misfire or very rapid heat release rate. Therefore, the development of an advanced in-cylinder feedback control will be required for commercialization of this technology.

Diesel HCCI combustion exhibits a narrow operating range [5,6]. As speed and load is increased diesel HCCI has a tendency to knock. Research work has been performed to expand the region of operation [7,8,9], but limits have not been able to extend to today's production levels. The present effort attempts to expand the operating region using a combination of VVA and possibly a form of variable compression ratio (VCR). In addition, a control system will be implemented to handle the complexity of in-cylinder pressure feedback control, VVA and VCR actuation control.

Results

The engine used in the present study is the International 6.4L V8. It is modified to target operation with equivalence ratios ranging 0.3-0.4 and EGR ratios of 40-50%. The engine displacement, with these targets of equivalence ratio and EGR, in conjunction with the air and cooling capabilities, will allow a maximum torque of 670 Nm (500 ft-lbf) at 2,000 rpm, corresponding to 12.6 bar BMEP. Figure 1 shows the engine lug curve and 50% load line. The engine system schematic for the lab setup is illustrated in Figure 2.

Fuel Injector bench testing was performed on a baseline injector and on the HCCI injectors. The first tested HCCI injector (16-hole) had a lower flow rate. For full open needle position the flow rate reduction is 14% (Figure 3). The driver which will substitute the power control module (PCM) drivers is a custom driver allowing for greater flexibility in voltage and charge energy to the piezo stack. The current levels can therefore be tailored to approximate the base driver as shown in Figure 4.

Turbocharger performance characteristics were finalized and hardware selected. Two configurations are available, a cooled and non-cooled inter-stage unit. The first combination gives improved turbine performance, the high-pressure unit operating at higher efficiency. The intake manifold temperatures are nearly identical owing to the performance of the charge air cooler and its capability to bring down the post compressor temperatures.

The EGR system is designed to handle 26 lb/m EGR mass flow while keeping cooling effectiveness to approximately 82%.

The VVA system provides an effective use of space and has minimum impact on the injection system (preserving original feed tube lengths). The arrangement

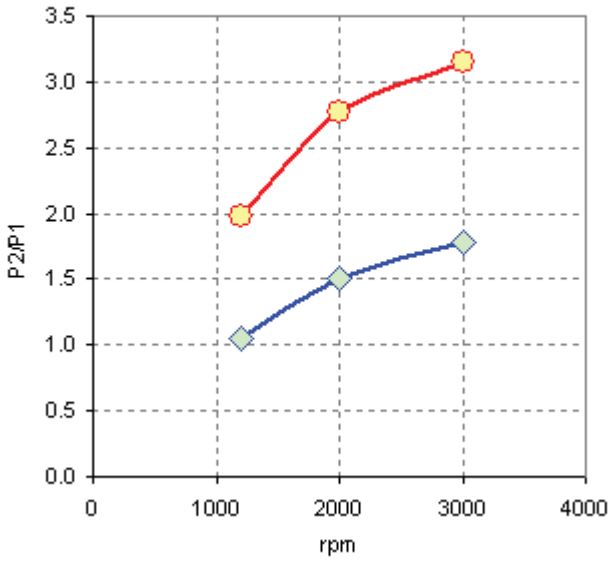


FIGURE 1. Engine Operating Conditions (Turbocharger Compressor Ratio; Top Line: 50% load; Bottom Line: Lug Curve)

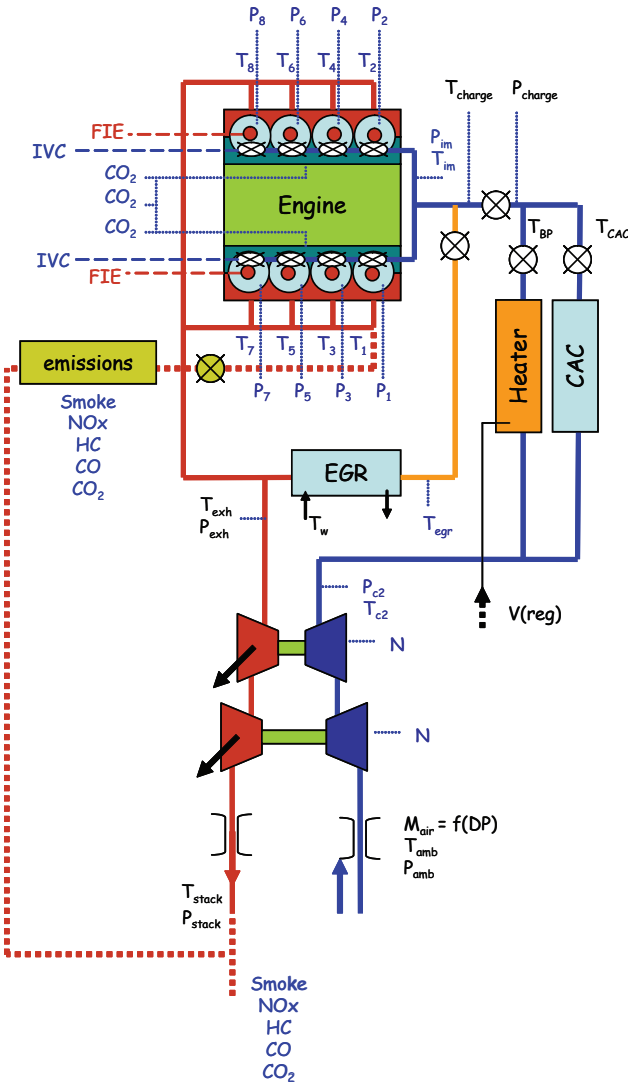


FIGURE 2. Engine Layout

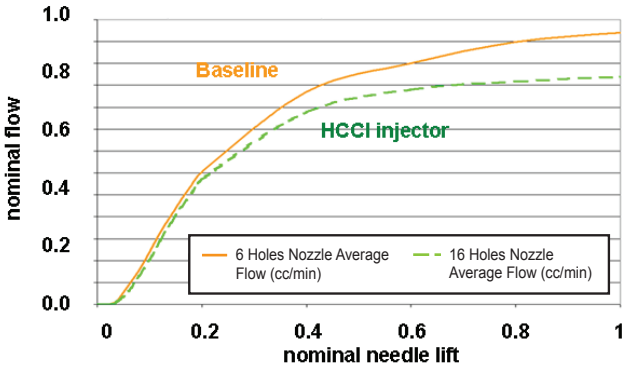


FIGURE 3. Injector Flow Comparison

allows for positioning of pressure sensors on rail and feed tubes. A new valve spacer and cover were adopted

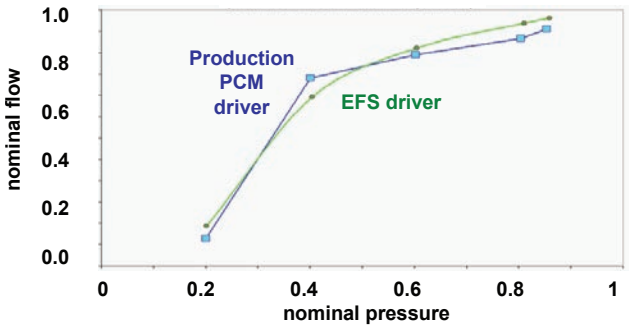
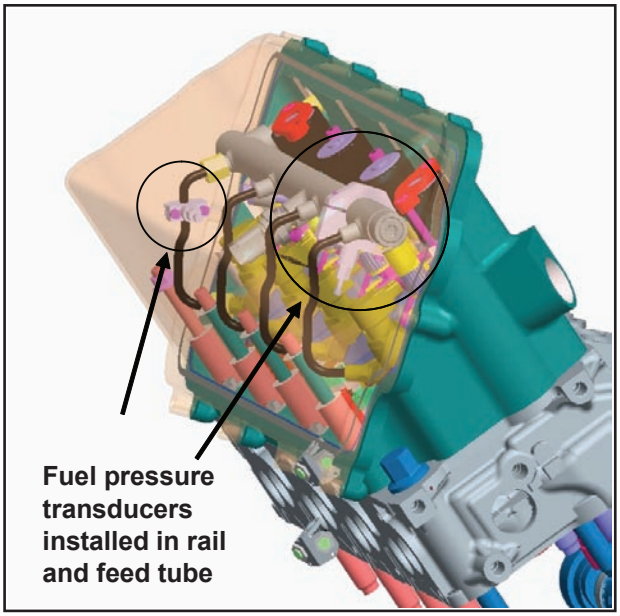


FIGURE 4. Effect of Driver on Injector Characteristics



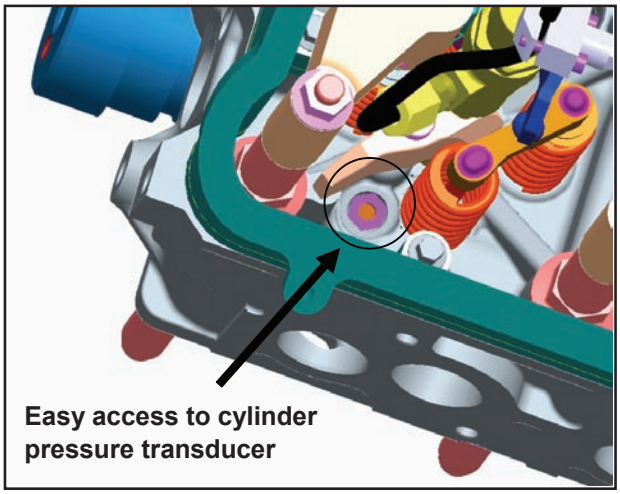


FIGURE 5. JVS Valve Actuation Packaged on a 6.4L V8 Cylinder Head

to accommodate the increase height (on the order of 50 mm) and allow easy access, including access to pressure transducers (Figure 5).

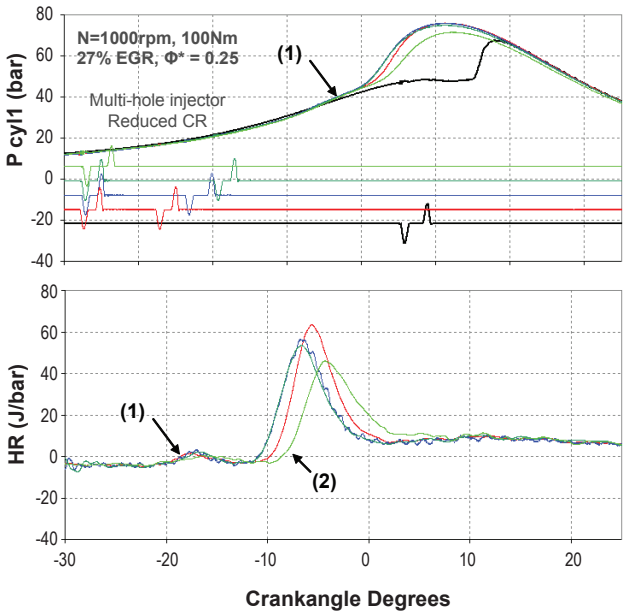


FIGURE 6. HCCI Combustion With Multiple Injection Strategies

Cylinder Head Modifications. The base engine was designed using inlet ports with relatively high swirl. As the HCCI engine would not require high swirl for mixing, an opportunity to improve the flow capacity of the ports was identified and achieved by setting a low swirl target of 0.5. The modifications yielded a 30% flow improvement.

Combustion Results. Though the nature of HCCI work is more properly within the scope of next phase of the project, the installation of new hardware and the ability to command the injection system by means of the rapid prototype system, served to explore the HCCI regime. The effect is shown in Figure 6. Under these conditions a cool flame is observed at 20º BTDC. Similar conditions with the base hardware did not show a cool flame.

Conclusions

- A baseline V8 engine was procured and delivered to support initial subsystem evaluation. Pistons and HCCI injectors were delivered. Turbocharger system has been delivered but awaits installation.
- VVA system has been designed and is awaiting fabrication (targeted for February 2007).
- FIE controller hardware has been procured. Fuels bench and injector calibration was initiated.
- Controller operates the engine subsystems, EGR, VGT, intake throttle valve (ITH), CAC and FIE satisfactorily; stable under steady-state conditions.
- Initial testing of the cylinder pressure engine management has been completed. Algorithms operate at 3,600 rpm. Cylinder pressure data is sampled at 0.5 degrees resolution.

The following Phase III (scheduled for November 2006 – March 2008) deliverables were also achieved in advance:

- Detailed design of modified cylinder head has been completed. Modified cylinder head is expected in December 2006.
- Control system has been commissioned on the engine. Engine controls system was implemented in engine on dyno with the ability to control the engine torque and start of combustion under steady-state conditions.

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1. Multicylinder Diesel Engine Design for HCCI operation, William de Ojeda, Alan Karkkainen, Diesel Engine Development, DEER 2006, August 20-24, Detroit, Michigan.

2. Development of a Multi-Cylinder Diesel Engine for HCCI Operation, William de Ojeda, SAE Homogeneous Charge Compression Ignition Symposium 2006, Sep. 25-26, San Ramon, California.

II.A.22 Heavy-Duty Stoichiometric Compression Ignition Engine with Improved Fuel Economy over Alternative Technologies for Meeting 2010 On-Highway Emissions

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Objectives

- Apply the stoichiometric compression ignition (SCI) concept to a 9.0 liter diesel engine.
- Obtain engine-out NOx and PM exhaust emissions so that the engine can meet 2010 on-highway emission standards by applying a three-way catalyst for NOx control and a particulate filter for PM control.
- Optimize the engine and air system to approach 50% thermal efficiency using variable valve actuation (VVA) and electric turbo compounding.
- Demonstrate that the engine with exhaust aftertreatment meets 2010 on-highway emission standards with maximum thermal efficiency.

Accomplishments

- Demonstrated that an advanced diesel engine can be operated at stoichiometric conditions with reasonable particulate and NOx emissions at full power and peak torque conditions.
- Calculated that the SCI engine will operate at 42% brake thermal efficiency without advanced hardware, turbocompounding, or waste heat recovery.
- Determined that exhaust gas recirculation (EGR) is not necessary for this advanced concept engine, and this greatly simplifies the concept.

Future Directions

Since the SCI concept has shown reasonable engine-out NOx and PM emissions with good fuel economy potential, the next critical issue is whether the three-way catalyst will provide the necessary NOx control. At the same time, further refinement of this engine concept is being conducted to improve the fuel efficiency. The near-term future work in rough chronological order is:

- Procure three-way catalyst and write software to control air/fuel (A/F) ratio to properly operate the catalyst.
- Determine if the three-way catalyst NOx efficiency will be acceptable (>95%).
- Improve combustion system based on computational fluid dynamics (CFD) results and experiments to increase combustion efficiency and reduce smoke.
- Optimize the air system for the lower flows inherent with stoichiometric operation.
- Order VVA system for engine control at lighter loads.
- Determine heat rejection and evaluate thermal loading on in-cylinder components.

Introduction

Various concepts have been proposed to meet the 2010 on-highway emission standards with improved fuel efficiency. The stoichiometric compression ignition (SCI) engine concept combines advantages of a diesel engine with simple, reliable exhaust aftertreatment to provide low emissions with superior fuel economy.

In this concept, a diesel engine operates at stoichiometric at all times so that a three-way catalyst can be used to control NOx to very low levels without adding additional fuel or other chemicals. Because the engine-out NOx emissions are reduced substantially by the catalyst, the combustion process in the cylinder can be improved to increase fuel efficiency. The reduced air flow and increased exhaust temperature due to stoichiometric combustion allow further engine changes to improve system fuel efficiency.

Approach

For this research a John Deere heavy-duty engine is being used. The initial task was to demonstrate a diesel engine running at stoichiometric to assess the viability of the concept. After conducting some air system simulation and computational fluid dynamic calculations of the combustion process, the engine was operated at full power and peak torque. Optimization of the combustion and air system is being conducted, and exhaust aftertreatment hardware and a VVA system will be procured.

The 2010 on-highway emission standards will be demonstrated using VVA and exhaust aftertreatment, and then an electric turbo-compounding system will be added. Further optimization will be conducted to obtain the goal of 50% overall engine thermal efficiency. Finally, the complete system will be integrated into a prototype vehicle and the performance and fuel economy of the advanced SCI engine will be evaluated.

Results

A John Deere six-cylinder 9.0 liter (9L) engine rated at 248 kW at 2100 rpm was used for testing. The air system and injection system were modified during development. In this first year of the project three series of engine tests were conducted.

In the first series several injector nozzles were evaluated at loads up to 50%, since the air system would not provide EGR at higher loads and therefore turbine inlet temperatures became excessive. With the preferred nozzles, smoke and particulate levels were acceptable, but the air system needed to be modified to provide the required EGR at higher loads.

For the second set of engine tests, the John Deere 9L engine was plumbed to use both high-pressure-loop EGR and low-pressure-loop EGR. However, it was found that there was an engine control stability problem when using the high-pressure-loop. Simulation work confirmed that this control instability was inherent with high-pressure-loop EGR. Using low-pressure-loop EGR, full load rated speed and peak torque conditions were obtained at stoichiometric A/F ratio, although considerable intake, exhaust, and charge cooler restriction had to be added to reduce the air flow to the proper level.

The smoke emissions were high using the production injection system at 200 MPa injection pressure, so six different nozzle configurations were evaluated at peak torque and rated power conditions, and some trends were observed. The smoke responded to normal combustion system variables like spray angle, hole number, injection duration, injection timing, etc., but remained high. As expected, smoke was very sensitive to equivalence ratio, so exhaust emissions were used to determine this. This is commonly referred to as the carbon balance method (CBM). NOx emissions were low, and therefore the 2010 on-highway standard should be easily achievable with a three-way catalyst. The engine brake specific fuel consumption (BSFC) was higher than expected because of the additional restrictions necessary to reduce the air flow. During the testing, cylinder pressure data was collected and provided to Ricardo and Purdue to incorporate into their modeling work.

With the six hole nozzles, test points were obtained near stoichiometric with approximately 750°C turbine inlet temperature (obtained by varying EGR percentage). This turbine inlet temperature limit was necessitated by the variable turbine geometry (VTG) turbocharger. Analysis of the data showed that smoke was quite sensitive to EGR percentage and that the EGR levels and exhaust temperatures were slightly different among the data points. Therefore, linear regressions were generated for both engine operating conditions (peak torque and rated power).

Regression results predicted smoke from the best nozzle at stoichiometric with 750°C exhaust temperature to be 5.6 Bosch at rated and 5.2 Bosch at peak torque. The conclusion from the analysis was that we needed further nozzle changes and reduced EGR (increased exhaust temperature). The strong effect of EGR on smoke suggested that eliminating EGR would greatly reduce the smoke, and results from other engine development activities without EGR have given smoke levels of 1 to 2 Bosch at stoichiometric, which should be acceptable for the diesel particulate filter (DPF). Therefore, means to allow engine operation with reduced EGR were sought. It was decided that using a water-cooled exhaust manifold would give reasonable turbine inlet temperature without EGR. Although this was expected to give acceptable smoke levels, NOx emissions became a concern. However, since the NOx removal efficiency of a three-way catalyst in diesel exhaust is unknown, the maximum acceptable NOx level is unknown.

The CFD model of combustion in the 9L engine was updated using the cylinder pressure data at rated power and peak torque from this second series of engine tests. The simulation predicted some of the PM changes with nozzle changes, but there were some discrepancies. A brief examination of changing the piston bowl shape did not indicate a significant improvement was likely.

Meanwhile, further refinement of the engine simulation with low-pressure-loop EGR indicated that 200 g/kWh BSFC (42% brake thermal efficiency) was achievable, although additional backpressure has to be added after the DPF in order to drive the clean EGR to the compressor inlet. Attention was shifted to the water-cooled exhaust manifold without EGR, and the heat release was changed to represent combustion

without EGR. The WAVE simulation predicted that without EGR 40 to 42% brake thermal efficiency was achievable even with exhaust aftertreatment. Also, this engine simulation work showed that VTG turbocharger with about twice the flow of the production turbocharger was needed to avoid excessive boost. Unfortunately, no VTG turbocharger was available with suitable turbine and compressor sizes. This is because unusually high exhaust energy is available with the SCI engine while only moderate boost levels and flows are needed from the compressor. Therefore, a larger fixed turbocharger with a pneumatically-operated wastegate on the turbine housing was used for the third series of engine tests. Although the air system was not optimal, the goal was to achieve proper in-cylinder conditions in order to determine the NOx and PM emissions. Then measured engine performance data can be adjusted using simulation to represent an air system designed for the SCI engine concept.

It was originally intended that the third series of engine tests would use the experimental Sturman S1.3 VVA system with elevated injection pressures. This is an intensified injection system that uses fuel at up to 120 MPa to drive a piston which pressurizes the injected fuel up to 300 MPa. Sturman Industries adapted the system to the Deere 9L engine with an electronic control unit (ECU) to drive the injectors, while the Deere ECU controlled the VTG turbocharger and EGR system. The engine with the injection system installed was tested for operability and shipped to Deere. However, injector and nozzle failures with the Sturman S1.3 system at about 240 MPa on the test stand at low hours have been a concern. The nozzle failures are apparently due to pressure spikes generated by the intensifier system, since the same nozzles have much longer life when used at the same pressure with the production common rail system. Sturman is exploring nozzle design alternatives. Because of the lack of robustness of the Sturman injection system, the third series of engine tests used experimental Denso G3 injectors, which are very robust at pressures above 220 MPa. To provide sufficient high-pressure fuel to operate these injectors, an available experimental setup using a gearbox to drive two Denso rail pumps was used initially. Unfortunately, the gearbox failed early in the testing, so a single pump was used for most of this test series, which limited the available rail pressure, especially at lower engine speeds.

The third series of engine tests was run without any EGR to reduce the smoke and particulates. To reduce the turbine inlet temperature to an acceptable level (750 to 800°C), a water-cooled exhaust manifold was installed. This manifold is used for marine versions of the 9L engine. Estimates indicated that the coolant heat rejection from the water-cooled exhaust manifold would be similar to the heat rejection from cooling the EGR in the previous setup. However, a future turbocharger design that will tolerate higher turbine inlet temperatures would reduce the need for exhaust cooling and improve the engine system efficiency.

In addition to the water-cooled exhaust manifold, a large wastegated turbocharger was installed, since the available VTG turbocharger had been unable to reduce the boost to the required level. Even with the wastegate wide open and the water-cooled exhaust manifold, it was found that the boost was excessive, so additional intake, charge cooler, and exhaust restrictions were added. A wide-range oxygen sensor was used to quickly set the operating conditions to stoichiometric, and with this sensor, we were able to consistently collect data very near to stoichiometric.

While maintaining stoichiometric A/F ratio, rail pressure and injection timing were varied at rated power and peak torque conditions. The test results are compared to previous data with EGR in Figures 1 and 2, where the results without EGR have high NOx and low smoke. It can be seen that the smoke goal was met without EGR, although NOx was higher than desired. However, the NOx goal was based on an assumed efficiency for the three-catalyst. If the NOx removal

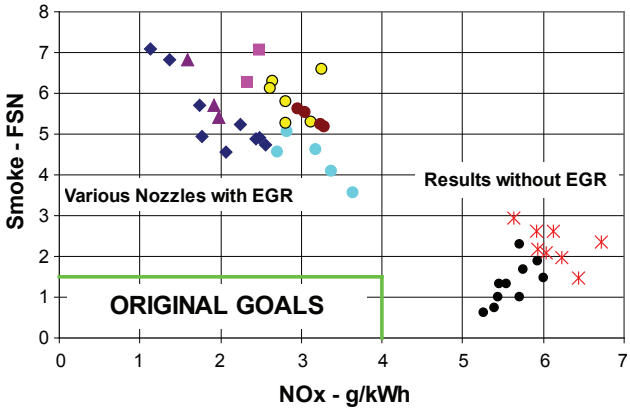


FIGURE 1. Comparison of Results from Second Test with EGR and Third Test without EGR at FLRS

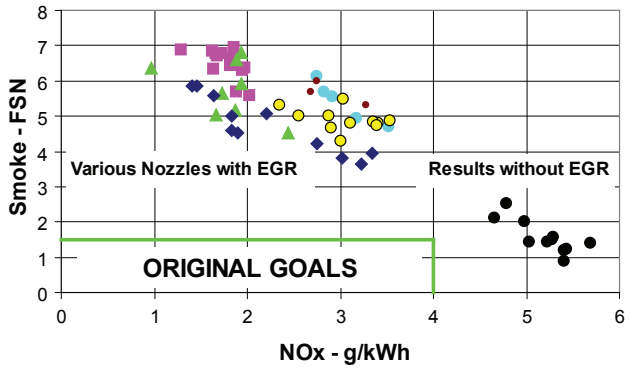


FIGURE 2. Comparison of Results from Second Test with EGR and Third Test without EGR at Peak Torque

efficiency is sufficiently high, the engine-out NOx of 5 to 6 g/kWh would be acceptable. Figure 3 shows engine-out emission results at full load rated speed (FLRS) and peak torque are within our revised goals. It should be noted that these emission results will be further improved with an optimized air system because the engine will generate more power while using the same amount of fuel and air. The results on the SCI engine without EGR are summarized by the rated power and peak torque operating points tabulated in Table 1. The results show reasonable NOx at 5.4 g/kWh and reasonable PM at 0.13 g/kWh. The measured BSFC is shown for reference, but it is high because of extra air system restrictions and an inefficient turbocharger with an open wastegate. WAVE simulations by Ricardo are being used to optimize the air system and predict the fuel economy with reasonable components and restrictions.

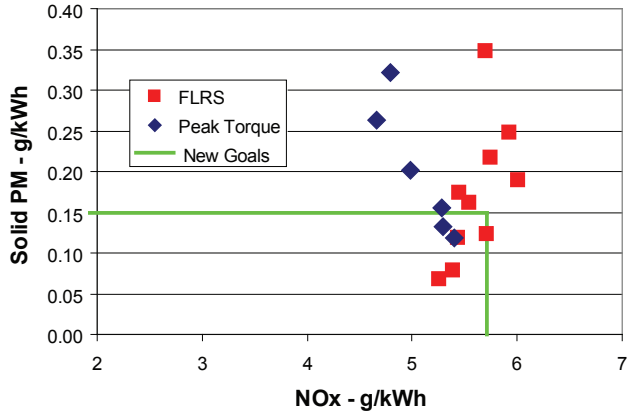


FIGURE 3. Engine-Out Emission Results without EGR

TABLE 1. Tabulated Summary of Operation at FLRS and Peak Torque without EGR

Speed	rpm	2100	1575
Torque	N-m	1124	1522
Smoke	FSN	1.0	1.2
Turbine Inlet	°C	798	767
O_2	%	0.5	0.5
HC	g/kWh	0.00	0.01
CO	g/kWh	16.1	26.9
NOx	g/kWh	5.4	5.4
PM	g/kWh	0.13	0.12
BSFC	g/kWh	*234.0*	*219.2*
Inlet Restr.	kPa	7.0	3.2
Intercooler Restr.	kPa	17.3	12.2
Exhaust Restr.	kPa	16.7	9.4

The recent tests of the SCI engine concept without EGR gave good combustion with reasonable NOx and smoke. Therefore, it does not appear that extremely high injection pressures will be necessary to have acceptable smoke and particulate emissions, although additional injector nozzles have been ordered and CFD calculations are being made to further improve combustion. Consequently, the problems with the Sturman injection system will not delay the project. Also, the elimination of EGR has greatly simplified the engine concept, although the addition of a water-cooled exhaust manifold increases heat rejection.

Now that reasonable smoke and particulate emissions have been obtained without EGR, the next major issue is control of NOx emissions. A three-way catalyst is being ordered and A/F ratio controls will be developed to operate the catalyst at stoichiometric in order to determine the efficiency of NOx removal. About 95% efficiency of NOx removal is needed, which is well within the capability of a three-way catalyst system operating on gasoline engine exhaust, but the efficiency on diesel exhaust may be lower.

Predictions of the engine efficiency are being made using the Ricardo WAVE model with heat release calculated from the engine running without EGR and reasonable air system components. The engine model will be modified to include the additional required air for the particulate filter and a turbocompound unit.

Conclusions

Although it is early in the development of the stoichiometric diesel engine concept, there are a number of significant findings:

- An advanced diesel engine can be operated at stoichiometric with reasonable particulate and NOx emissions.
- The low boost requirements and absence of EGR make this SCI engine concept attractive.
- The reduced engine air flow and reduced exhaust flow at high temperature provide advantages for further system optimization to improve fuel economy.
- Stoichiometric engine operation may allow higher specific output, i.e. smaller engine displacement, than other advanced diesel engine concepts providing the same power.
- A three-way catalyst efficiency of about 95% is needed to meet the NOx standards.
- Brake thermal efficiency of 50% with electric turbocompounding and optimization should be obtainable.

FY 2006 Publications/Presentations

1. Winsor, Richard E. and Baumgard, Kirby J., Stoichiometric Compression Ignition (SCI) Engine Concept was presented at the 12th Diesel Engine-Efficiency and Emissions Research (DEER) Conference in Detroit, MI on August 23, 2006.

II.A.23 Demonstration of Air-Power-Assist (APA) Engine Technology for Clean Combustion and Direct Energy Recovery in Heavy-Duty Applications

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Objectives

Demonstrate an APA engine technology that enables 15% fuel economy improvement for heavy-duty refuse truck applications.

Accomplishments

- APA engine functional specifications were completed.
- Vehicle simulation with APA technology showed 4-18% efficiency improvement over a wide range of driving cycles.
- Low temperature exhaust gas recirculation (EGR) circuit offered additional 3-4% efficiency improvement in vehicle simulation tests.

Future Directions

- Integrate the hydraulic valve actuator (HVA) system with Volvo MD11 engine for baseline testing.
- Upgrade the HVA system and install air handling system.
- Develop hybrid engine control strategy.
- Perform testing of low-temperature EGR circuits for improved engine efficiency.

Introduction

The concept in this project is to use the engine to convert braking energy into compressed air stored in an on-board tank [1]. Later, during acceleration, the engine is powered by the stored compressed air with or without burning diesel fuel to get up to speed or until the compressed air is depleted. Once the vehicle has attained a cruising speed, the engine is back to a conventional diesel engine. The positive pumping work performed by compressed air during the intake stroke is added to the work performed by combustion gas during the gas expansion stroke. The additional work performed by the compressed air permits a reduction in the quantity of fuel needed to achieve the required engine power. In this way, the engine efficiency is increased, and the vehicle fuel economy is improved [2]. The high boost pressure during engine acceleration helps reduce the emissions of particular matter. In addition, smaller quantities of fuel burned in each cylinder during each cycle lead to lower peak temperatures, which result in lower NOx emissions. The noise from the sudden exhaust gas blow-down process during engine braking is reduced by minimizing the pressure difference across the engine valves, and the reduced noise is further muffled by the air tank. This provides a solution to the noise issue that a conventional engine brake has. Therefore, regenerative compression braking can be utilized in the areas where conventional engine braking is prohibited due to its noise pollution. This facilitates greater usage of the engine brake, which in turn helps save fuel and reduces the frequency of brake service with its associated costs. In summary, an APA engine absorbs the vehicle kinetic energy during braking, puts it into storage in the form of compressed air (air compressor mode), and reuses it to assist in subsequent vehicle acceleration (air motor mode). The energy saving principle of this technology is similar to that of the electric hybrid technology, except that the high capital cost for an electric hybrid drive train is avoided.

Approach

A GT-Power™ engine simulation model was constructed to predict engine efficiency based on the second-law thermodynamic availability at various operating conditions and optimization of valve timing was achieved as well. The engine efficiency map generated by the engine simulation was then fed into a simplified vehicle model to predict fuel consumption of a refuse truck on a simple collection cycle. Design

and analysis work supporting the concept of retrofitting an existing HVA system with the modifications that are required to run the HVA system with APA functionality was completed. An APA engine with HVA system will be implemented to validate the fuel economy improvement.

Results

APA engine functional specifications and component design were completed in this year. A general view of the entire APA air handling system from the "exhaust side" and "intake side" of the engine is shown in Figures 1 and Figure 2, respectively. In this view, one can see the exhaust three-way valves, compressor bypass valve system, air tank and associated piping. The 2010-spec EGR cooler can be seen below the turbocharger. For the purpose of the test cell demonstration, this cooler will be remotely mounted. The 2010-spec cold-side EGR valve and intake three-way valve on the intake side of the engine is shown in Figure 2.

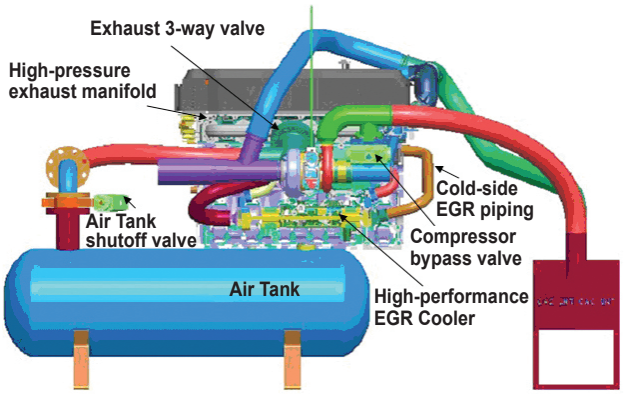


FIGURE 1. APA Air Handling System General View (Exhaust side)

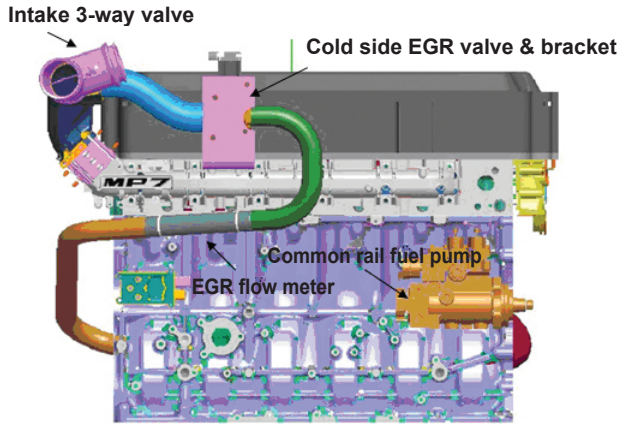


FIGURE 2. APA Air Handling System General View (Intake side)

The brake specific fuel consumption (BSFC) benefit of improved EGR cooling has been proven in testing. An MD11 engine was run through two screening tests, one with a standard EGR cooler and one with improved cooling fin geometry. The EGR cooler with improved cooling fins reduced the EGR cooler outlet temperature by ~30°C versus the stock cooler in the 'seasoned' condition. The improved EGR cooler had the effect of moving the NOx/BSFC trade-off line, making it possible to re-optimize to run at a more efficient point at the same NOx. Testing results showed that a 30°C reduction in EGR cooler outlet temperature results in ~1.5% (3 g/kWh) BSFC improvement at U.S. 2007/U.S. 2010 engine-out NOx levels. An improved EGR cooler design has been tested for the MD11 that promises a 60°C reduction in EGR outlet temperatures versus the stock U.S. 2007 cooler. Based on the temperature/BSFC correlation of 1.5% per 30°C temperature reduction, additional 3% fuel economy improvement was achieved with this new cooler design.

Vehicle simulation results are shown in Table 1 with APA technology showing a 4–18% fuel economy improvement over a wide range of driving cycles (14 Driving Cycles). Additional 3–4% of fuel economy improvement in all driving cycles was observed by combining low temperature EGR with APA technology in vehicle simulation. Over 15% fuel economy improvement is shown from four driving cycles, New York City Transit Bus, Manhattan Bus cycle, Central Business District and Simple Refuse of Volvo Powertrain North America (VPTNA) cycle with APA technology plus the low temperature EGR cooler circuit. This APA technology showed improvement of fuel economy on various driving cycles and improvement of fuel economy; APA technology, however, strongly depends on driving cycle.

TABLE 1. Estimated Efficiency Improvement From Vehicle Simulation

> 15%
[10%, 15%]
< 10%

Vehicle Simulation with ADVISOR

Driving Cycles	base (mpg)	APA (mpg)	% Increase	APA + LT EGR (mpg)	% Increase
Heavy-Duty Cycles					
WVU City Driving Schedule	3.51	3.87	10%	3.98	13%
WVU Suburban Driving Schedule	4.48	4.87	9%	5.02	12%
WVU Interstate Driving Schedule	6.62	6.98	5%	7.19	9%
Urban Dynamometer Driving Schedule	4.43	4.79	8%	4.93	11%
Central Business District (CBD_Truck)	3.37	3.80	13%	3.92	16%
City Suburban Cycle & Route (CSC)	3.91	4.34	11%	4.47	14%
New York Composite	2.96	3.48	18%	3.58	21%
WHM	3.04	3.35	10%	3.45	14%
Bus Cycles					
New York City Transit Bus	2.18	2.57	18%	2.63	21%
Manhattan Bus cycle	3.04	3.56	17%	3.66	20%
Central Business District (CBD14)	4.63	5.05	9%	5.21	12%
BAC cycle - Transit coach	4.04	4.21	4%	4.34	8%
VPTNA cycles					
Simple refuse	1.09	1.23	13%	1.27	16%
30-day cycle	3.04	3.31	9%	3.40	12%

Conclusions

Fuel economy improvement with APA technology depends highly on the driving cycle. Fourteen driving cycles over a wide range of applications were simulated. Overall, 4–18% efficiency improvement was observed with APA technology. Specifically, Central Business District, New York City Transit Bus, Manhattan Bus cycle, and Simple Refuse cycles demonstrated over 15% efficiency improvement with APA technology and low temperature EGR cooler circuit.

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FY 2006 Publications/Presentations

Publications

1. Tai, C. et al., "Demonstration of Air-Power-Assist Engine Technology for clean combustion and direct energy recovery in heavy duty application", Phase I Final Report, January 2006.

2. Tai, C. et al., "Demonstration of Air-Power-Assist Engine Technology for clean combustion and direct energy recovery in heavy duty application", Phase II Quarterly Report, July 2006.

3. Tai, C. et al., "Demonstration of Air-Power-Assist Engine Technology for clean combustion and direct energy recovery in heavy duty application", Phase II Final Report, October 2006.

Presentations

1. Tai, C., "APA project technical review", DOE Phase I final review presentation, Hagerstown, MD, Nov. 2005.

2. Tai, C., "APA project technical review", DOE Phase II final review presentation, Hagerstown, MD Sep. 2006.

II.B.1 Fundamental Studies of NOx Adsorber Materials

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Objectives

- Develop a practically useful fundamental understanding of NOx adsorber technology operation.
- Focus on chemical reaction mechanisms correlated with catalyst material characterization.
- Interact with Oak Ridge National Laboratory (ORNL) project aimed at development of 'aging' protocols (Bruce Bunting), and actively participate in the Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) lean-NOx trap (LNT) subgroup. This latter activity now includes an additional 3-way collaboration between ORNL (Stuart Daw and coworkers), Sandia National Laboratory-Livermore (Rich Larson), and Pacific Northwest National Laboratory (PNNL).
- Transfer the developing fundamental understanding to industry via the CLEERS activity as well as periodic technical meetings with industry scientists and engineers.

Accomplishments

- Determined the practical significance of our previously discovered two morphological 'forms' of the storage Ba-phase – a 'monolayer' phase and a 'bulk' phase. Notably:
  - the "monolayer" morphology is found to decompose at lower temperature in vacuum and in a reducing atmosphere than "bulk" nitrates;
  - the "monolayer" Ba-phase is also easier to 'de-sulfate';
  - the formation of a high-temperature (deactivating?) $BaAl_2O_4$ phase requires BaO coverages above 1 monolayer; and
  - the morphology model at least partially explains relatively small use of Ba species (often <20%) in storing NOx during typical lean-rich cycling.
- Water was found to have a profound effect on the relative distribution of Ba-species morphologies, but may not be practically important at typical LNT operating conditions.
- Studies provided important information regarding the chemical mechanisms of processes occurring during the rich phase of LNT operation.
- We have identified possible methods for restoring the performance of LNTs deactivated by $BaAl_2O_4$ formation, via controlled water exposures.
- One new invention disclosure, and numerous publications (9), invited talks (5), and other presentations (7) have resulted from this project in the past year (see below list).

Future Directions

- BaO morphology studies
  - Effects of CO_2 and effects of both CO_2 and H_2O on morphology changes during NOx uptake and release. Temperature programmed x-ray diffraction (TP-XRD) studies to be performed at National Synchrotron Light Source (NSLS) as beamtime becomes available.
  - *In situ* transmission electron spectroscopy (TEM) studies to watch morphology changes in real time.
  - Effects of additional catalyst components (e.g., ceria as used in CLEERS Umicore material), and alternative support materials (e.g., MgO and $MgAl_2O_4$).
  - Role of Pt/BaO interface for optimum NOx storage.
- Detailed characterization (e.g., Fourier transform infrared, TEM) of alternative materials.
- Studies of CLEERS Umicore samples.
  - CLEERS performance protocol experiments.
  - Nitrogen balance experiments (mechanism(s) of reductive regeneration).

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 lean-NOx trap, 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 barium oxide (BaO) supported a high surface area alumina (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 test, 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 3 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 hrs. State-of-the-art techniques such as X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM)/energy dispersive spectroscopy (EDS), Fourier transform infrared (FTIR), Brunauer, Emmett and Teller (BET)/ pore size distribution, and temperature programmed desorption/reaction (TPD/TPRX), available at PNNL, 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 NSLS, at Brookhaven National Laboratory. The detailed experimental set-up and protocol have been discussed elsewhere [3,4].

Nitrogen Balance Experiments

We also utilize a recently constructed experimental apparatus for conducting nitrogen balance experiments on core samples of monolith-supported LNT catalysts. *As far as we know, our studies represent the only quantitative measurement of nitrogen balance for LNT operation conducted to date* [5]. This year, we have continued studies of a degreened (16 hrs in air at 700°C in 10% H_2O at Oak Ridge National Laboratory) commercial LNT catalyst manufactured by Umicore (provided by Umicore through ORNL as part of the CLEERS activity). This Umicore catalyst contains the precious metals Pt, Pd and Rh (in descending quantities), added ceria and zirconia (for oxygen storage) and BaO for NOx storage.

In prior work, we found for the first time that the reduction of stored NOx by H_2 in a commercial LNT catalyst produces primarily N_2 with smaller quantities of N_2O. For insufficiently long rich periods, the adsorbed NOx builds up until the lean-cycle NOx storage is drastically reduced, degrading the overall performance significantly. Under these conditions, the catalyst never fully removes stored NOx, and NO and NO_2 are observed throughout the entire lean-rich cycle. During overly long rich periods, NOx is never observed but, unfortunately, NH_3 is. Compared to an optimized rich cycle length, similar amounts of N_2 are produced early in the rich period, but its production drops off significantly once the stored NOx is depleted. Thus, the appearance of ammonia is an excellent indication that nitrogen production from stored NOx is complete, and that the optimal rich period has been reached or exceeded. Importantly, the proper choice of the rich period length prevents the production of significant amounts of NH_3 altogether. In our prior studies, a small but noticeable

amount of N_2O was unavoidably produced. In this report, we will emphasize work on other elements of the project.

Results

In last year's report we 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 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. In this year's work, we have determined a number of important practical consequences of these cyclic morphology changes. In particular:

- From TPD experiments, the "monolayer" morphology is found to decompose at lower temperature in vacuum and in a reducing atmosphere than "bulk" nitrates [4,6];
- "Monolayer" Ba-phase is also easier to 'de-sulfate' [7];

The morphology cycle of BaO/A_2O_3 in NO_2 in NO

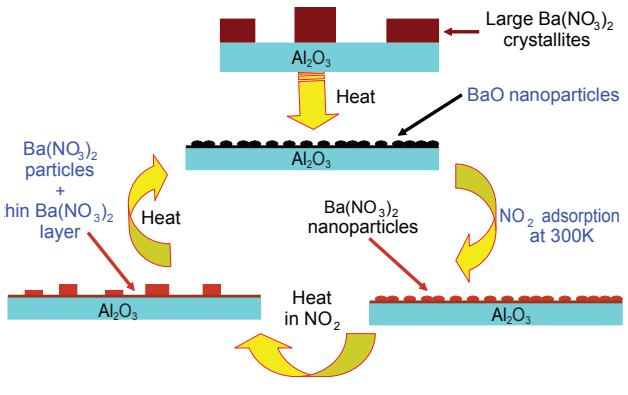


FIGURE 1. Schematics of the cycle of morphology changes taking place during NO_2 uptake and release on BaO/Al_2O_3 NO_x storage/reduction materials.

- Formation of a high-temperature (deactivating?) $BaAl_2O_4$ phase requires BaO coverages above 1 monolayer [8]; and
- 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 also studied the effect of water on these morphology changes (manuscripts in preparation). In the following, we highlight a few of these areas of recent work.

The Effect of Ba-Loading and Water on the Formation and Stability of $BaAl_2O_4$

It is widely reported that BaO and Al_2O_3 react at high temperature (>800°C) to form an aluminate phase, $BaAl_2O_4$ (for example, see [10] and references therein). However, there is considerable disagreement about the effectiveness of the $BaAl_2O_4$ phase for NOx storage. We have studied the effect of barium loading on $BaAl_2O_4$ formation for various BaO/Al_2O_3 samples. As illustrated in Figure 2, 2 (Figure 2a) and 8 (Figure 2b) wt% BaO/Al_2O_3 samples showed essentially no detectable morphological changes upon high temperature thermal treatment, while $BaAl_2O_4$ formation occurred readily for a 20 wt% one (Figure 2c). Because the 8 wt% sample contains approximately just enough BaO to completely cover the alumina surface (*i.e.*, is ≈ 1 monolayer, ML), these results led us to the conclusion that a surface (monolayer) BaO phase is stable to high temperature thermal treatment, while a more 'bulk-like' BaO phase provides the source of Ba for $BaAl_2O_4$ formation.

Recently, Gorte and coworkers [11] reported the formation of a bulk $Ba(NO_3)_2$ phase when NO_2 is adsorbed onto both moderate (~500°C) and high temperature (≥600°C) calcined BaO/Al_2O_3 materials, the latter containing $BaAl_2O_4$ as the primary Ba-containing phase observable in XRD. These authors further claimed that BaO and $BaAl_2O_4$ appear to be equally effective as NOx storage materials, both being able to fully utilize the Ba content to form stoichiometric $Ba(NO_3)_2$ upon NO_2 exposure at room temperature. Although the reaction of $BaAl_2O_4$ with NO_2 and O_2 to form $Ba(NO_3)_2$ is exothermic, to our knowledge this was the first report that such a dramatic phase change could occur upon room temperature NO_2 adsorption. However, the authors do acknowledge possible uncharacterized effects of H_2O on their results. Considering the importance of barium phases as active sites for NOx storage, we investigated these processes in more detail [10] with specific emphasis on the effect of NO_2 adsorption and subsequent water treatment on the phase changes of $BaO(x)/Al_2O_3$ (x = 8 and 20 wt%) materials by using XRD and solid state ^{27}Al magic-angle spinning (MAS) nuclear magnetic resonance (NMR). Furthermore, we followed the changes in NOx adsorption capacity of the

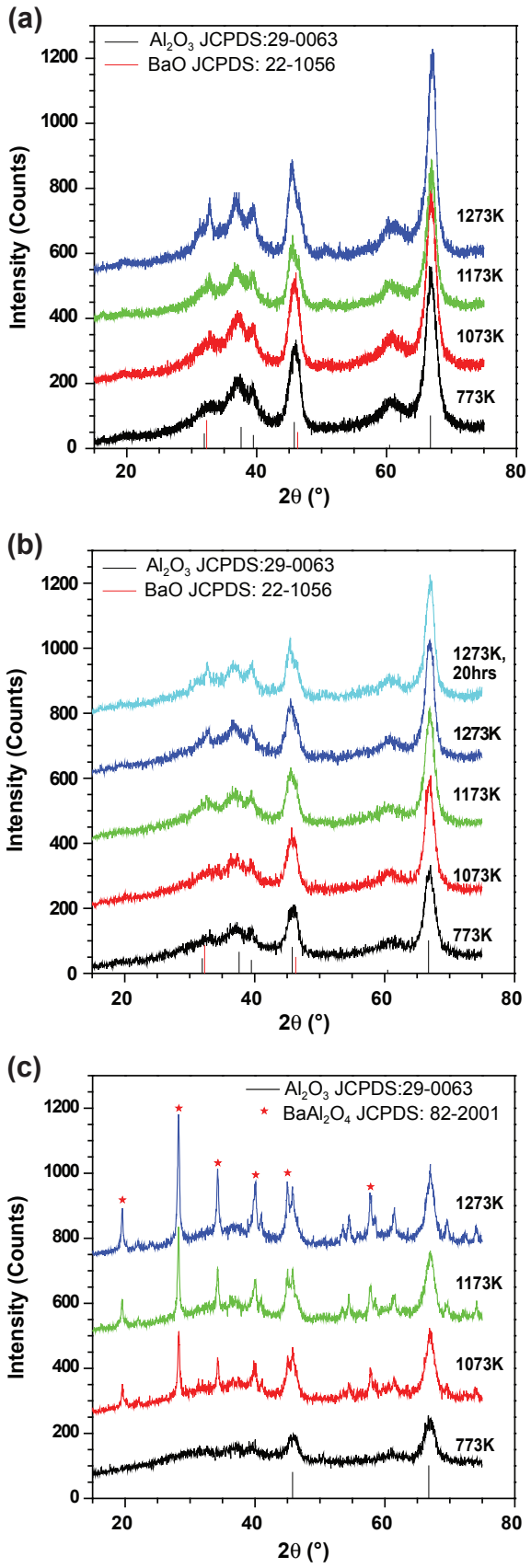


FIGURE 2. XRD spectra of 2% (A), 8% (B) and 20 wt% BaO/Al_2O_3 (C) NSR catalysts after calcination for two hours to different temperatures.

resulting materials in TPD experiments subsequent to NO_2 exposure at room temperature.

After calcination in dry air at 1000°C, the XRD and solid state ^{27}Al MAS NMR results confirm that stable surface BaO and bulk $BaAl_2O_4$ phases are formed for 8 and 20 wt% BaO/Al_2O_3, respectively. Following NO_2 adsorption on either high-temperature treated sample, we observed little if any evidence for $Ba(NO_3)_2$ formation, in contrast to the recent results of Gorte and coworkers [11]. However, when water was added to the thermally aged samples after NO_2 exposure, the formation of bulk crystalline $Ba(NO_3)_2$ particles was observed in both samples. For example, Figure 3 shows solid state ^{27}Al MAS NMR of 20% BaO/Al_2O_3 samples following various treatments, with peak assignments made on the basis of model compounds. The spectrum obtained from the 20 wt% BaO/Al_2O_3 material after calcination at 1000°C for 10 hrs (Figure 3a) shows three peaks arising from Al_2O_3 (peaks at 3 and 63 ppm) and $BaAl_2O_4$ (at 70 ppm) – note that there is an insufficient amount of Ba (20 wt%) to fully transform the alumina into $BaAl_2O_4$. When NO_2 is adsorbed at room temperature, there is no change in the ^{27}Al MAS NMR spectrum as shown in Figure 3b, consistent with our XRD results [10]. Thus, both the XRD and NMR data demonstrate that the $BaAl_2O_4$ phase is not altered significantly by room temperature NO_2 adsorption. However, when the sample is treated with water at room temperature (Figure 3c), aluminum

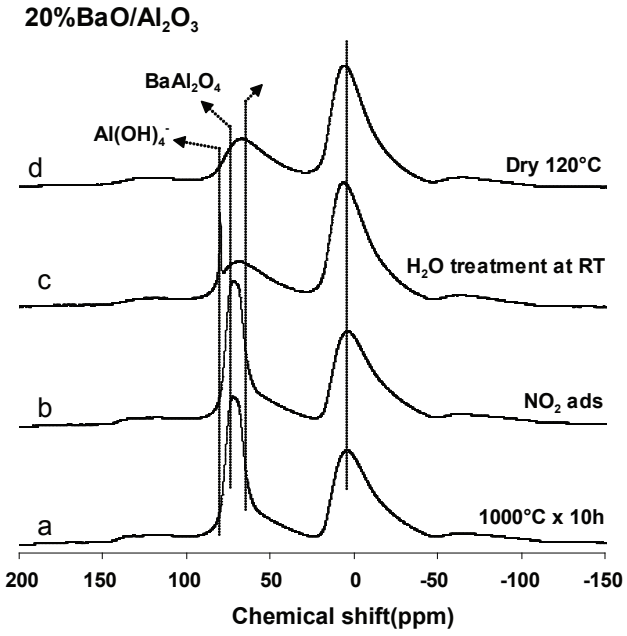


FIGURE 3. Solid state ^{27}Al MAS NMR spectra of a 20 wt% BaO/Al_2O_3 sample treated at 1000°C for 20 hrs (a) exposed to NO_2 at room temperature (b) and following a subsequent room temperature H_2O treatment (c). Spectrum (d) was obtained after an additional drying step at 120°C for sample (c).

species from $BaAl_2O_4$ completely disappear and a new peak, assigned to $Al(OH)_4^-$, develops. The $Al(OH)_4^-$ species readily converts to alumina by dehydration when the sample is dried in an oven at 120°C as shown in Figure 3d. NO_2 TPD results demonstrate a significant loss of uptake for the 20 wt% model catalysts upon thermal treatment indicating that formation of $BaAl_2O_4$ results in LNT deactivation. However, the just described phase transformations upon subsequent water treatment gave rise to the partial recovery of NOx uptake, demonstrating that such a water treatment of thermally aged catalysts can provide a potential method to regenerate LNT materials.

Effects of Water on BaO Morphology and NOx Uptake

The effects of H_2O and CO_2 on the uptake of NOx over BaO/Al_2O_3-based storage systems have been recognized and reported. However, the extent of the effects of these compounds on the NOx uptake, and the mechanisms by which these compounds influence NOx uptake are still widely debated. For this reason, we have initiated studies of the effects of water on the morphology of BaO/Al_2O_3-based NOx storage materials using FTIR, TPD, and TR-XRD techniques [12].

The results of this multi-spectroscopy study reveal that, in the presence of water, surface Ba-nitrates convert to bulk nitrates, and water facilitates the formation of large $Ba(NO_3)_2$ particles. For example, Figure 4 shows a series of FTIR spectra obtained during step-wise H_2O exposure to NO_2-saturated 8 wt% BaO/Al_2O_3 samples demonstrating dramatic changes in the spectra upon water exposure. Specifically, the intensities of the infrared bands characteristic of surface nitrates (1294 and 1582 cm^{-1}) gradually decreased with increasing amounts of H_2O introduced, while those of the bulk nitrates (1325 and 1434 cm^{-1}) increased. After the 7th H_2O dose, the intensities of peaks due to surface Ba-nitrate species almost completely diminished, while those of the bulk Ba-nitrates reached their maxima. This process is completely reversible; *i.e.*, after the removal of water from the storage material, a significant fraction of the bulk nitrates re-convert to surface nitrates (Figure 5 summarizes the just-described morphology changes). The amount of NOx taken up by the storage material is, however, essentially unaffected by the presence of water, regardless of whether the water was dosed prior to or after NO_2 exposure. Based on the results of this study, we are now able to explain most of the observations reported in the literature on the effect of water on NOx uptake on similar storage materials.

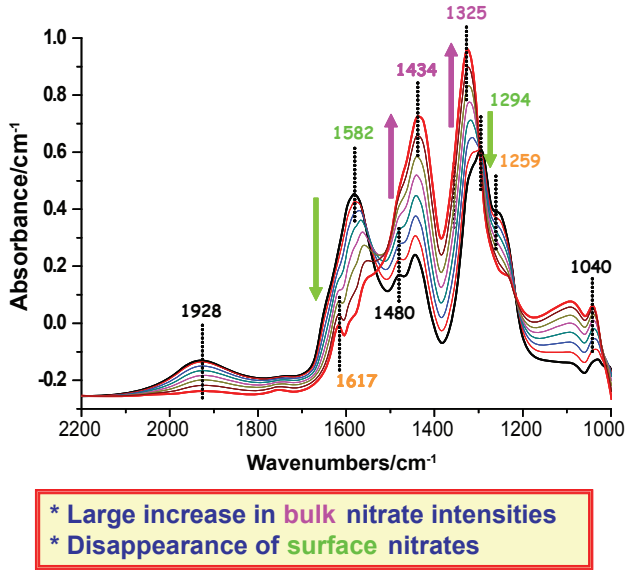


FIGURE 4. Infrared spectra collected during the step-wise H_2O adsorption at 300 K on NO_2/8 wt% BaO/Al_2O_3 (each H_2O dose was 1 Torr).

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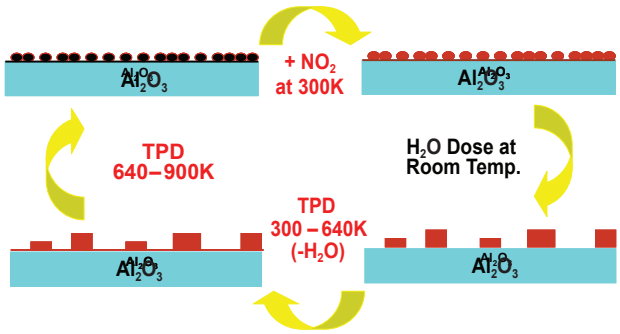


FIGURE 5. Schematics of changes in the cycle of morphology changes as a result of water exposure.

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FY 2006 Presentations

Invited

1. C.H.F. Peden (invited presenter), C.M. Wang, J.H. Kwak, D.H. Kim, J. Szanyi, R. Sharma, and S. Thevuthasan, "In-Situ TEM Study of Morphological Evolution of Emission Control Catalysts During Operation", presentation at the NSF Workshop on "Dynamic in-situ electron microscopy as a tool to meet the challenges of the nanoworld", Tempe, AZ, January, 2006.

2. C.H.F. Peden (invited presenter), J. Szanyi, D.H. Kim, J.H. Kwak, "The Adsorption and Reaction of NOx (NO and NO_2) on BaO/Al_2O_3 Storage/Reduction Materials", presentation at Ford Research Laboratories Seminar, Detroit, MI, March, 2006.

3. C.H.F. Peden (invited presenter), J. Szanyi, D.H. Kim, J.H. Kwak, "The Adsorption and Reaction of NOx (NO and NO_2) on BaO/Al_2O_3 Storage/Reduction Materials", presentation at Topsøe Company, Copenhagen, Denmark on April, 2006.

4. J. Szanyi (invited presenter), D.H. Kim, J.H. Kwak, J.C. Hanson, and C.H.F. Peden, "In-Situ Synchrotron Studies of BaO/Al_2O_3 NOx Storage/Reduction Materials for Vehicle Emission Control", presentation at the 2006 National Synchrotron Light Source (NSLS) Annual Meeting, Upton, NY, May, 2006.

5. C.H.F. Peden (invited presenter), "Fundamental Studies of Catalytic NOx Vehicle Emission Control", Presentation at the University of California, Santa Barbara, CA, August, 2006.

Contributed

6. D.H. Kim, J.H. Kwak, J. Szanyi, T. Szailer, J.C. Hanson, and C.H.F. Peden, "Understanding of NOx storage/release mechanism over Pt-BaO/Al_2O_3 lean NOx trap catalysts", presentation at the AIChE Annual Meeting, Cincinnati, OH, November, 2005.

7. C.M. Wang, J.H. Kwak, D.H. Kim, J. Szanyi, R. Sharma, S. Thevuthasan, and C.H.F. Peden, "In-Situ TEM Study of Morphological Evolution of $Ba(NO_3)_2$ Supported on α-$Al_2O_3(0001)$", presentation at the MRS Fall Meeting, Boston, MA, November, 2005.

8. C.H.F. Peden, J. Szanyi, D.H. Kim, J.H. Kwak, "The Adsorption and Reaction of NOx (NO and NO_2) on BaO/Al_2O_3 Storage/Reduction Materials", presentation at at PacifiChem 2005, Honolulu, HI, December, 2005.

9. J. Szanyi, C.H.F. Peden, D.H. Kim, J.H. Kwak, X. Wang, W.S. Epling, and J.C. Hanson, "The Effect of Water on the Adsorbed NOx species over BaO/Al_2O_3 NOx Storage Materials: A Combined FTIR and In Situ Time-Resolved XRD Study", presentation at the 2nd International Congress on Operando Spectroscopy, Toledo, Spain, April, 2006.

10. R.S. Disselkamp, D.H. Kim, J.H. Kwak, C.H.F. Peden, J. Szanyi, R.G. Tonkyn, and X. Wang, "Recent Results from PNNL Studies of NOx Adsorber Materials", presentation at the 9th CLEERS Workshop, Dearborn, MI, May, 2006.

11. R.G. Tonkyn, R.S. Disselkamp, and C.H.F. Peden, "Mechanistic Studies of the Reduction of Stored NOx on BaO/Al_2O_3-Based Lean-NOx Traps", presentation at the 9th CLEERS Workshop, Dearborn, MI, May, 2006.

12. C.H.F. Peden, J. Szanyi, D.H. Kim, J.H. Kwak, X. Wang, W.S. Epling, and J.C. Hanson, "The Effect of Water on the Adsorbed NOx species over BaO/Al_2O_3 NOx Storage Materials: A Combined FTIR and In Situ Time-Resolved XRD Study", presentation at the 232nd National Meeting of the American Chemical Society, San Francisco, CA, September, 2006.

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1. Szailer, T.; Kwak, J.H.; Kim, D.H.; Szanyi, J.; Wang, C.; Peden, C.H.F. "Effects of Ba Loading and Calcination Temperature on $BaAl_2O_4$ Formation for Ba/Al_2O_3 Storage and Reduction Catalysts." Catal. Today **114(1)** (2006) 86-93.

2. Tonkyn, R.G.; Disselkamp, R.S.; Peden, C.H.F. "Nitrogen Release from a NOx Storage and Reduction Catalyst." Catal. Today **114(1)** (2006) 94-101.

3. Disselkamp, R.S.; Tonkyn, R.G.; Chin, Y.-H.; Peden, C.H.F. "A Multiple-Site Kinetic Model to Simulate $O_2 + 2\ NO \leftrightarrow 2\ NO_2$ Oxidation-Reduction Chemistry on Pt(100) Catalysts." J. Catal. **238(1)** (2006) 1-5.

4. Szailer, T.; Kwak, J.H.; Kim, D.H.; Hanson, J.; Peden, C.H.F.; Szanyi, J. "Reduction of Stored NO_x on Pt/Al_2O_3 and $Pt/BaO/Al_2O_3$ Catalysts with H_2 and CO." J. Catal. **239(1)** (2006) 51-64.

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Special Recognitions & Awards/Patents Filed/ Patents Issued

1. Ja Hun Kwak, Do Heui Kim, Xianqin Wang, Janos Szanyi, and Charles H.F. Peden, "New Desulfurization Process for Suppression of Pt Sintering of Sulfated Lean NOx Traps." PNNL Invention Disclosure #15330-E, filed in August, 2006.

II.B.2 Mechanisms of Sulfur Poisoning of NOx Adsorber Materials

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- Randy Stafford, John Stang, Alex Yezerets, Neal Currier - Cummins Inc.
- Hai-Ying Chen, Howard Hess, Andy Walker - Johnson Matthey

Objectives

- Develop and apply characterization tools to probe the chemical and physical properties of 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

- Mechanisms of thermal aging as a function of gas composition (reducing or oxidizing).
  - As noted by others, we find that thermal deactivation is very sensitive to the atmosphere (*i.e.*, oxidizing or reducing). Additional studies aimed at understanding these differences were initiated this year.
  - Samples treated with H_2, which results in the smaller Pt particles, show much higher activity than ones treated under oxidizing conditions, again supporting the correlation between Pt particle size and NOx storage activity.
- Robust methods for Pt particle size measurement in aged catalysts.
  - Based on prior work, the issue of Pt sintering as a primary cause of lean-NOx trap (LNT) performance degradation was clearly established. Thus, it has become a primary concern to establish 'routine' methods to determine Pt particle size in aged parts from the field in order to clearly establish their mode of failure.
  - Low Pt accessibility after H_2 reduction, as determined by H_2 chemisorption methods, does not correlate with NOx uptake activity. Rather, it is likely evidence of the strong Pt-Ba interactions that reduce the effectiveness of the H_2 chemisorption method for determining Pt particle size.
- The chemical mechanisms of the sulfur removal processes.
  - In previous year's work, we have identified conditions for effective removal of sulfur while also minimizing thermal degradation. This year, we have initiated studies of the sulfur removal mechanisms in order to provide guidance for further optimization of the required periodic sulfur removal processes.
  - As noted by others, CO_2 and H_2O significantly enhance the reductive removal of sulfur species and reduce the formation of a 'refractory' BaS phase. Experiments aimed at determining the chemical mechanisms of these effects have been initiated.
  - When H_2O is present in the desulfation step, the evolution of sulfur containing species is enhanced, regardless of the nature of the reductant.
  - The initial barium morphology differences play a crucial role in determining the extent of desulfation and the temperature at which it occurs, therefore, it was found that the removal of sulfur is significantly easier at lower barium loading.
- Three public presentations and two manuscripts have been cleared for release by CRADA partners. One of the manuscripts has appeared (in the Journal of Physical Chemistry B, 110 (2006) 10441.), and the other has been accepted for publication and will appear soon in the journal, Industrial & Engineering Chemistry Research.

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 H_2 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.
- Continue development of LNT thermal history diagnostics techniques
  - Establish reference treatment conditions that can be applied to aged parts with minimal additional changes.
  - More detailed studies to investigate the Pt-Ba interaction.
- Apply to real-life engine "aged" samples.
- Continue to improve mechanistic understanding of sulfur removal processes.
  - Identify important desulfation intermediates.
  - Effects of sulfur concentration on Pt accessibility and barium phase changes.

Introduction

The NOx adsorber (also known as lean-NOx trap – 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 [1]. 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 (EPA'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 are being 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 further note here that while program progress for the entire year is summarized above in the "Accomplishments" section, we present below more detail about results obtained in this last year in three specific areas: i) the effect of barium loading on the desulfation process; ii) the design of a reaction protocol to specifically investigate desulfation behavior; and iii) the effect of water on desulfation processes.

Approach

In a microcatalytic reactor system (Figure 1), 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 (4 minutes)", which measures NOx removal efficiencies for the first 4 minutes of the lean-period.

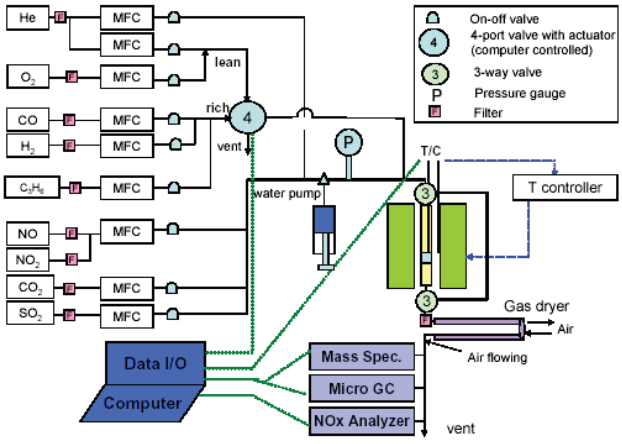


FIGURE 1. Schematic of the Microreactor Constructed for this Project's Studies

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 are able to identify optimum de-sulfation treatments to rejuvenate catalyst activities (a new manuscript describing this protocol is currently undergoing review by the CRADA partners).

State-of-the-art catalyst characterization techniques such as X-ray diffraction (XRD), transmission electron microscopy (TEM)/energy dispersive spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS), thermal gravimetric analysis (TGA), Brunauer-Emmett-Teller (BET)/pore size distribution, and temperature programmed desorption/reaction (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, H_2 TPRX (temperature programmed reaction), 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 adsorber material as a function of desulfation process.

Results

Effect of Barium Loading on the Desulfation of Pt-BaO/Al_2O_3

We have previously shown that NOx adsorption/desorption chemistry is strongly dependent on the loading of barium on the basis of Fourier Transform Infrared Spectroscopy (FTIR) and NO_2 TPD experiments [2]. With reference to these results, we addressed an important question about how the sulfation and desulfation chemistry varies as a function of barium content in the LNT formulation. For this, we performed a multi-technique study, using H_2 temperature programmed reaction, synchrotron time resolved X-ray diffraction, sulfur K-edge X-ray absorption near-edge spectroscopy (XANES), and transmission electron microscopy (TEM).

Our previous work [2] has clearly shown that two kinds of barium nitrate species (surface and bulk barium nitrates) are formed upon NOx uptake, and the relative distribution of these nitrate species depends on the barium loading. In particular, an 8 wt% BaO/Al_2O_3 sample will contain primarily surface nitrates, while a significant quantity of both surface and bulk nitrates were present for a 20 wt% BaO/Al_2O_3 sample following NOx adsorption. As H_2 TPRX results demonstrate in Figure 2, sulfated Pt-BaO(8)/Al_2O_3, consisting of predominantly of surface BaO/$BaCO_3$ species, displays

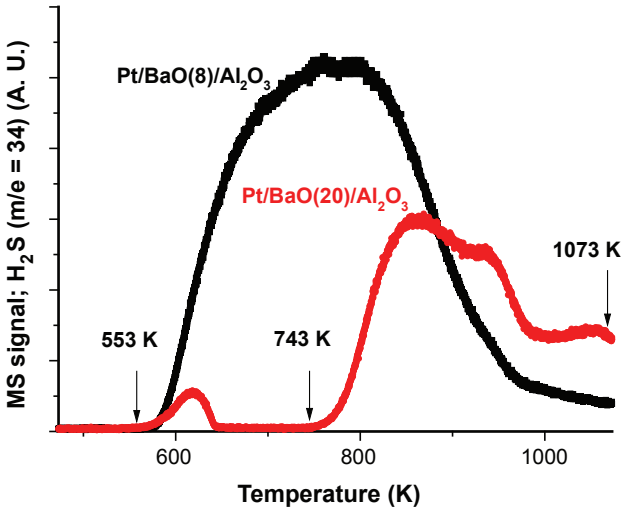


FIGURE 2. H_2 TPRX Spectra for 5 g/L Pt-BaO(8)/Al_2O_3 and 5 g/L Pt-BaO(20)/Al_2O_3 Samples

more facile desulfation by H_2 at lower temperature than sulfated Pt-BaO(20)/Al_2O_3, a material containing primarily bulk BaO/$BaCO_3$ species. Furthermore, after desulfation the amount of residual sulfur species on the former material is much less than on the latter as evidenced by S K-edge XANES and TEM/EDX results. After high temperature desulfation for both samples, residual sulfur exists in a reduced form, primarily as fairly large BaS particles. This suggests that the initial morphology differences between these two samples plays a critical role in determining the extent of desulfation and the temperature at which it occurs, potentially providing important information for the development of more sulfur resistant LNT catalyst systems.

A Reaction Protocol to Investigate Desulfation Behavior for Lightly Sulfated Samples

In the previous year, we demonstrated that a newly developed reaction protocol provided a useful tool to optimize desulfation conditions for deactivated LNT catalysts. Because actual LNT catalysts will experience frequent regenerations, we modified the reaction protocol to determine how repeated regenerations will affect the recovery of NOx performance. In other words, how easily are sulfur species removed for the case of successive sulfations and regenerations? NO_x uptake was measured in the presence of SO_2 for 2 hrs, followed by regeneration at 600°C in the absence of SO_2. These two steps were repeated six times until the total amount of sulfur deposited onto the materials was 4 g/L. For comparison purposes, the reaction was performed without SO_2 to identify the effects of thermal deactivation during these successive treatments at 600°C (not shown). In this latter case,

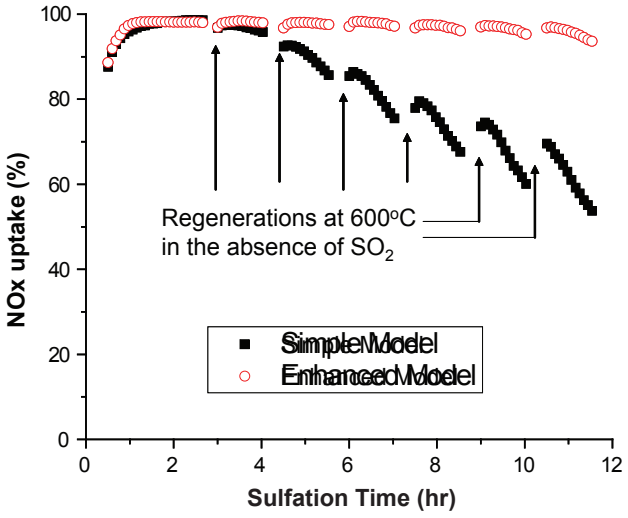


FIGURE 3. Change of NOx uptake with time during repeated sulfation and regeneration over simple model and enhanced model samples.

the NO_x uptake for 4 min was not changed for either sample; therefore, we can exclude the effects of thermal deactivation on performance during these successive sulfation and regeneration processes at 600°C. Figure 3 shows the change of NOx uptake as a function of sulfur exposure. The break in the sets of data points indicates the regenerations at 600°C in the absence of SO_2. For the case of the simple model sample, sulfur appears to deposit on the sample, even after successive regeneration treatments at 600°C, resulting in deactivation. Although there is a slight increase after each of the regeneration processes, the NOx uptake decreases rapidly. On the other hand, the enhanced model sample shows only a slight decrease in NOx uptake performance after multiple regenerations. Up to the sulfation level of 1 g/L, the NOx uptakes of the two samples are essentially identical. However, after several successive sulfation followed by regeneration, the differences becomes larger, demonstrating that the enhanced model sample has a much more significant ability to remove the low amounts of sulfur.

Role of H_2O in the Desulfation Process

We have recently been studying the effects of H_2O during desulfation processes as a function of the reductant (*i.e.*, H_2, CO or hydrocarbons-HCs) used. Regardless of the nature of the reductant, the presence of H_2O has a dramatic effect on the evolution of the sulfur containing species during, and also results in the higher desulfation activity. For example, Figure 4 shows the compositional change in the evolving gases during the desulfation steps of the enhanced model sample using CO as the reductant, either in the absence or presence of H_2O. For the H_2O-free case, only COS was formed, via reaction between CO and sulfates. On the other

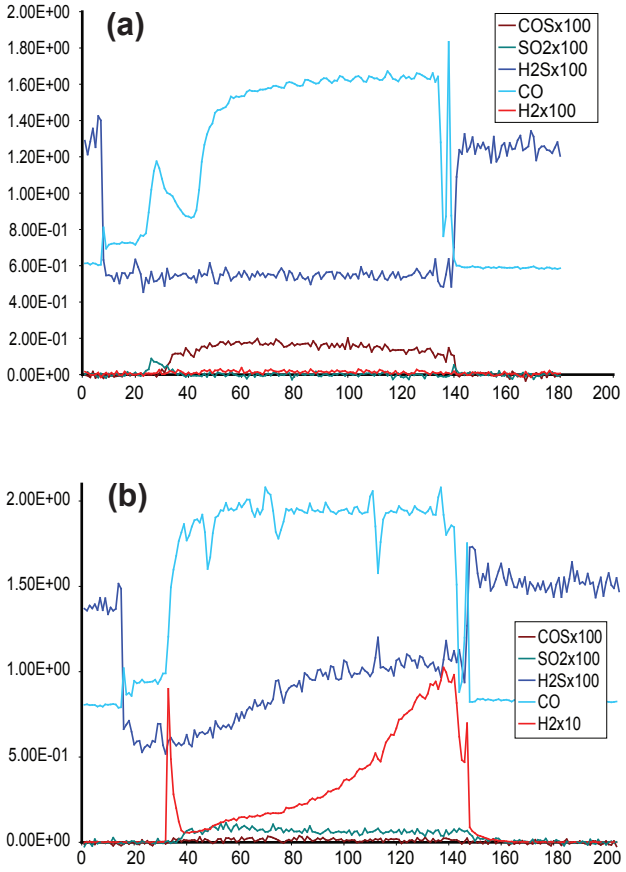


FIGURE 4. Change of composition of the gas phase with time during regeneration of the enhanced model sample at 600°C with CO, in the absence (a) or presence (b) of H_2O.

hand when H_2O is present, H_2 is generated from the water-gas-shift reaction (WGS) between CO and H_2O. The formed hydrogen is more actively involved in the desulfation process than CO, resulting in the formation of H_2S and SO_2, as in the case when hydrogen was present in the reductant stream. Although not shown, C_3H_6 also generates hydrogen via, in this case, the steam reforming (SR) reaction with water. Therefore, it can be summarized that water is an essential component for desulfation processeses, by facilitating the formation of hydrogen via the WGS and SR reactions, and also by reacting with BaS (as described above), thereby decomposing this otherwise refractory sulfur compound that would otherwise reduce the performance of LNTs for NOx storage and reduction.

Conclusions

PNNL and its CRADA partners from Cummins Inc. and Johnson Matthey are carrying 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 complete

desulfation of the barium species in Pt-BaO(20)/Al_2O_3 is difficult due to the relative inaccessibility of sulfate species in the interior region of the particulate Ba phase. Therefore, it was found that the lower barium loadings provide for more optimum conditions for the removal of sulfur and, correspondingly, reduced deactivating effects. Use of a modified reaction protocol enables us to compare the relative performance of various LNT samples after regeneration processes for light sulfated conditions. The reaction protocol is easily modified to also give information about the regeneration characteristics of the samples. H_2O promotes desulfation process by generating the hydrogen arising from the WGS or SR reaction when CO or C_3H_6, respectively, are used as reductants.

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II.B.3 Characterizing Lean NOx Trap Regeneration and Desulfation

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Objectives

- Establish relationships between exhaust species and various lean-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

- Improved data quality and experimental method.
- Investigated mitigation of fuel penalty with LTC-based regeneration.
- Studied sulfur effects:
  - Characterized intra-catalyst reductant utilization.
  - Determined effect of sulfur on unregulated species.
  - Determined impact of sulfur on regeneration strategy performance.
- Examined additional LNT formulations:
  - Two model catalyst formulations.
  - Umicore gasoline direct injection (GDI) catalyst (CLEERS focus group).
- Presented progress at DEER 2006.
- Collaborated with CLEERS:
  - Presented at CLEERS workshop.
  - Participated in LNT focus group.
  - Uploaded data from engine experiments to CLEERS website.
- Continued ongoing discussions with industry peers and Manufacturers of Emission Controls Association (MECA) partner(s).
- Presented papers at 2005 SAE Fall Powertrain & Fluid Systems Conference and 2006 Congress:
  - Presented N_2 Selectivity paper (SAE 2005-01-3876) at SAE Fall Powertrain & Fluid Systems Conference.
  - Presented LTC regeneration paper (SAE 2006-01-1416) at SAE Congress.
- Submitted paper for 2006 SAE Fall Powertrain & Fluid Systems Conference.

Future Directions

- Study Sulfation/Desulfation:
  - Multiple catalysts with same formulation.
  - Desulfation frequency study.
- To investigate improved LNT regeneration strategy performance related to the following parameters:
  - Smoke
  - Torque perturbations
  - Reductant slip (HC and CO)
  - Engine out NOx flux
  - Attempt to increase the fuel specific NOx reduction (lower fuel penalty)

Introduction

As part of the Department of Energy's strategy to reduce imported petroleum and enhance energy security, the Office of FreedomCAR and 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 (EPA) 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 nobel metal catalysts to N_2. The momentary fuel-rich environment in the 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. NOx regeneration is normally a 2-4 second event and must be completed approximately every 30-90 seconds (duration and interval dependent on many factors; e.g., load, speed, and temperature).

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.

Different strategies for introducing the excess fuel for regeneration can produce a wide variety of hydrocarbon and other species. One focus of this work is to examine the effectiveness of various regeneration strategies in light of the species formed and the LNT formulation. Another focus is to examine the desulfation process and quantify catalyst performance after numerous sulfation/desulfation cycles. Both regeneration and desulfation will be studied using advanced diagnostic tools.

Approach

A 1.7-L Mercedes common rail engine and motoring dynamometer have been dedicated to this activity. The engine is equipped with an electronic engine control system that provides full-bypass of the original engine controller. 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 hydrogen and NOx at five locations within the LNT monolith using a spatially resolved capillary inlet mass spectrometer (SpaciMS). Fourier transform infrared (FTIR) sampling capability has also been improved with dilution and intra-catalyst extraction options. In addition to these set-up changes, we've increased the statistical population size by (1) running the experiments in triplicate, (2) using dedicated engine-out (EO) and tailpipe (TP) five gas benches, with one bench that sweeps from EO to TP in six steps, providing six data sets of EO-to-TP NOx reduction efficiency (NRE), (3) utilizing a remotely operated sample switching system that allows for rapid data acquisition, and finally (4) developing MATLAB code to rapidly reduce the large quantities of data collected.

Three regeneration strategies have been studied with the goal of introducing a broad range of species to the LNT catalyst. Two of the strategies use throttling to reduce the intake air flow, and in turn they reduce the exhaust air:fuel ratio (AFR). Excess fuel is then introduced into the cylinder to produce a rich AFR. The first of these two strategies applies excess fuel by extending the main fuel pulse and delaying it in crank angle time (delayed extended main or DEM). The second strategy introduces the excess fuel in a late cycle post injection at 80 degrees ATDC (Post80). In addition to these two strategies, a third strategy uses EGR in place of throttling to reduce intake air flow and exhaust AFR. The EGR is increased to approximately 55% while the pilot injection is disabled and the main injection timing is advanced to stabilize the combustion. These changes drive the engine into an advanced combustion regime referred to as low temperature combustion (LTC). LTC is characterized by simultaneous low NOx and low PM emissions. Once the engine is operating in the LTC regime, a nominal amount of excess fuel is applied to the main fuel pulse to produce a rich AFR. These strategies are used to study catalysts under quasi-steady conditions, that is steady load and speed but with periodic regeneration.

Activities for FY 2006 can be categorized into three main areas:

- Assessment of the utilization of LTC for reducing fuel penalty associated with LNT regeneration.
- Quantification of the performance impacts of sulfation and desulfation.
- Assessment of catalyst formulation impacts using model and commercial LNTs.

Future work will include bench-scale and diffuse reflectance infrared Fourier-transform spectroscopy (DRIFTS) characterization of LNT monoliths, wafers, and/or powders. Results from the engine experiments will be used to help define more meaningful bench scale methods. The ability to correlate bench-scale and engine test stand measurements will be enhanced by using the exact same catalyst formulations in some cases.

Results

Summary of LTC Regeneration Reduced Fuel Penalty Study – Previous work at ORNL has shown that LTC regeneration has a superior fuel specific NOx reduction (FSNR – grams of NOx reduced per gram of

excess fuel used to regenerate) versus both DEM and Post80. This portion of the study focused on performing an in-depth investigation of the relative benefits of LTC regeneration, which had the lowest fuel penalty, to the DEM regeneration, which had the best NRE.

Integrating the engine-out molar reductants for the three strategies, a decreasing trend in H_2 mass was noted from DEM to Post80 (P80) to LTC, respectively. In addition, the NRE for these strategies follows the same trend. Previous observations have indicated that H_2 production for a given strategy dictates the NRE of the LNT [1]. As the LTC strategy has the lowest H_2 level, it is not surprising that it also has the lowest NRE. In order to capitalize on the superior FSNR but improve the NRE, methods were investigated that would lead to increased H_2 production for the LTC regeneration strategy. The first method studied involved doubling the rich period to increase the H_2 mass delivered per regeneration. The second method studied involved halving the lean period to reduce the mass of NOx stored and therefore, increasing the mass of H_2 delivered per gram of NOx.

Figure 1 shows the DEM (3/30) and LTC (6/30) cases. The nomenclature in parentheses indicates the rich period duration and the total cycle time in seconds (as such, 3/30 indicates a 3 second rich pulse on a 30 second cycle). DEM (3/30) has a NRE slightly below 90%, compared to the LTC (6/30) NRE of about 95%. Worthy of note is that, even with improved NRE, the LTC strategy still has on the order of five times better FSNR. Furthermore, although there is only a 6-7% difference in NRE, this DEM case would actually have twice the tailpipe emissions of this LTC strategy for equivalent engine-out NOx emissions.

Figure 2 compares DEM (3/60) and LTC (6/60). Under conditions in which there is only a need for 75% NRE, these two cases would be a closer comparison. For these data, the LTC strategy has nearly 35 times better FSNR. This research has been published in SAE 2006-01-1416 [2] and the reader is encouraged to review this publication for more detail.

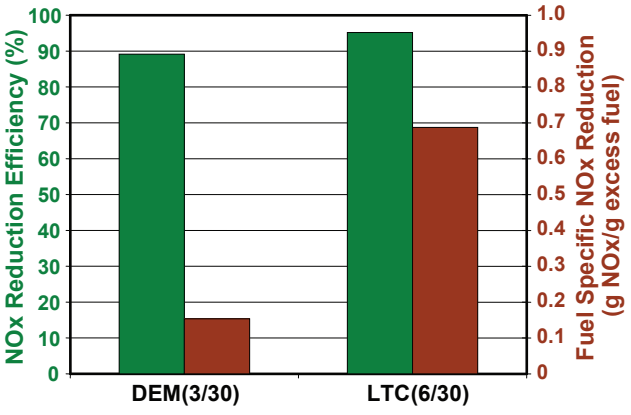


FIGURE 1. NRE and FSNR for DEM (3/30) and LTC (6/30) Strategies

Summary of Sulfation/Desulfation Effects – The deleterious impact of LNT sulfur poisoning is well known but not well understood. In order to better understand how sulfur affects LNTs performance, a set of experiments was completed to produce a range of sulfur poisoning levels. Following the sulfur poisoning measurements, the LNT was desulfated in order to study the effect of high temperature aging. Finally, an LNT of the same formulation, which had been exposed to several high temperature desulfations, was evaluated for comparison.

Figure 3 shows the NRE performance of four strategies as the LNT is progressively sulfur poisoned and then desulfated. The strategies included a DEM and Post80 regeneration with a 20 second cycle time and a DEM and Post80 with a 60 second cycle time. It can be seen that the 60 second Post80 strategy is not only the least effective strategy, it is also the strategy that is most affected by sulfur poisoning and desulfation aging.

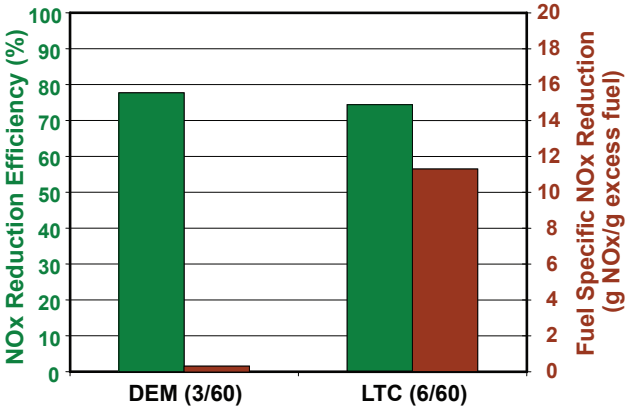


FIGURE 2. NRE and FSNR for DEM (3/60) and LTC (6/60) Strategies

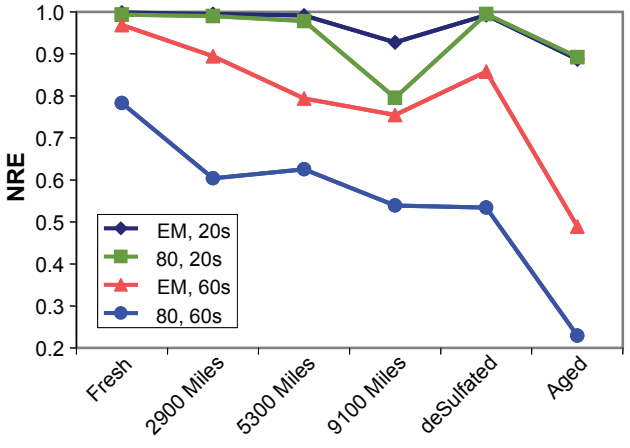


FIGURE 3. Sulfuation, Desulfation and Aging Effects on NOx Reduction Efficiency

When studying the utilization of the reductants as they progress through the LNT, the data indicate that the sulfur loading state has little effect on the level of unused reductants at the exit of the LNT. However, as seen in Figure 4 for the Post80 20 second cycle, the production of ammonia is affected by the level of sulfur. The ammonia formation after desulfation was higher for all four strategies. Since the reductant to NOx ratio did not change dramatically, it is suspected that thermal sintering of the sorbate may be the cause of the higher ammonia production. Findings reported by Castoldi et. al. [3] show that ammonia formation corresponds with higher sorbate loading.

Finally, in both the DEM and Post80 20 second cycles, it was observed that H_2 was being generated in the catalyst. This H_2 production is most likely due to catalytic processes such as partial oxidation of HCs or reforming processes such as the water-gas-shift reaction. Figure 5 shows the "excess intra-catalyst H_2 produced" in regeneration, defined here as the tailpipe H_2 minus the minimum intra-catalyst H_2. Internal H_2 production shows rapid degradation with sulfur loading, and a regain in production after desulfation for the 20 second strategies. The aged catalyst measurements indicate that multiple sulfation/desulfation cycles continue to reduce internal H_2 production. This indicates that LNT control strategies depending on internal H_2 generation to optimize reductant utilization may lose effectiveness with aging. This research has been published in SAE 2006-01-3423 [4] and the reader is encouraged to review this publication for more detail.

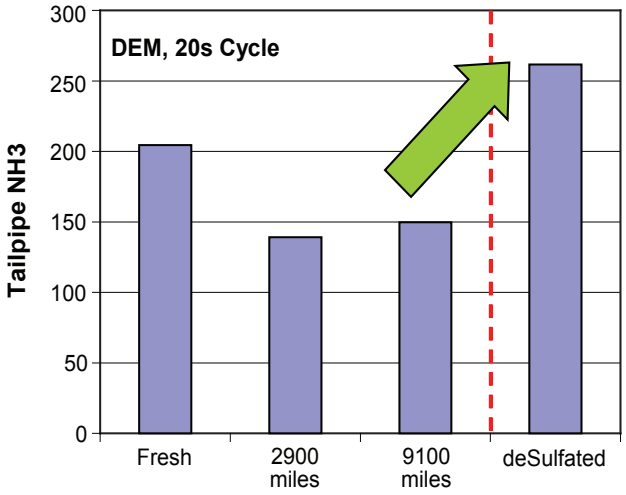


FIGURE 4. Tailpipe Ammonia Increases after Desulfation

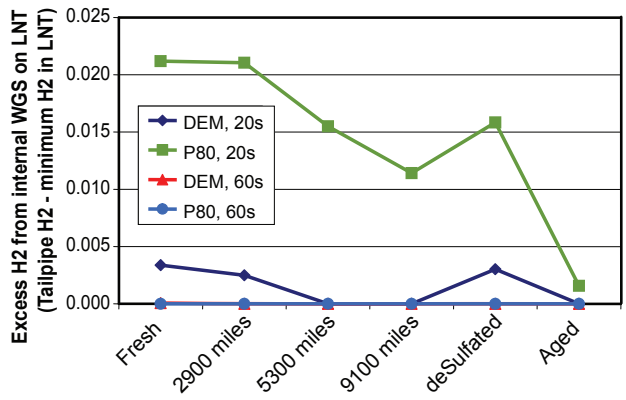


FIGURE 5. Excess Intra-Catalyst H_2 Production during Regeneration as a Function of Sulfation, Desulfation and Aging

Summary of Model and Commercial Catalyst Study – Experiments are underway to help understand the effects of catalyst formulation on NOx reduction performance. Two model LNT catalysts with differing barium loadings and a commercial GDI catalyst are being examined. These formulations have been suggested by the CLEERS LNT focus group. Full characterizations of these alternate formulations will be performed, including intra-catalyst measurements during four regeneration strategies. Preliminary results indicate similar trends for all three formualtions, although there are definite quantitative differences. The availability of the results for the two different model catalysts will also be a valuable contribution to CLEERS.

Conclusions

Strategies for in-cylinder regeneration have been developed for studying reductant chemistry effects on LNTs. Notable conclusions are as follows:

- LTC regeneration produces lower PM levels than typical lean/EGR operation, and considerably less than DEM.
- Low fuel consumption for LTC regeneration yields superior fuel specific NOx reduction:
  - Increasing frequency and duration of regeneration improves NOx reduction for LTC with minimal fuel penalty.
- Preliminary data indicates that regeneration with LTC has the potential for producing equivalent NOx reduction to DEM and P80 regeneration, but with 5x-35x more efficient fuel utilization:
  - Additional improvements in NOx conversion, fuel efficiency, PM generation, and torque smoothing are possible with further effort.
- In general, reductant utilization in LNT only slightly changed with sulfation/desulfation:
  - The LNT zone impacted by sulfur does tend to move downstream with repeated sulfation/desulfation and aging.

- NH_3 formation increased after desulfation:
  - There are indications that sorbate migration/ coarsening occurred at higher desulfation temperature.
- Strategies with high HC and low H_2/CO (Post80) may depend on intra-catalyst H_2/CO production for regeneration:
  - Sulfation/desulfation degradation of catalytic function may have greater impact on regeneration strategies that rely in intra-catalyst H_2/CO production.
- Preliminary model and commercial catalyst data with different formulations indicate similar trends but different quantitative performance.

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II.B.4 Development of Chemical Kinetics Models for Lean NOx Traps

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Objectives

- Identify a set of elementary (microkinetic) surface reactions that can account for the observed behavior of a lean NOx trap (LNT) during both the storage and regeneration phases of operation.
- Optimize the kinetic parameters associated with these reactions by matching model predictions with laboratory reactor data.
- 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

- Assembled, from literature and intuition, a comprehensive Chemkin-format reaction mechanism for LNT regeneration.
- Coupled the Chemkin plug flow reactor code with the Sandia-developed APPSPACK optimization code in order to automate the process of parameter estimation.
- Found an optimized, thermodynamically consistent set of kinetic parameters for the regeneration mechanism by fitting model predictions to the results of pseudo-steady state reactor experiments conducted at Oak Ridge National Laboratory (ORNL).

Future Directions

- Repeat the mechanism assembly and parameter optimization process for the NOx storage phase of normal LNT operation.
- Augment the regeneration mechanism with reactions for additional kinds of reductants, in particular hydrocarbons.
- Introduce reactions needed to describe sulfur poisoning and desulfation.

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. Lean NOx traps (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. However, 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 for both phases of LNT operation.

Our work thus far has been focused primarily on modeling the regeneration chemistry in an LNT. This is due to the existence of a large set of bench-scale reactor data taken at ORNL that is ideally suited to the modeling tools that we have available. For the same reason, we have treated the reduction of stored NOx only by H_2 and CO, even though hydrocarbon reductants are also used in practice. Needless to say, much remains to be done before a comprehensive kinetics model for LNT behavior is available.

Approach

The first step in constructing the regeneration mechanism is to assemble a tentative set of elementary reaction steps and associated mass-action kinetic parameters. Information from the catalysis literature is used where available, but some reactions and parameter values are simply hypothesized in order to obtain a comprehensive set. For a given proposed mechanism and a given set of experimental conditions, the steady-state flow through a single monolith channel is simulated with the Chemkin-based PLUG code to obtain a predicted set of exit concentrations for all gas-phase species. After this is done for all experiments in the ORNL data base, an overall average deviation between the predicted

and measured results is computed. This is used as the objective function in an optimization routine that adjusts the kinetic parameters in order to obtain the best possible fit to the data. Finally, superfluous reactions are identified by dropping candidates one at a time from the mechanism, repeating the optimization procedure, and observing the degradation in the overall fit.

A very significant complication in this parameter estimation process arises from the fact that not all of the parameters can be varied independently if thermodynamic consistency is to be maintained. Specifically, a well-defined number of the equilibrium constants for the surface reactions must be constrained so as to be consistent with the known thermodynamics of the gas-phase species. In addition, all of the activation energies, whether varied independently or computed from thermodynamic constraints, are required for physical reasons to be non-negative. The optimization of the kinetic parameters is therefore a very large and complex problem, but it is made feasible by the availability of the Sandia-developed APPSPACK code running on a massively parallel computing platform.

Results

While it is possible that the regeneration mechanism will undergo further refinements if necessary to accord with new data, the current version is quite acceptable in that it satisfies all constraints and provides a reasonably good fit to all of the ORNL data sets simultaneously. Even though all chemistry is assumed to occur on the catalyst surface, the mechanism involves both gas-phase and surface species. The former include the typical components of engine exhaust as well as the desired and unwanted products of aftertreatment: O_2, NO, NO_2, CO, H_2, CO_2, N_2, H_2O, N_2O, and NH_3. The surface species are those thought to exist on the precious metal (nominally Pt) sites responsible for regeneration: *(Pt), O(Pt), NO(Pt), NO_2(Pt), CO(Pt), H(Pt), N(Pt), OH(Pt), H_2O(Pt), NH(Pt), NH_2(Pt), NCO(Pt), and NH_3(Pt). The first of these is simply an empty site available for adsorption. Taking place among these species are 24 elementary reaction steps, all of them reversible; some are gas-surface interactions, while the remainder involve only surface species. In the former category are adsorption/desorption reactions for all gas-species except N_2O; the adsorptions of O_2, H_2, CO_2, and N_2 are assumed to be dissociative. The remaining gas-surface reactions are

$$H_2O(Pt) + CO(Pt) = 2H(PT) + CO_2$$
$$N(Pt) + CO = NCO(Pt)$$
$$NCO(Pt) + H_2O(Pt) = NH_2(Pt) + CO_2 + *(Pt)$$
$$2NO(Pt) = N_2O + O(Pt) + *(Pt)$$
$$NO_2(Pt) + CO(Pt) = NO(Pt) + CO_2 + *(Pt)$$
$$N_2O + H(Pt) = N_2 + OH(Pt)$$
$$NO(Pt) + NH_2(Pt) = N_2O + 2H(Pt)$$

The first of these is essentially the well-known water-gas-shift reaction, which can in principle account for the ability of CO to reduce NOx to NH_3 in the presence of H_2O. However, the experimental data suggest that a different route is actually operative at low temperatures, and the second and third reactions above provide such a pathway through an isocyanate surface intermediate. The existence of such a species has been confirmed by direct observation at ORNL.

The mechanism is completed by the following eight reactions involving only surface species:

$$NO(Pt) + O(Pt) = NO_2(Pt) + *(Pt)$$
$$NO(Pt) + *(Pt) = N(Pt) + O(Pt)$$
$$H(Pt) + O(Pt) = OH(Pt) + *(Pt)$$
$$H(Pt) + OH(Pt) = H_2O(Pt) + *(Pt)$$
$$N(Pt) + H(Pt) = NH(Pt) + *(Pt)$$
$$NH(Pt) + H(Pt) = NH_2(Pt) + *(Pt)$$
$$NH_3(Pt) + *(Pt) = NH_2(Pt) + H(Pt)$$
$$NH_3(Pt) + O(Pt) = NH_2(Pt) + OH(Pt)$$

With the exception of the last reaction, which is an atom transfer that provides a route for ammonia oxidation, these are simply surface decomposition/recombination processes that are almost certain to occur on the catalyst.

As noted above, the proposed mechanism is quite successful in reproducing a large body of experimental data generated at ORNL. Although the experiments were conducted separately from this project, a brief description of them should be given here in order to make clear the kind of situation that the mechanism was used in modeling. In each experiment, a reactant gas of specified composition was made to flow through a core sample of a commercially available LNT catalyst. Each feed mixture included CO_2, H_2O, and N_2 in amounts typical of engine exhaust, together with a lesser amount of one of the following reactant combinations: NO/H_2, NO/CO, NO_2/H_2, NO_2/CO, N_2O/H_2, N_2O/CO, NH_3/O_2, NH_3/NO, NH_3 alone, H_2 alone, or CO alone. During each experiment, the temperature was ramped slowly from below 100°C to 500°C in order to generate pseudo steady-state conversion data over a wide range of temperatures. Chemiluminescent analyzers and Fourier transform infrared (FTIR) spectroscopy were used to measure the concentrations of key species in the outlet stream, and these values provided the basis for comparison with the reactor simulations.

A comprehensive review of the modeling results is not possible here, so we will discuss just a few of the most interesting cases. Figures 1 and 2 show

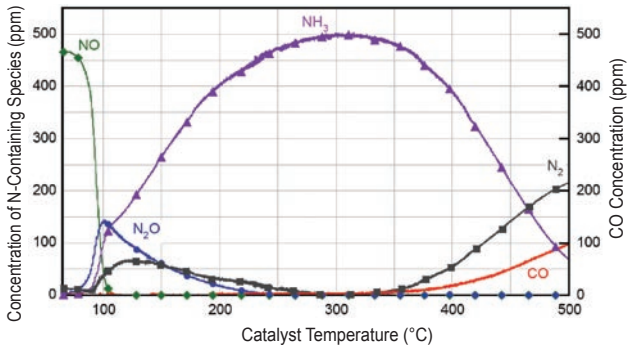


FIGURE 1. Experimental Outlet Concentrations for a Feed Stream Containing 1:2.5 NO/H_2

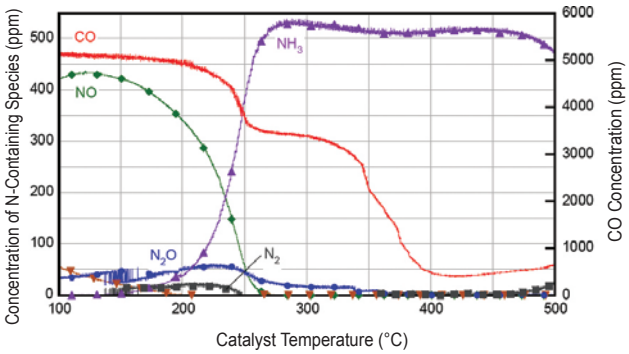


FIGURE 3. Experimental Outlet Concentrations for a Feed Stream Containing 1:10 NO_2/CO

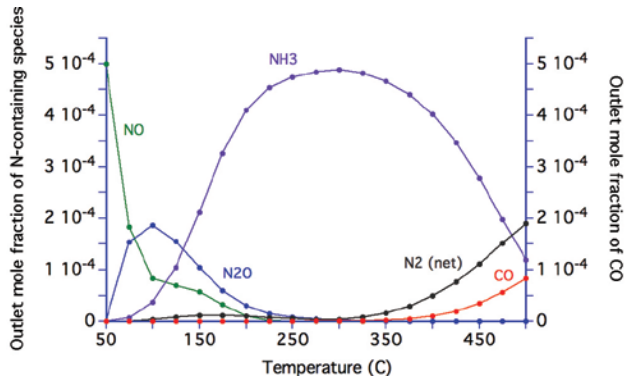


FIGURE 2. Computed Outlet Concentrations for a Feed Stream Containing 1:2.5 NO/H_2

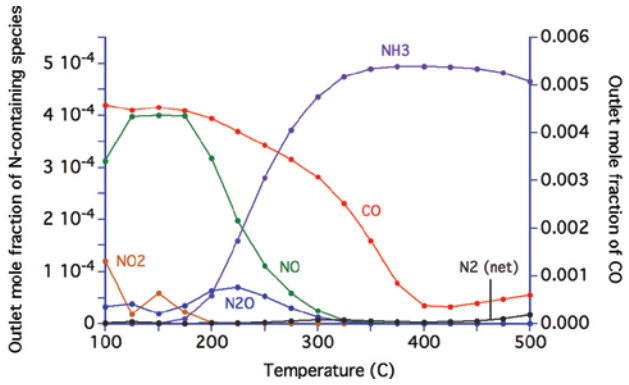


FIGURE 4. Computed Outlet Concentrations for a Feed Stream Containing 1:10 NO_2/CO

the experimental data and the model predictions, respectively, for the case in which the feed stream contains NO and H_2 in a 1:2.5 ratio. Obviously, the excess amount of H_2 gives rise to a strong tendency to form the reduction byproducts N_2O and NH_3 rather than the nominally desired N_2, although it should be mentioned that NH_3 is actually the desired product in some novel applications of this technology. In any case, it can be seen that the model (and, by inference, the chemical mechanism) is able to capture all of the general trends, including the eventual decomposition of NH_3 at high temperatures. The role of kinetics is crucial here, as equilibrium calculations show essentially no NH_3 at temperatures above 300°C.

Figures 3 and 4 show results for a feed that contains NO_2 and CO in a 1:10 ratio. Again, the large excess of reductant causes large amounts of NH_3 to be formed at sufficiently high temperatures, although this is still a kinetically-driven phenomenon: ironically, NH_3 appears in significant amounts at equilibrium only *below* 250°C. However, the most interesting aspect of this case is the striking two-step drop in the outlet CO concentration that is seen experimentally. Clearly, the first step is closely tied to NH_3 formation, while the second is not. The experiment in which CO is fed by itself confirms that the high-temperature drop is due to the water-gas-shift reaction, so we conclude that the NH_3 formation seen here is attributable to some other pathway. The most reasonable choice is the isocyanate scheme mentioned earlier; its incorporation into the overall mechanism allows the model to reproduce the experiment fairly well, although the intermediate plateau in the CO level is largely absent.

Finally, Figures 5 and 6 show results for a feed stream containing a 1:2 mixture of NH_3 and O_2. Even though the primary purpose of the regeneration mechanism is to simulate reduction of NOx, these results show that the mechanism is sufficiently robust to describe a process as different as NH_3 oxidation; note that NH_3 is present at low temperatures and NO at high temperatures, in direct contrast with Figures 1 and 2.

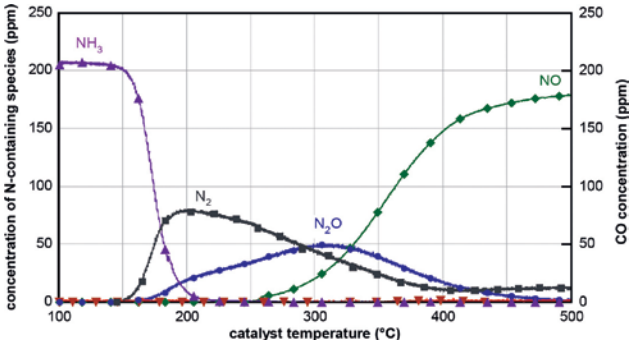


FIGURE 5. Experimental Outlet Concentrations for a Feed Stream Containing 1:2 NH_3/O_2

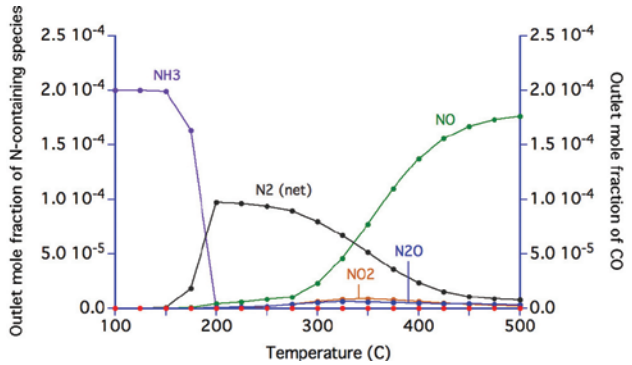


FIGURE 6. Computed Outlet Concentrations for a Feed Stream Containing 1:2 NH_3/O_2

Neither species is present at equilibrium, as all nitrogen appears simply as N_2.

Conclusions

- The chemistry occurring on the precious metal sites of a lean NOx trap can be simulated quite well with a reasonably compact (24-step) elementary reaction mechanism.
- Both water-gas-shift and isocyanate pathways for CO consumption are necessary to explain experimental results over a wide range of temperatures.
- Optimization of very large sets of kinetic parameters in the presence of constraints is time-consuming but feasible with newly available software and parallel processing machines.

FY 2006 Publications/Presentations

1. R. S. Larson, "Simulation of byproduct formation during regeneration of lean NOx traps," CLEERS LNT Focus Group Meeting, January 24, 2006.

2. R. S. Larson, V. K. Chakravarthy, C. S. Daw, and J. A. Pihl, "Modeling Kinetics of NH_3 and N_2O Formation in Lean NOx Traps," Ninth CLEERS Workshop, Dearborn, MI, May 4, 2006.

3. R. S. Larson, V. K. Chakravarthy, J. A. Pihl, and C. S. Daw, "Modeling the regeneration chemistry of lean NOx traps," 12th Diesel Engine-Efficiency and Emissions Research (DEER) Conference, Detroit, MI, August 24, 2006.

4. R. S. Larson, "Update on LNT Regeneration Mechanism," CLEERS LNT Focus Group Meeting, September 19, 2006.

5. R. S. Larson, V. K. Chakravarthy, J. A. Pihl, and C. S. Daw, "Modeling chemistry in lean NOx traps under reducing conditions," SAE paper 2006-01-3446.

II.B.5 Advanced Engine/Aftertreatment System R&D

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Cooperative Research and Development Agreement (CRADA) Partner:
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Alan Karkkainen

DOE Technology Development Manager:
Kenneth Howden

Objectives

- Improve the effectiveness and efficiency of lean-NOx traps (LNTs) by understanding the role and fate of various hydrocarbon (HC) species in LNT regeneration through engine experiments.
- Define pathways to reduce catalyst deactivation and fuel penalty from sulfation and desulfation processes by examining fully-formulated LNT catalysts in bench reactors.
- Study advanced combustion regimes and thermodynamic cycles using infinitely variable intake and exhaust valve timing on a camless engine prototype.

Accomplishments

- Determined (in engine-based LNT experiments) that light alkenes are preferred HC species for LNT regeneration, followed by mono-aromatics. Branched alkanes are poorly utilized by LNTs.
- Examined engine-aged LNT samples in ORNL reactors. Results show sulfur remnants in front of the catalyst, as well as significant differences in front and rear surface area, NOx storage capacity, and NOx conversion.
- Removed camless engine prototype from International vehicle and installed in ORNL engine-dynamometer lab.

Future Directions

- Continue to study LNT chemistry at bench scale, to improve understanding of sulfation/desulfation. The ability to desulfurize the catalyst is foremost to commercial success of LNT technology.
- Commission camless engine at ORNL facility, explore interaction between advanced low-temperature combustion modes (lower NOx and PM) and overexpansion (improved efficiency).

Introduction

Heavy and light-duty emissions standards call for significant reductions in NOx emissions by 2009-2010. The LNT catalyst is a promising technology to help meet these stringent new NOx standards, but there are many open issues that must be resolved prior to commercialization. One of the most important issues is sulfur poisoning. Even with the nationwide availability of 15 ppm sulfur diesel fuel, the LNT will require effective sulfur management. The catalyst's high affinity for sulfur will require periodic desulfation. Desulfation requires high temperature and fuel-rich conditions. Managing the desulfation such that thermal damage is avoided is very important to the life of the aftertreatment system. Prior work in this Cooperative Research and Development Agreement (CRADA) project has focused on understanding the regeneration and desulfation processes through engine experiments with full-scale aftertreatment devices. Ongoing work with the LNT technology at ORNL will focus on bench-scale experiments to better understand the fundamentals.

A second focus of the CRADA will involve use of a unique camless engine prototype with infinitely variable valve timing, to study more conventional variable valve timing approaches. Using valve timing to trap exhaust gas (internal exhaust gas recirculation, or EGR) will be examined as a means to bring about advanced combustion modes such as low-temperature combustion. Overexpansion as a means to greater thermal efficiency or other thermodynamic cycles unique to the diesel engine will also be explored.

Approach and Results

Under this CRADA, experiments at ORNL have focused on in-pipe or in-exhaust (after turbo) fuel injection for LNT regeneration. ORNL developed a PC-based controller for transient electronic control of EGR valve position, intake throttle position, and actuation of fuel injectors in the exhaust system. Diesel oxidation catalysts (DOCs) in conjunction with a catalyzed diesel particle filter (CDPF) and LNT have been evaluated under quasi-steady-state conditions while sampling for HC species at multiple locations in the exhaust system.

Previously reported studies examined fuel cracking upstream of a 14 liter LNT by using the CDPF alone and in conjunction with a 5.0 liter DOC. Gas chromatograph mass spectrometry (GC-MS) and Fourier transform infrared (FTIR) spectroscopy were used to speciate the hydrocarbons entering and exiting the LNT catalyst. Results showed high utilization of light alkenes and mono-aromatics, and poor utilization of branched alkanes. Follow-on experiments utilized pure compounds (1-pentene, toluene, and iso-octane) to confirm the rank order of HC species for LNT regeneration [1].

The LNT was also desulfated on the engine, using throttling, EGR, and in-pipe injection of diesel fuel. This desulfation was conducted at a "road load" condition to demonstrate that desulfation might be accomplished during normal driving.

This year, small one-inch long core samples were taken from the front and rear of the 14 liter LNT as shown in Figure 1. These samples were analyzed by several methods to elucidate the desulfation effectiveness and aging effects. Figure 2 shows results of diffuse reflectance infrared fourier transform spectroscopy (DRIFTS) analysis on the front and rear samples. A small amount of washcoat was scraped from each sample for DRIFTS analysis. The large sulfate peak noted on the front sample indicates the presence of sulfur, while the rear sample shows little or no sulfur. Additional analysis on fresh and sulfated samples is planned and will allow further understanding of the sulfation and desulfation processes for this catalyst formulation. Additional samples from the core of this catalyst will also be examined.

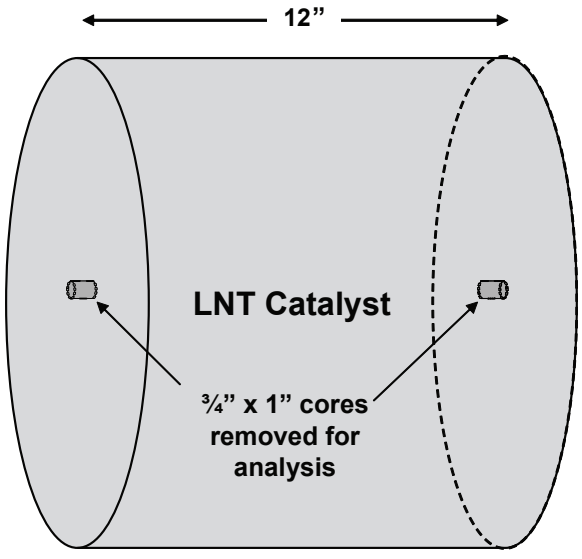


FIGURE 1. LNT Schematic Showing Location of Core Samples Removed for Bench Analysis

Other bench-scale analyses included N_2 physisorption for surface area measurements using a static constant volume sorption apparatus (method of Brunauer, Emmett and Teller), precious metal sizing by X-ray diffraction (XRD), and NOx storage and conversion using small cores in a microreactor. During desulfation, the temperature in the rear of the LNT was at least 50°C higher than in the front. This higher temperature apparently leads to a loss of surface area in the rear; the front sample measured some 23 m^2/g while the rear had been reduced to 16. Also, the average precious metal particle size in the front was 3.9 nm, while the rear showed signs of sintering with an increase to 4.5 nm. In addition, both XRD and DRIFTS analysis indicate the presence of $BaCO_3$ in the rear, while only trace amounts were observed in the front sample, most likely due to the overwhelming presence of $BaSO_4$.

Figure 3 shows the comparative NOx storage for the front and rear samples at three different temperatures. The figure shows that the stored sulfate causes a significant loss of storage capacity at 400°C on the front sample. The loss of storage capacity at 400°C directly relates to the most stable storage sites of the LNT, i.e., weak storage sites and stable storage sites are utilized at the lower temperatures, but only the more stable sites are utilized at the higher temperature. Therefore, these results show that the remaining sulfates are preferentially blocking the most stable sites of the LNT. These

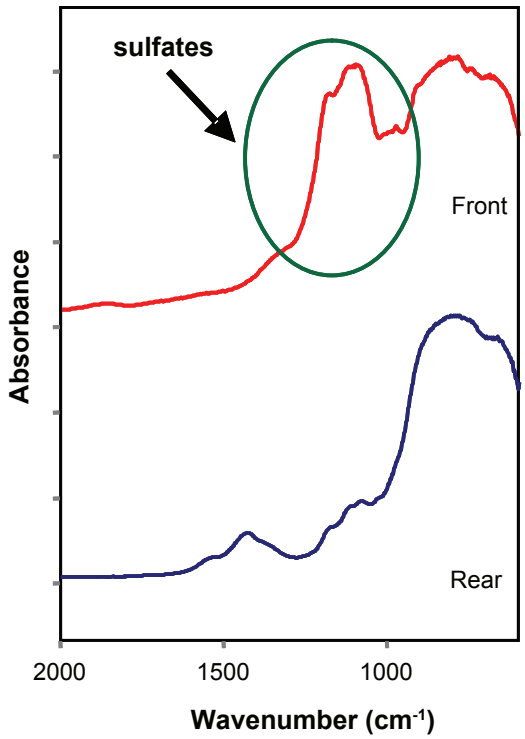


FIGURE 2. DRIFTS Spectra from Front and Rear LNT Samples Show Prominent Sulfate Peak in Front Sample

results also relate directly to the desulfation process. Because the front section of the catalyst did not reach temperatures high enough to remove the most stable sulfates, the most stable nitrate storage sites are thus preferentially blocked.

The presence of sulfate and the loss of surface area also impact the NOx conversion efficiency, shown in Figure 4. These data were collected using a modified CLEERS protocol [2]. The front of the catalyst has superior NOx conversion at the lower temperature, while the rear sample is better at the higher temperature. These results suggest that the precious metal sintering limits the performance at the lower temperatures more than the loss of NOx storage sites. This observation is supported by the fact that LNT performance is limited at lower temperatures by NO to NO_2 oxidation, a reaction that is heavily dependent on precious metal surface sites. Conversely, the improved performance for the rear of the catalyst at 400°C can be attributed to the higher

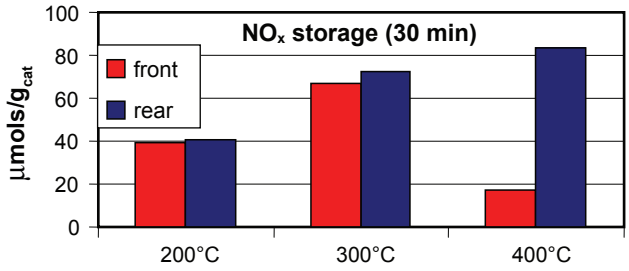


FIGURE 3. NOx Storage Capacity as a Function of LNT Temperature

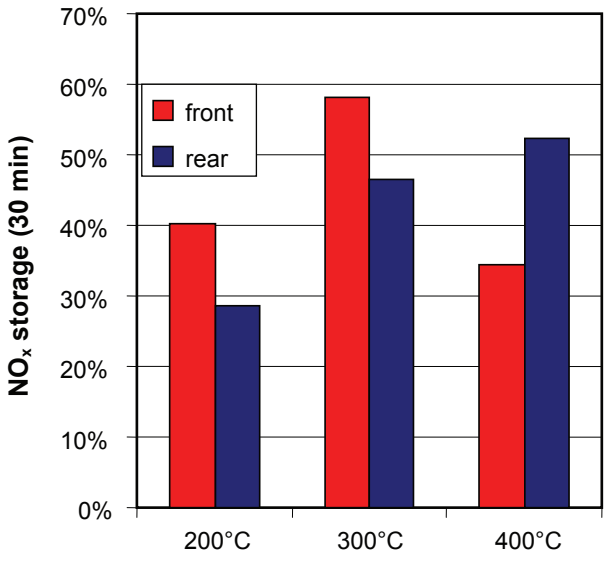


FIGURE 4. NOx Conversion of Front and Rear LNT Core Samples in Micro-reactor

NOx storage capacity. Again, analyses of fresh samples will provide more insight into the significance of these results.

In addition to the bench-scale LNT studies at ORNL, a camless engine prototype has been setup for advanced combustion studies. In FY 2006 this camless engine prototype was removed from an International truck and installed in place of the International T444E V8 diesel previously used in the engine-based LNT studies. Engineers from International visited ORNL on three occasions to train ORNL staff on the camless hardware and software, to assist with the engine removal, and to help commission the engine in the ORNL dynamometer cell. Difficulties with the transition from vehicle to dynamometer cell precluded engine operation before the end of the FY. These difficulties were resolved and the engine was successfully started early in FY 2007.

Conclusions

During this CRADA activity, experiments on LNT regeneration have been conducted with diesel fuel and three pure compounds to examine the HC sensitivity of the catalyst system. A LNT desulfation was conducted at a road-load condition with diesel fuel spray for reductant. Core samples from the engine-aged LNT have been examined in ORNL bench reactors. A camless engine prototype has been removed from an International truck and installed in an ORNL dynamometer cell. Notable conclusions are the following:

- Light alkenes and monoaromatics appear to be preferred by the LNT.
  - Pentene is the most efficient compound examined, followed by toluene.
  - Iso-octane is very poorly utilized by the LNT.
- Laboratory reactor analyses of engine-aged LNT samples suggest:
  - Higher temperatures at the rear of the catalyst during desulfation are believed to be responsible for more complete sulfur removal and precious metal sintering (coarsening).
  - Presence of sulfur in the front of the catalyst impacts performance at higher temperatures where storage capacity is most important.
  - Precious metal coarsening in the rear of the LNT catalyst impacts performance most notably at lower temperatures, where the NO to NO_2 oxidation and NO_2 to N_2 reduction limits performance.

References

1. FY 2005 Progress Report for Advanced Combustion Engine Technologies, Energy Efficiency and Renewable Energy, Office of FreedomCAR and Vehicle Technologies, "Advanced Engine/Aftertreatment System R&D," pp. 169-174, January 2006.

2. FY 2005 Progress Report for Advanced Combustion Engine Technologies, Energy Efficiency and Renewable Energy, Office of FreedomCAR and Vehicle Technologies, "Cross-Cut Lean Exhaust Emission Reduction Simulation (CLEERS)," pp. 218-226, January 2006.

II.B.6 Advanced CIDI Emission Control System Development

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Subcontractors:

- FEV Engine Technology, Inc., Auburn Hills, MI
- ExxonMobil Research and Engineering Company (EMRE), Paulsboro, NJ

Objectives

Develop and demonstrate a highly efficient exhaust emission control system for light-duty compression ignition direct injected (CIDI) engines to meet Federal Test Procedure (FTP) Tier 2 emissions standards (0.07 g/mi NOx, 0.01 g/mi particulate matter, PM) with minimal fuel economy penalty and 120k mi durability.

Accomplishments

- The project was completed and the final technical progress report was filed.
- Tier 2 Bin 5 emission levels were achieved for non-methane hydrocarbons (NMHC), CO, and PM at 120k miles using a selective catalytic reduction (SCR) system and catalyzed diesel particulate filter (CDPF) with a mid-size diesel engine on a 6,000 lbs gross vehicle weight rating (GVWR) light-duty truck (LDT). Weighted tailpipe NOx on the FTP for light-duty vehicles (FTP-75) was 0.128 g/mi.
- With a more active diesel oxidation catalyst (DOC), the 120k mile SCR system reduced NOx emissions to 0.091 g/mi, which corresponded well to lower-mileage results under similar conditions. This confirmed the durability of the copper/zeolite SCR catalyst.
- Tier 2 Bin 5 levels for NOx were achieved using an improved SCR catalyst aged in the laboratory for the equivalent of 120k miles. The tailpipe NOx emissions were 0.061 g/mi when tested with a more active DOC.
- Post mortem analyses of the 120k mile catalysts revealed non-uniform aging.
- Improvements were made to the DOC and SCR models

Future Directions

The project is concluded. No further work is planned.

Introduction

Reducing particulate matter (PM) and NOx emissions are primary concerns for diesel vehicles required to meet 2007 Federal Tier 2 and California Low Emission Vehicle II (LEVII) emission standards (Table 1). These standards represent a 90-95% reduction from Federal Tier 1 diesel standards.

TABLE 1. 2007 FTP Emission Standards* (passenger cars and light-duty vehicles)

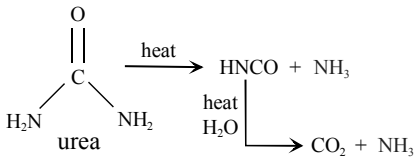
	50k mi		*120k mi*	
Standard (g/mi)	**NOx**	**PM**	**NOx**	**PM**
LEVII	0.05	----	0.07	0.01
Tier 2, Bin 5	0.05	----	0.07	0.01

*Supplemental FTP standards not included.

The high oxygen content of diesel exhaust makes onboard NOx control complicated. The technology with the most potential to achieve 90+% NOx conversion with minimal or no fuel economy penalty is SCR with an ammonia-based reductant such as aqueous urea. Ammonia-SCR has been used extensively for stationary source NOx control [1]. The main reactions are shown below:

Feasibility of using aqueous urea on vehicles has been proven by past work at Ford [2,3], Volkswagen [4], Mack Truck [5] and DaimlerChrysler [6].

urea decomposition:



NO_x reduction:

$$4NO + 4NH_3 + O_2 \longrightarrow 4N_2 + 6H_2O$$
$$6NO_2 + 8NH_3 \longrightarrow 7N_2 + 12H_2O$$
$$2NH_3 + NO + NO_2 \longrightarrow 2N_2 + 3H_2O$$

Control of diesel PM is accomplished with a periodically regenerated ceramic filter, usually called a catalyzed diesel particulate filter, or CDPF. The filter may be washcoated with precious metal to help oxidize HC and collected soot. A DOC may also be placed upstream of the filter to further aid in filter regeneration. The DOC also provides reduction in hydrocarbon (HC) and carbon monoxide (CO) emissions, as well as NO oxidation for more durable SCR function.

Approach

At Ford, improved supplier catalysts were tested in laboratory flow reactors for aged conversion levels. The best performing system that included a DOC, SCR catalyst, and CDPF was aged and tested on an engine dynamometer at FEV. Development and evaluation of improved SCR catalysts continued. Ultra-low-sulfur diesel fuel (<15 ppm S) was used for all aging and testing. Tests of the aged system were performed on a 6,000 lbs GVWR LDT. Appropriate exhaust gas sensors and control strategies were tested for durable system function. System modeling played an important role in design and analysis of performance.

Results

Catalyst system aging to the equivalent of 120,000 miles was completed on the engine dynamometer at FEV. Total time on the engine was 2,544 hours. The CDPF was regenerated a total 643 times, each typically lasting ten minutes, including six minutes with the SCR catalyst at high temperature (over 600°C). In all, the SCR catalyst spent 64 hours at high temperature during the durability phase.

The catalysts were installed on the LDT for emissions testing. Issues with engine control prevented using the rapid warm-up strategy that had proven effective in enabling NOx emissions approaching Tier 2 Bin 5 with fresh catalysts. Average tailpipe emissions from FTP-75 testing showed that non-methane organic gases (NMOG) and CO emissions were within Tier 2 Bin 5 limits, but the NOx emissions were higher than fresh and at 50k mi, with 74% conversion and 0.128 g/mi tailpipe NOx over the FTP-75 cycle (see Figure 1). The CDPF continued to be effective at meeting the regulated level of PM with 0.0012 g/mi, and it effectively converted any NH_3 slip from the SCR catalyst.

In order to determine which component was responsible for the decreased emission performance, combinations of low-mileage and 120k mi SCR and DOC catalysts were tested. The low mileage DOC with the aged SCR improved NOx emissions to the level reported at 50k mi: 0.091 g/mi NOx with 85% conversion efficiency. This indicated that the decreased performance of the aged emission system was due

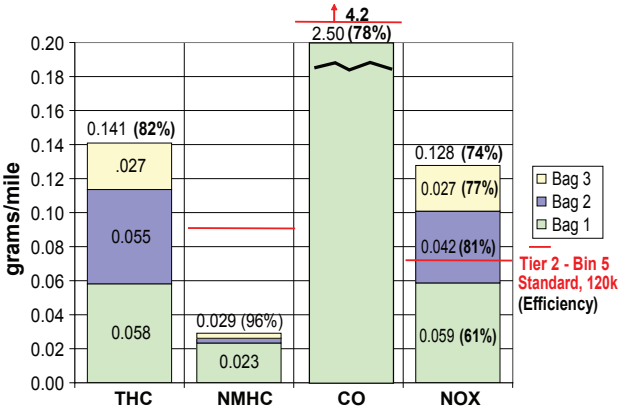


FIGURE 1. FTP-75 performance of the 120k mi aged catalyst system on the 6,000 lb light-duty truck without rapid system warm-up.

primarily to deterioration of the DOC, and that the copper/zeolite SCR catalyst was durable to 120k mi.

A newer SCR catalyst with improved low-temperature performance was aged in the laboratory at 670°C under lean conditions for 64 hours. This catalyst was installed on the LDT, and with the aged DOC NOx emissions were improved to 0.081 g/mi. With the more active DOC this catalyst met the Tier 2 Bin 5 NOx limit, with 0.061 g/mi over the FTP-75, even without an engine capable of running a rapid warm-up strategy (Figure 2).

A detailed post-mortem analysis of the 120k mi DOC, SCR and CDPF components showed non-uniform aging of the DOC and SCR catalysts due to exotherms from DPF regeneration and poisoning by oil additives. HC, CO, and NO oxidation activity and surface area of the rear portion of the DOC were reduced compared to the inlet, indicating exposure to high temperatures. The front face of the SCR was especially degraded in NOx performance compared with the rest of the brick. Laboratory flow reactor results are shown in Figure 3 for different parts of a core sample taken from the SCR. The activity of the outlet sample correlated well with a lab-aged sample. There was evidence to suggest contamination by urea-related deposits as an additional aging factor. The CDPF was intact and its washcoat showed evidence of thermal aging. Some ash and soot were found in the inlet channels, as expected.

Semi-empirical DOC and DOC+SCR system models were developed further during the course of the project. The DOC model was used to study the effect of formulation and volume on the amount of NO_2 generated and the resulting SCR NOx conversion. A more detailed SCR model was developed, incorporating energy and mass balances, NH_3 oxidation and several selective NH_3 reactions with NOx. The kinetic parameters were calibrated using NH_3 adsorption and desorption experiments and other laboratory flow

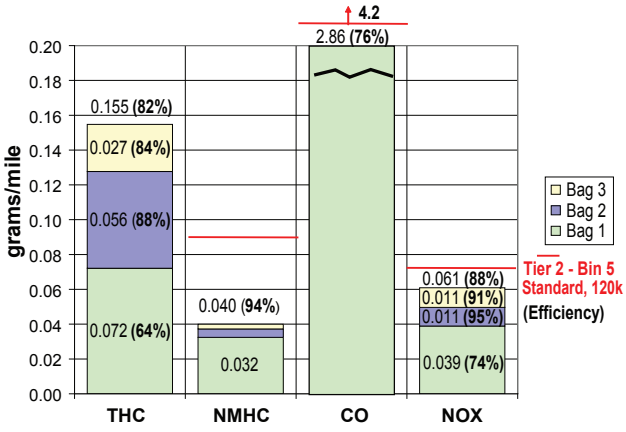


FIGURE 2. FTP-75 performance of the improved SCR catalyst with low-mileage DOC.

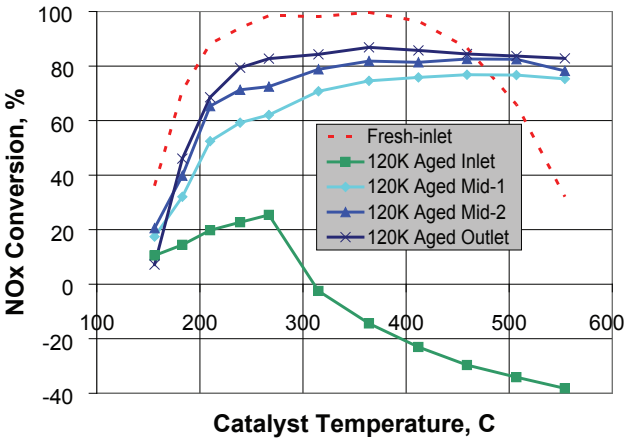


FIGURE 3. NOx activity of core taken from 120k engine-aged SCR catalyst, SV=30,000/hr, NO only.

reactor data. Model performance was validated by comparing predictions to vehicle test results, as in Figure 4. The model predictions gave direction for improving urea control and selecting catalyst components, and helped to explain the vehicle emission results.

Conclusions

- Catalyst system aged to the equivalent of 120k mi on an engine dynamometer met Tier 2 Bin 5 for NMHC, CO, and PM. The engine was not capable of running a rapid warm-up cold start strategy, resulting in a tailpipe NOx level of 0.128 g/mi.
- DOC deterioration was found to be responsible for most of the decrease in NOx performance, indicating that the copper/zeolite SCR was durable to 120k mi.

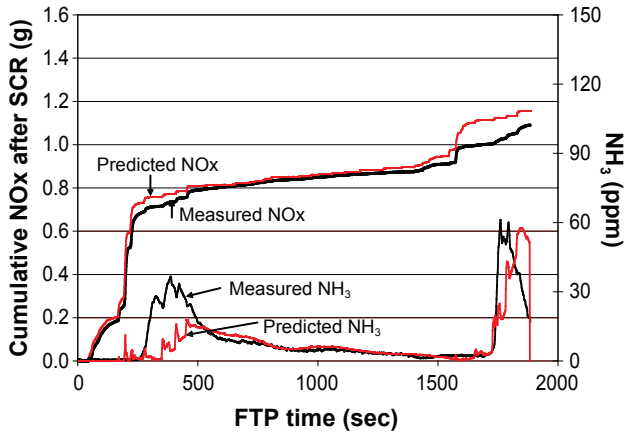


FIGURE 4. Vehicle NOx and NH_3 emissions measured after the improved lab-aged SCR catalyst, compared to model predictions for an FTP-75 test.

- The test vehicle met the Tier 2 Bin 5 NOx limit with a more active DOC and an improved SCR catalyst aged to 120k mi equivalent.

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II.B.7 Fundamental Sulfation/Desulfation Studies of Lean NOx Traps, DOE Pre-Competitive Catalyst Research

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Objectives

- Provide a better understanding of the fundamental deactivation mechanisms that result during regeneration and desulfation
  - Investigate ways to limit the impact of these mechanisms
- Transfer this information to teams to:
  - Improve the material
  - Improve the desulfation methods
  - Improve simulation of the processes

Approach

- Effort is pre-competitive
  - Allows open dissemination of results and data
- Study deactivation mechanism fundamentally
- Evaluate deactivation from sulfur poisoning and de-sulfation
  - Employ moderate levels of sulfur (15 ppm SO_2) to more accurately mimic engine levels
  - Desulfation under controlled temperature ramps
- Employ multiple analytical techniques to monitor activity and morphology effects
  - Investigate surface species (DRIFTS) and their reactivity
  - Monitor activity over typical operating range, 200-400°C with powder reactor
  - Investigate morphological effects with (BET, X-ray defraction [XRD], Chemisorption)

Accomplishments

- Presented recent efforts at Delphi, CLEERS, and ACE Review (poster)
- Identified multiple sulfate species on both Ba- and K-based lean-NOx traps (LNTs) that are dependent on time and temperature
- Titrated sulfur poisoning in both DRIFTS and kinetic reactor to evaluate poisoning potential of fast and slow sites.
- Correlated sulfation degree to desulfation species
- Demonstrated linear loss in storage sites with sulfation
- Published FY 2005 results in refereed journal (Catalysis Today)
- Characterized catalysts for morphological and bulk changes

Future Directions

- Verify sulfates form near Pt then migrate during rich phase
- Perform detailed sulfation/desulfation experiments on washcoated catalyst sample in translational diffuse reflectance infrared Fourier-transform spectroscopy (DRIFTS) reactor with spatially resolved capillary inlet mass spectrometer (Spaci-MS)
  - Investigate fast desulfation to potentially drive off weakly bound sulfates before they convert to strongly bound sulfates
- Determine sulfation/desulfation behavior of mixed Ba/K model catalysts
  - Investigate which phase preferentially adsorbs sulfates first
- Investigate effects of doping storage phase with other alkali/alkaline components to affect sulfate stability

Introduction

Several efforts previously investigated under the Cummins/Oak Ridge National Laboratory (ORNL) Cooperative Research and Development Agreement (CRADA) which are pre-competitive have been transferred to this project. This allows

open dissemination of those research results, without confusing issues of CRADA protected information, and frees up CRADA funds to investigate protected topics. The transferred efforts connect kinetic rates with optical spectroscopy areas. Nevertheless, the two projects will continue to work closely to address both competitive and pre-competitive research issues.

The complex heterogeneous nature of production catalyst washcoats critically obscures research of fundamental mechanisms. Model catalyst materials represent only a component of production materials, but allow isolation of individual fundamental processes; these include detailed mechanisms for desorption and poisoning, intermediate existence and role, and reduction details. Hence, this project primarily employs model catalyst materials for experimental investigation of fundamental catalyst phenomena.

Approach

Under future vehicle regulations, the efficiency of a diesel engine system will also 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. Modeling/simulating processes is an effective way to develop efficient systems, and basing the model on fundamental chemistry is critical for it to be transportable and broadly-useful to industry; parametric-based models will not fill the need.

The emphasis of this project is to improve detailed understanding of mechanisms limiting catalyst performance. Work closely with catalyst-industry representatives to identify and investigate pre-competitive catalyst-performance issues of broad relevance across the catalysis industry. Specific objectives are to improve the fundamental understanding of adsorption, reduction, poisoning processes and the influence on catalyst morphology. The objectives of this project are consistent with those of the Diesel Cross-Cut Team regarding details of sulfur poisoning and catalyst morphology effects.

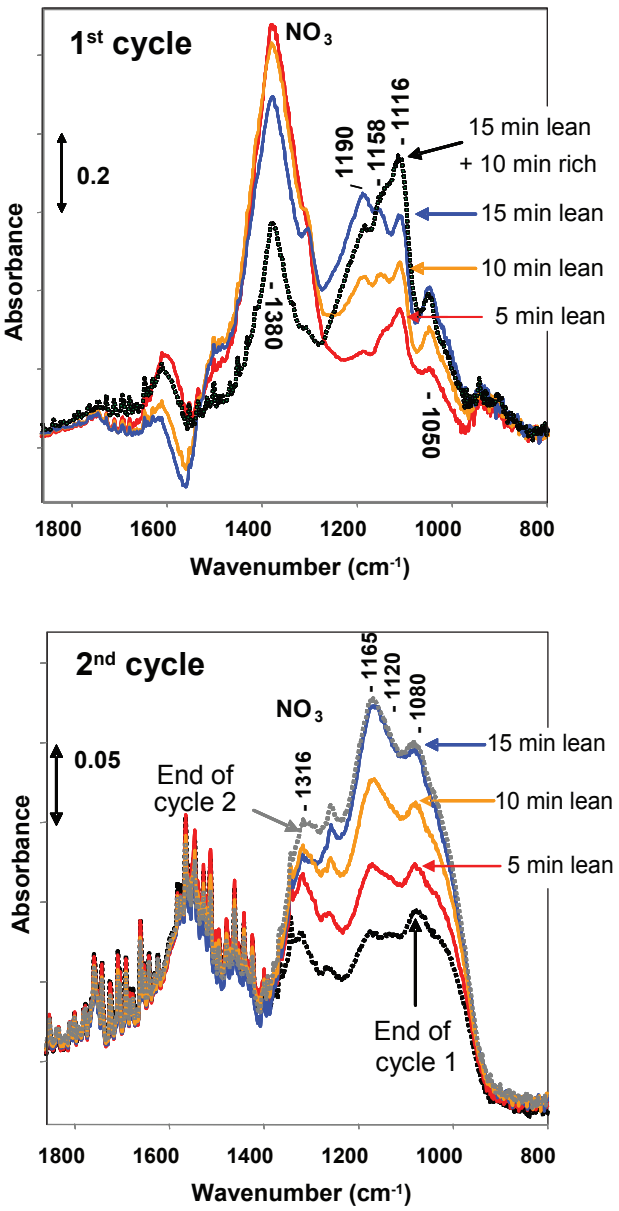


FIGURE 1. DRIFT spectra of sulfation on K-based LNT during cycles of 15 minutes lean and 10 minutes rich. (a) First cycle shows initial sulfation, and (b) second cycle shows LNT as it becomes completely poisoned and nitrate formation ceases.

Results

The results this year have been focused on studying SO_2 adsorption on the storage (Ba or K) and catalytic (Pt) sites of LNTs. We have identified a precursor to permanent sulfate formation on both Ba- and K-based LNTs using DRIFTS. This is illustrated for the K-based LNT in Figure 1a where sulfates are initially observed forming at 1116 cm^{-1} in conjunction with the nitrates at 1380 cm^{-1}; eventually the sulfates at 1158 and 1190 cm^{-1} begin to form as the nitrates begin to diminish. When all nitrate formation ceases during the second cycle (Figure 1b) the sulfate at 1165 cm^{-1} dominates the spectra. Also of interest in these initial spectra is the transformation of sulfates when switching from lean to rich (peaks at 1190 and 1158 cm^{-1} decrease while 1116 cm^{-1} increases). This view contrasts the widely held notion that sulfates are highly stable and immobile, i.e they form in the storage medium and do not change until desulfation. These initial findings were the basis for the bulk of the efforts this year and attempted to answer key questions regarding sulfate stability with respect to degree and temperature of sulfation.

The Ba-based LNT effort this year was focused in the DRIFTS reactor by performing 6.5-minute lean and 30-second rich cycles with 15 ppm of SO_2 flowing at all times; temperatures evaluated were 200, 300, and 400°C. Multiple sulfur groups were observed for these experiments, but specific spectral identification has not been finalized to date. The first observation for Ba-based LNTs regarded sulfur's impact on nitrate storage. At 200°C, the overall nitrate storage was not impacted by SO_2 until the LNT was heated to 500°C, i.e. the sulfur adsorbed as a spectator that required "activation" at higher temperatures to remove nitrates and impact storage capacity. At 300°C, surface nitrates were immediately impacted upon SO_2 addition, and at 400°C bulk nitrates incurred the largest impact. Observations were also detected with respect to Pt surface sites. The Pt-CO bond is visible during the rich-phase of these experiments; it can be an indicator of active Pt sites. When SO_2 is included in the flow the intensity of this bond steadily decreases at all temperatures; however, when SO_2 is removed it recovers. This is indicative of SO_2 masking the Pt surface sites and limiting reactivity.

The K-based LNT effort this year included efforts in the DRIFTS reactor and the powder-based microreactor. Three distinct sulfate forms were observed with DRIFTS on the K-based LNT (listed in order of increasing stability): ionic sulfate, monodentate sulfate and bidentate sulfate. Figure 2 shows the peak areas associated with these sulfates while sulfating at 200, 300, and 400°C with an intermittent mild desulfation at 500°C (the max allowed temperature in the DRIFTS reactor). These plots indicate for each temperature the degree of sulfation continues throughout the experimentation, i.e. no sulfate groups are removed during the mild "desulfation" at 500°C. Also, although the less-stable ionic sulfate is a dominant feature initially, heating tends to transform it into the more stable bidentate sulfate. These two key observations are somewhat disappointing, but continue to illustrate that the sulfate forms on LNTS continue to be mobile, and in future experiments we are hoping to demonstrate the possibility to desulfate the less stable form quickly before it can transform into the more stable bidentate sulfate. This will also more accurately mimic engine-based desulfation efforts, but will require some reactor modifications.

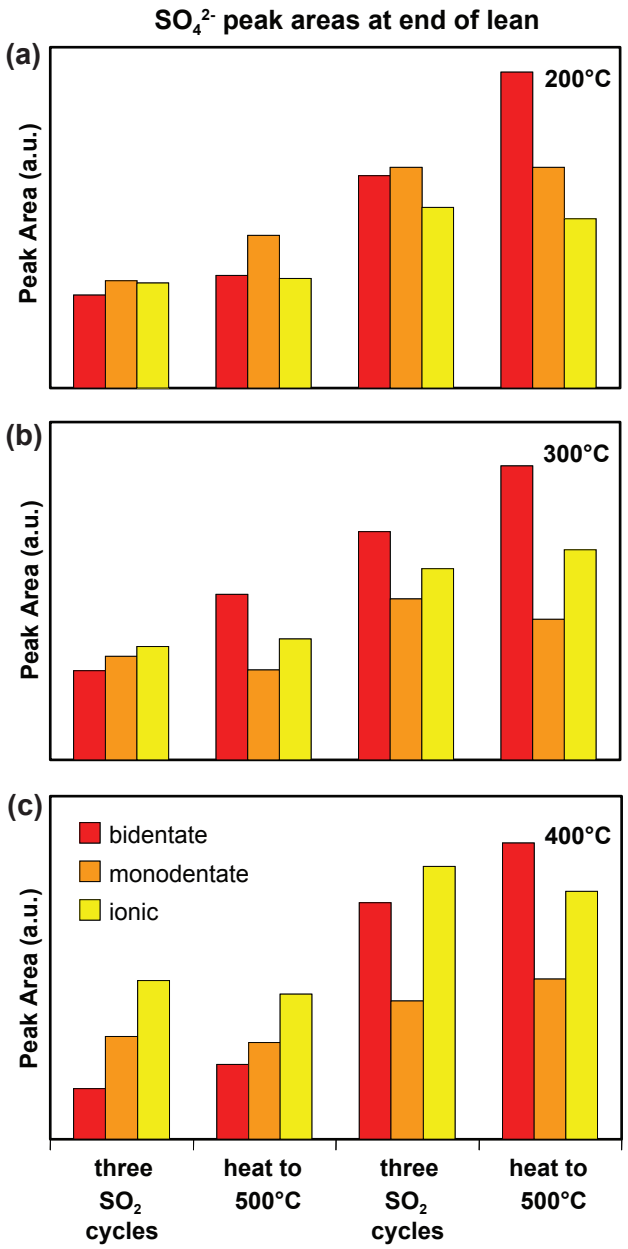


FIGURE 2. DRIFTS peak areas of sulfur groups—(■) bidentate, (■) monodentate, and (■) ionic—that form during incremental sulfation of K-based LNT catalysts. Areas are determined at the end of the lean cycle.

Analyzing sulfates only describes part of the process, thus it is important to also analyze the effects on nitrates. The general observations at 200 and 300°C for the K-Based LNTs are that the active NOx storage, i.e. the amount of NOx that is stored and then released for a given cycle, is relatively constant during the initial sulfation experiments. This is depicted graphically in Figure 3 using the light bars. The impact of sulfur on the overall amount of nitrates stored on the LNT, i.e. the nitrates that are stored but not necessarily released during the rich-phase, is depicted in Figure 3 using the dark bars. It is evident at all temperatures that the overall capacity begins to decrease as soon as SO_2 is introduced; however, the effective storage is not immediately impacted at 200 and 300°C. At 400°C, where nearly all of the storage sites are participating in active NOx storage, the impact on overall storage is immediately observed. This DRIFTS reactor-based observation is also observed in the micro reactor results. Figure 4 shows the overall NOx conversion in the microreactor as a function of exposure time.

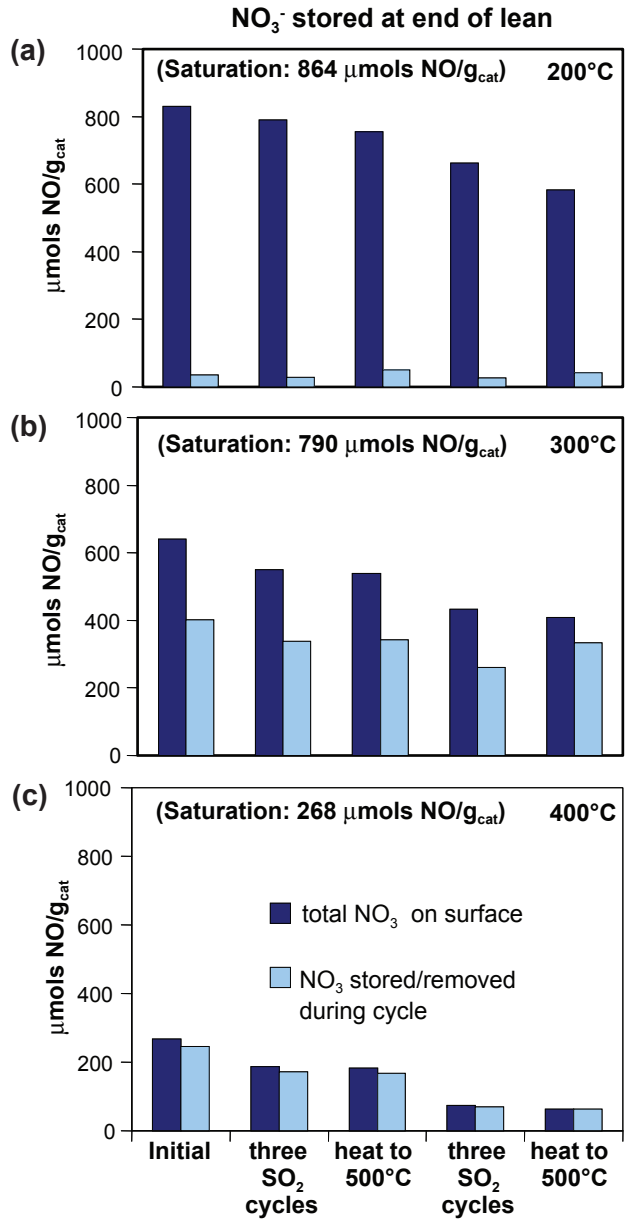


FIGURE 3. Quantified DRIFTS analysis of active nitrates (▭) and overall nitrate storage (■) during incremental sulfation of K-based LNT catalysts. Values are determined at the end of the lean cycle.

At each temperature there is a level period where the NOx conversion is not impacted, then after a period of about 4 hours the NOx conversion decreases almost linearly; the rate of deactivation varies proportional to temperature.

The low levels of SO_2 used to sulfate the catalyst did not allow for accurate measurements of sulfur uptake, so it was difficult to monitor the degree of sulfation directly. However, during the desulfation a large amount of SO_2 and H_2S are desorbed and detection possible. From this, a sulfur collection efficiency can be estimated based

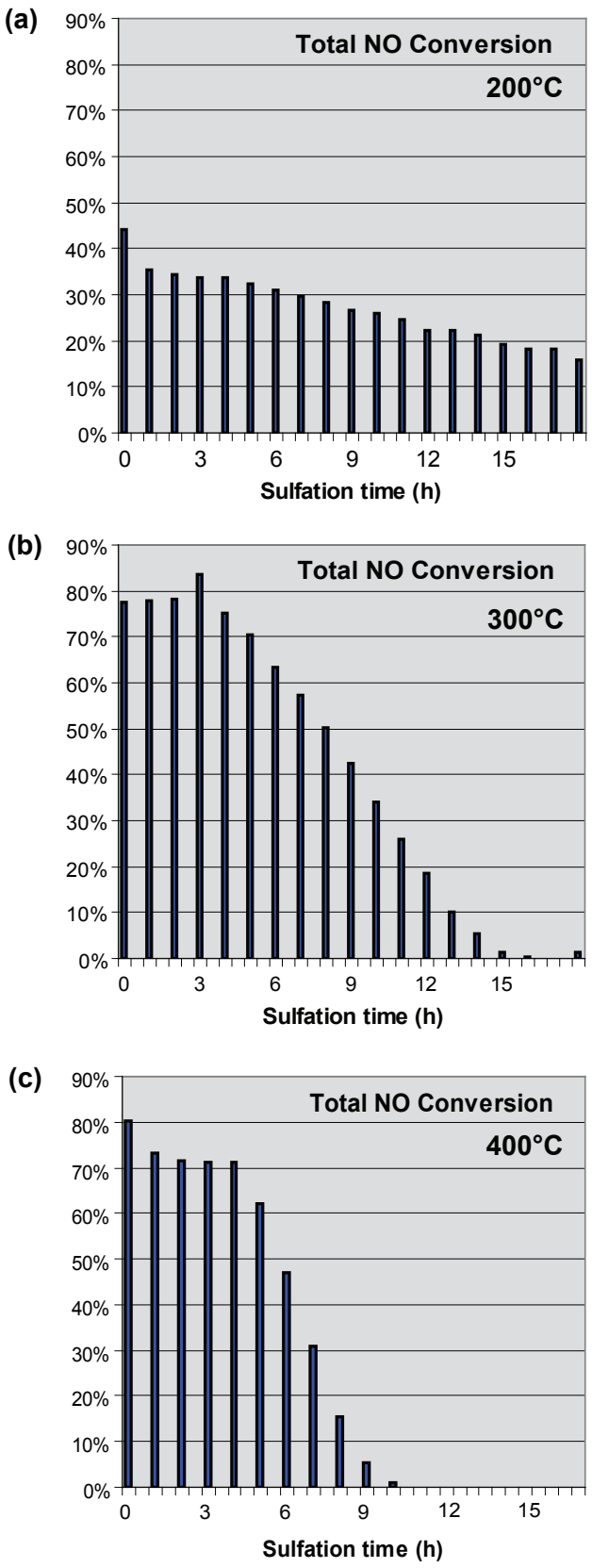


FIGURE 4. NOx Conversion as a function of LNT poisoning using 15 ppm SO_2 at (a) 200°C, (b) 300°C, and (c) 400°C.

on time and temperature. The desulfation results are listed in Table 1, where it is apparent sulfur is trapped much more effectively at 300°C, and much of the SO_2 is not collected at 200°C and 400°C. The desulfation procedure regains much of the activity as demonstrated in Figure 5.

TABLE 1. Summary of desulfation products and their respective temperature of peak formation. Desulfation conditons: 400 to 800°C at 10°C/min, 5,625 ppm CO, 3,375 ppm H_2, 5% H_2O, 5% CO_2, and 30k, h^{-1}.

Sulfation Temperature (°C)	Sulfation Time (h)	H_2S Released (μmols)	Peak Temperature (°C)	SO_2 Released (μmols)	Peak Temperature (°C)
200	18	1.4	750	5.7	760
300	3	1.8	760	1.3	760
300	18	5.0	750	18.0	500+760
400	18	1.1	750	2.6	760

Incremental sulfation studies in the DRIFTS reactor show that the initially formed sulfate generally transitions to the more stable sulfate upon heating to 500°C rather than being removed. Powder reactor efforts corroborated this result as the lightly sulfated LNT does not desulfate below 750°C. A key observation from the sulfation studies was the ability of the LNT to maintain its active sites during the incremental addition of SO_2. This has implications to modeling efforts and consequently systems control, since it suggests that sulfates that form near Pt can migrate to another less-active site. This view contrasts the notion of sulfates being highly stable and immobile, and suggests that LNTs can withstand a significant level of sulfur without a major impact on overall conversion. This observation is most significant at 200 and 300°C where there are a significant number of storage sites that are not used during lean/rich cycling. This result has also been independently corroborated in the powder reactor for all temperatures. The powder reactor study also showed that the collection efficiency of SO_2 varied significantly with temperature with the most efficient collection of sulfur at 300°C; however, sulfur has the fastest and most significant impact on NOx conversion at 400°C.

The reduced funding level this year did not allow for efforts to go forward with our DRIFTS reactor that enables *in-operando* investigation of surface species along the length of washcoated sample. The reactor is designed to allow flow between the infrared window and the sample. The catalysts sample can have dimensions that are 25 mm wide and a length of up to 300 mm. This reactor is designed to allow surface investigations along the axial length of washcoated samples. When coupled with Spaci-MS this reactor will be a powerful tool that will allow a direct correlation between observed surface species and gas-phase concentrations.

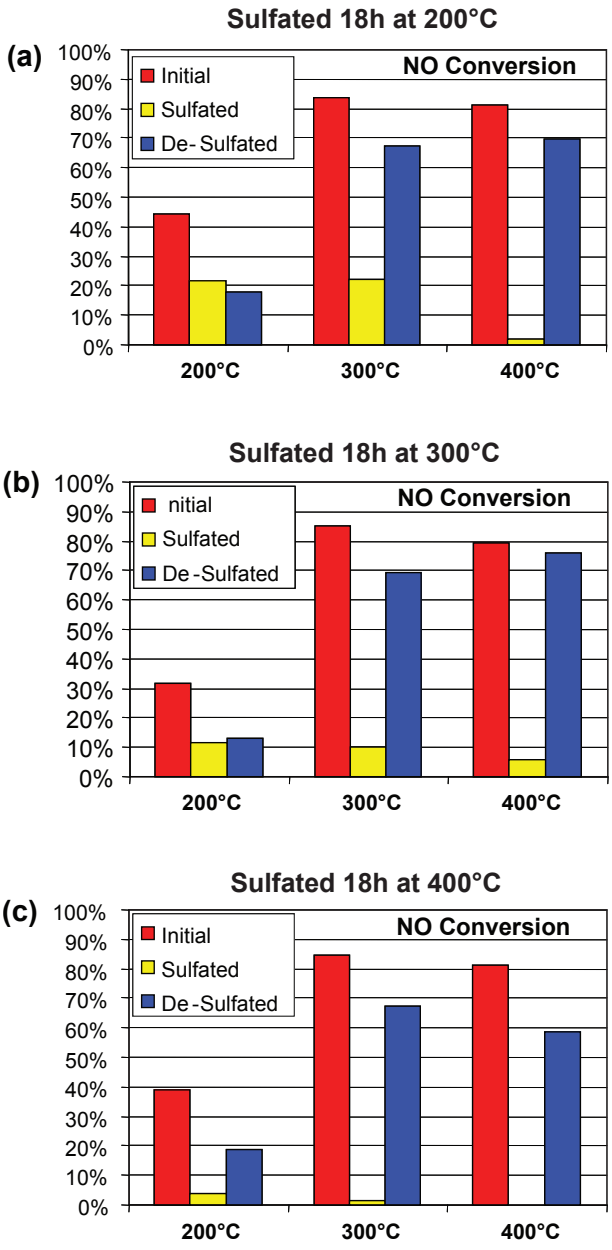


FIGURE 5. NOx conversion before sulfation (■), while completely poisoned (■), and after 800°C desulfation (■); sulfation using 15 ppm SO_2 at (a) 200°C, (b) 300°C, and (c) 400°C.

Conclusions

- Three sulfate forms observed on LNTs
  - Form depends on temperature, degree of sulfation and lean/rich condition
- All sulfur leaving the engine is not trapped
  - Rates of sulfation vary with temperature
  - Additional T-dependent data being generated

- Model must account for two types of sites
  - Fast and slow sites are relevant to rates of sulfation
  - Fast sites appear to be less impacted by initial sulfation
  - Surface mobility is a key factor
- Sulfation degree and relative impact is temperature dependent
  - SO_2 stored at 400°C is more detrimental to performance than SO_2 collected at 200 or 300°C

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II.B.8 NOx Control and Measurement Technology for Heavy-Duty Diesel Engines

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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

- Characterized detection limit of various analytical methodologies for real-time on-engine measurement of oil dilution.
- Quantified details of CO regeneration of lean-NOx traps (LNTs) and function of the water-gas-shift reaction (WGSR). Regeneration CO pulsing results in dynamic surface carbonate formation which displaces surface water resulting in dynamic gas-phase water pulses. Comparing isocyanate (NCO) and WGSR pathways for NH_3 formation; WGSR does not appear to be a primary pathway.
- Characterized nature of spatially resolved capillary inlet mass spectrometer (SpaciMS) capillary flow, for improved calibrations and system design for mitigation of intra-capillary condensation.
- Improved the robustness of phosphor thermography fiber probe tips, and signal-to-noise ratio (SNR) of the instrument.

Future Directions

- Apply oil-dilution diagnostic for real-time on-engine measurements with various operating conditions.
- Quantify engine-system nonuniformities and mitigation strategies.
- Quantify selected LNT sulfation effects.
- Investigate selected nitrogen-selectivity issues related to LNT regeneration and hybrid catalyst systems.
- Develop and improve analytical techniques as necessary.

Introduction

A combination of improved technologies for in-cylinder and aftertreatment control of NOx emissions are required to efficiently meet 2010 emission regulations. These include advanced combustion and associated engine hardware and controls, improved catalyst systems, and overall system management improvements. The development and application of enhanced diagnostic tools is required in order to realize these technology improvements. For instance, unique diagnostics developed in this Cooperative Research and Development Agreement (CRADA) have been used by the partners to resolve the network, sequence and distribution of catalyst reactions via intra-reactor species and temperature measurements; this detailed understanding in combination with other more conventional analysis has proven critical to system implementation. Similarly, the partners have applied these diagnostics outside the CRADA to quantify the performance of EGR and other hardware for improved system efficiency. These types of applications of advanced analytical techniques are required to obtain the detailed understanding of specific system components and the integrated systems in order for the manifold of technologies required for meeting efficiency and emissions targets to work effectively in concert.

Approach

- Apply advanced analytical capabilities to improve the efficiency of diesel-engine-catalyst systems.
- Engine-based research focuses on detailed barriers to diesel market penetration.

- Bench-based research is focused on detailed catalyst reactions, interactions of various reactions, their distribution through the device, and the efficacy of various operation strategies.
- Both the engine and bench research are designed to provide the requisite insight necessary to improve the efficiency of diesel systems.

Results

DOE goals support development of robust and deployable engines using advanced combustion regimes that provide simultaneous high efficiency and low particulate and NOx emissions. Certain advanced combustion regime approaches can result in dilution of engine oil with fuel resulting in chronic irreversible hardware degradation. Current analytical approaches for quantifying oil dilution (e.g., ASTM D 3524-04) are off-line measurements and do not provide the desired detection limit. On-engine real-time measurements of oil dilution would hasten development of robust advanced engine systems that meet DOE goals.

The CRADA team has evaluated a range of analytical approaches to assess their applicability for the desired *in situ* oil-dilution measurement. Optical (ultra-violet/visible, near-infrared, mid-infrared, laser-induced fluorescence, total synchronous fluorescence) and electrical impedance spectroscopy methods based on natural diesel and oil mixtures have a detection limit of approximately 1% v/v diesel in oil which is not sufficient. Compared to our previous work with oil dilution in gasoline systems [1], diesel dilution of oil is complicated by the similarity of the two constituents. Bench results based on incorporation of commercial fuel dyes indicate this to be a possible route for realizing the analytical specifications. This methodology is amicable to optical-fiber based systems, on-engine and real-time analytical systems.

In previous CRADA work the nature of CO regeneration of LNT catalysts and the role of the WGSR has been investigated. That work demonstrated that CO appears to directly regenerate LNT catalysts, and that the WGSR is a lower-priority reaction that apparently occurs in the wrong place and at the wrong time to effect regeneration (see publications). That work also indicated several interesting intra-catalyst water dynamics. The first of these is that when available, the WGSR initially uses surface water and may ultimately cause a gas-phase water sink as the surface is rehydrated to continue the reaction. The second is that dynamic gas-phase water sources can occur spatially and temporally coincident with oxidizing fronts. These results suggest that gas-phase CO_2 generation from oxidation of CO results in catalyst-surface carbonate formation and subsequent displacement of surface water into the gas-phase; this was indicated by gas-phase water generation synchronous with missing gas-phase CO_2. In follow-on work we eliminated several complicating reactions by pulsing CO_2 or oxygen directly into a stream of humidified nitrogen. In a manner consistent with the interpretation of earlier results, gas-phase water generation scaled with the amplitude of the CO_2 pulse. Catalyst temperature had little effect on the efficiency of surface-species displacement, and no displacement was observed with oxygen pulsing. This is further evidence that surface carbonate formation can displace water from the catalyst surface into the gas phase. Consequently, the obtained results further support our conjecture that the water-gas-shift reaction is probably not relevant to primary NOx release/reduction during LNT regeneration: CO acts directly to release/reduce NOx and the resulting CO_2 product displaces surface H_2O which cannot be consumed via water-gas-shift reaction.

WGSR is also potentially relevant to NH_3 generation, and experiments were performed to investigate WGSR and NCO pathways during LNT regeneration. Figure 1 shows species transients from a LNT under various flow conditions. From 900 to ~960 s the feed consists of NO_2+H_2O+N_2. From ~960 to ~1150 s the feed is CO+N_2. From ~1150 to ~1270 s the feed is N_2, and beyond ~1270 s the feed is H_2O+N_2. An NH_3 puff is observed at the first flow switching event that could be attributable to WGSR or NCO pathway; however, the amplitude of this feature does not scale with the temperature dependence of the WGSR. There is no NH_3 formation in the absence of water during regeneration conditions. Transient NH_3 generation is also observed at the final feed switch without CO and as H_2O is turned on. The results suggest surface NCO hydrolysis to be the primary pathway for NH_3 generation.

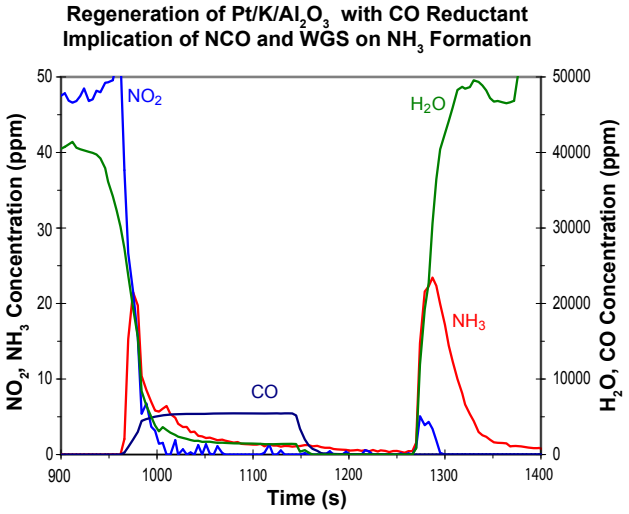


FIGURE 1. FTIR Measured Transient LNT-Effluent Species Pool with Varying Feed Composition to Investigate the Origin of NH_3

The SpaciMS is an instrument developed in the CRADA that has been applied extensively both within and outside the CRADA and on DOE and industry sponsored projects to further DOE energy efficiency goals. Experiments were performed to better understand the nature of sample flow in the SpaciMS capillaries. This improved understanding is needed to improve measurement quantification and better specify capillary conditions to mitigate intra-capillary sample condensation. Capillary flow is generally not well understood based on discussions with industry leaders in the vacuum and capillary technologies areas, university professors and a Fellow of the American Vacuum Society. Experiments were performed to characterize the transit time of various gas mixtures. These measurements show that capillary flow follows mixture bulk viscosity; hydrogen and methane flow faster than oxygen and nitrogen, and helium behaves more like nitrogen than hydrogen. Moreover, little chromatography effect was observed. A step-edge of H_2 in N_2 flow faster than does N_2, but the mixture constituents arrive at approximately the same time; in the mixture H_2 arrives slightly earlier than N_2, but the predominant effect is from mixture composition and hence viscosity. This work will continue in conjunction with flow modeling to better understand capillary flow and its implications on SpaciMS measurements.

Optical-fiber based phosphor thermography has been refined and used in the CRADA to quantify *in situ* intra-catalyst transient temperature distributions. In combination with the SpaciMS this provided a rich description of the catalyst chemistry in terms of local species and temperature. This significantly benefits the understanding and modeling of these complex systems important to DOE's efficiency goals. Methodologies to produce robust, minimally invasive, phosphor-tipped optical fibers have been investigated. Deposition methodologies for multi-component oxide phosphors can change the nature of the phosphor and be limited. A method using fine attrition-milled phosphor in conjunction with a thermally cured ceramic adhesive has proved superior to previous methodologies. Using the new method, coated fibers have survived repeated experiments up to 1,000°C and involving fiber-probe translation.

Conclusions

- Dye additives appear to provide a pathway to realizing oil-dilution specifications
- CO appears to directly regenerate LNT catalysts
- WGSR is of secondary importance to LNT-catalyst regeneration
- WGSR is not a primary pathway for NH_3 generation
- SpaciMS capillary flow does not appear to follow Hagen-Poiseuille flow
- SpaciMS capillary flow is proportional to sample bulk viscosity
- SpaciMS capillary flow shows little chromatography effect
- Improved phosphor deposition methods provide more robust phosphor-thermography probes

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1. Jae-Soon Choi, William P. Partridge and C. Stuart Daw (2005). "Spatially-resolved in situ measurements of transient species breakthrough during cyclic, low-temperature regeneration of a monolithic $Pt/K/Al_2O_3$ NOx storage-reduction catalyst," Applied Catalysis A 293, 24-40; doi:10.1016/j.apcata.2005.06.025.

2. Jae-Soon Choi, William P. Partridge, William S. Epling, Neal W. Currier, and Thomas M. Yonushonis (2006). "Intra-channel evolution of carbon monoxide and its implication for the regeneration of monolithic $Pt/K/Al_2O_3$ NOx storage-reduction catalyst," Catalysis Today 114, 102-111; doi:10.1016/j.cattod.2006.02.011.

3. William P. Partridge, "Spatially Resolved Capillary-Inlet Mass Spectrometry: Instrument Details and Applications," Centre for the Theory and Application of Catalysis (CenTACat), Queen's University Belfast, Belfast, Ireland, June 7, 2006.

4. Bill Partridge, Jae-Soon Choi, William S. Epling, Neal W. Currier, Tom Yonushonis, "Intra-Reactor Measurements of Transient Species Distributions," The Instrumentation, Systems and Automation Society EXPO 2006, Houston, Texas, October 17, 2006.

5. Jae-Soon Choi, Vitaly Prikhodko, Kalyan Chakravarthy, Stuart Daw, "Assessing Monolith Length Effect on LNT Performance," 9th CLEERS Workshop, University of Michigan, Dearborn, May 4, 2006.

Special Recognitions & Awards/Patents Issued

1. Invited seminar at Queen's University Belfast, Ireland, Centre for the Theory and Application of Catalyst (CenTACat) on in-operando intra-reactor SpaciMS species measurements; see item 3 in FY 2006 Publications/Presentations.

II.B.9 Off-Highway Engine Emission Control with High System Efficiency

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John Fairbanks

Objectives

- Demonstrate Tier 3 emission levels with fuel consumption at 195 g/kWh or less by optimizing injection control with urea-SCR.
- Achieve particulate matter emission levels less than 0.02 g/kWh.
- Optimize NOx emissions using an advanced urea-SCR system.

Accomplishments

- Achieved interim Tier 4 NOx emissions and final Tier 4 particulate matter (PM) emissions for an off-highway diesel engine using a combination of advanced injection control coupled with urea selective catalytic reduction. This represents a >90% reduction in NOx and PM emissions over the baseline setting.
- Discovered that the total PM emissions are reduced by 50% by the urea-SCR catalyst. This effect was maintained during high rates of urea application (up to stoichiometric level flow). Evaluated the influence of fuel sulfur concentration on the performance of a urea-SCR system and PM emissions.
- Evaluated the influence fuel sulfur level, injector orifice design and catalyst systems.

Future Directions

- Conduct an investigation of particulate formation and chemistry as a function of rail pressure and urea-SCR dosing.
- Optimize the efficiency of a 2007 Deere diesel engine equipped with open control, variable geometry turbocharger (VGT), and exhaust gas recirculation (EGR) to enable excursions into advanced combustion regimes.
- Assess waste heat recovery potential using a combination of experimental evaluation and advanced modeling.
- Install and evaluate a prototype reformer for a lean-NOx (LNT) study on the 2007 Deere engine.

Introduction

Tier 3 federal standards for new off-highway diesel engines require that NOx and PM levels be regulated to 4 g/kWh and 0.2 g/kWh, respectively, for engines between 130 and 560 kW. The phase-in period for Tier 3 compliance is set to begin in 2006 and to be completed by 2008. Urea-SCR has been shown to effectively reduce NOx emissions for on-highway applications, but needs to be thoroughly evaluated for off-highway engines since both engine design and operating conditions are different. The utilization of advanced injection systems and controls are to be evaluated for improvements in both PM emissions and fuel efficiency. This project seeks to develop and evaluate emission control methodologies with the goal of identifying pathways to meet interim Tier 4 and retrofit solutions.

Approach

During FY 2006, this Cooperative Research and Development Agreement with Deere & Company was renewed with a focus on maintaining or improving fuel economy while meeting Tier 4 emissions levels for NOx and PM. The initial approach was to assess the efficacy of utilizing high fuel rail pressures to lower PM emissions. Because NOx emissions increase with high rail pressure, an advanced urea-SCR system was evaluated to determine its effectiveness to lower NOx emissions to Tier 4 levels. The test protocol followed the ISO 8178 C1 test cycle for off-highway engines. Data were collected for a range of urea delivery rates, up to and exceeding the stoichiometric value. The particulate matter was evaluated as a function of rail pressure. The PM was also evaluated during the urea-SCR process to determine chemistry changes that might result during the urea-SCR process.

Results

The influences of rail pressure and urea-SCR on the resulting NOx and PM emissions are shown in Figure 1. Increasing the rail pressure to values approaching

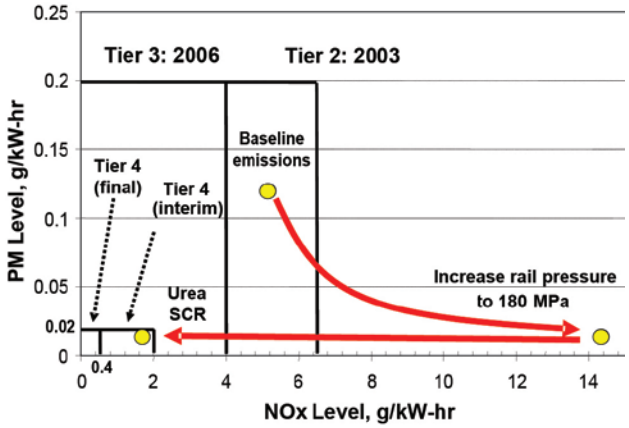


FIGURE 1. PM versus NOx Emissions for an Off-Highway Diesel Operated at High Fuel Rail Pressures and Utilizing Urea-SCR

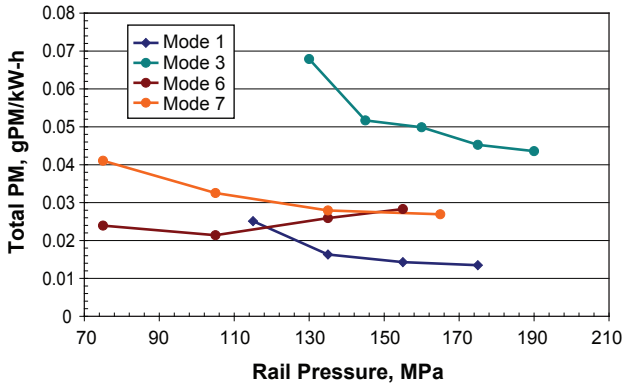


FIGURE 2. Total PM as a Function of Rail Pressure and Engine Operation

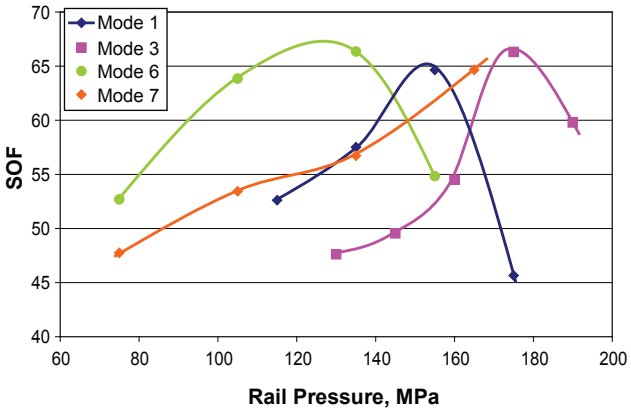


FIGURE 3. SOF of the Collected PM as a Function of Rail Pressure and Engine Operation

180 MPa decreased the total PM to less than 0.02 g/kWh; however, the NOx emissions were increased from a starting value of 5 g/kWh to almost 15 g/kWh. Under high rail pressure, the application of urea-SCR was effective at lowering the NOx emissions to 1.75 g/kWh, which meets the interim Tier 4 limits. The results show that the high rail pressure/urea-SCR approach was successful at meeting the Tier 4 PM and interim Tier 4 NOx emissions for off-highway diesels.

Further analysis of the PM structure and chemistry were performed as a function of rail pressure for four of the ISO 8178 test points shown in Table 1. The total PM and SOF results are shown as a function of rail pressure in Figures 2 and 3, respectively. Although the total PM mass was observed to decrease for Modes 1, 3, and 7 with increasing rail pressure (as shown in Figure 2), the effect appears to be marginal. For Mode 6 the mass initially decreased slightly when raising the pressure to 100 MPa. At high pressures however, the Mode 6 PM mass was observed to gradually increase with higher rail pressures. Analysis of the collected PM indicated that the soluble organic fraction (SOF) was very high for each condition as shown in Figure 3. For modes 1, 3, and 6 the SOF of the PM was observed to increase initially, reach a peak value, and then decrease with increasing rail pressure. The reason for this is not known, but is probably related to fuel droplet size and jet penetration distance.

TABLE 1. Description of Modal Test Points

ISO 8178 Mode	Engine Speed, rpm	Torque, ft-lbs
1	2,400	400
3	2,400	200
6	1,400	352
7	1.400	235

The total PM was also collected for Mode 6 while applying urea to lower the NOx emissions. The results shown in Figure 4 indicate that the total PM mass can be significantly reduced by the urea-SCR catalyst. This reduction is significant even during high rates of urea application, up to and including overspray conditions. The accompanying gas chromatography-mass spectrometry results indicate that high pressures generate a large SOF, which is eliminated (via oxidation) by the catalysts is relatively unaffected during urea-dosing.

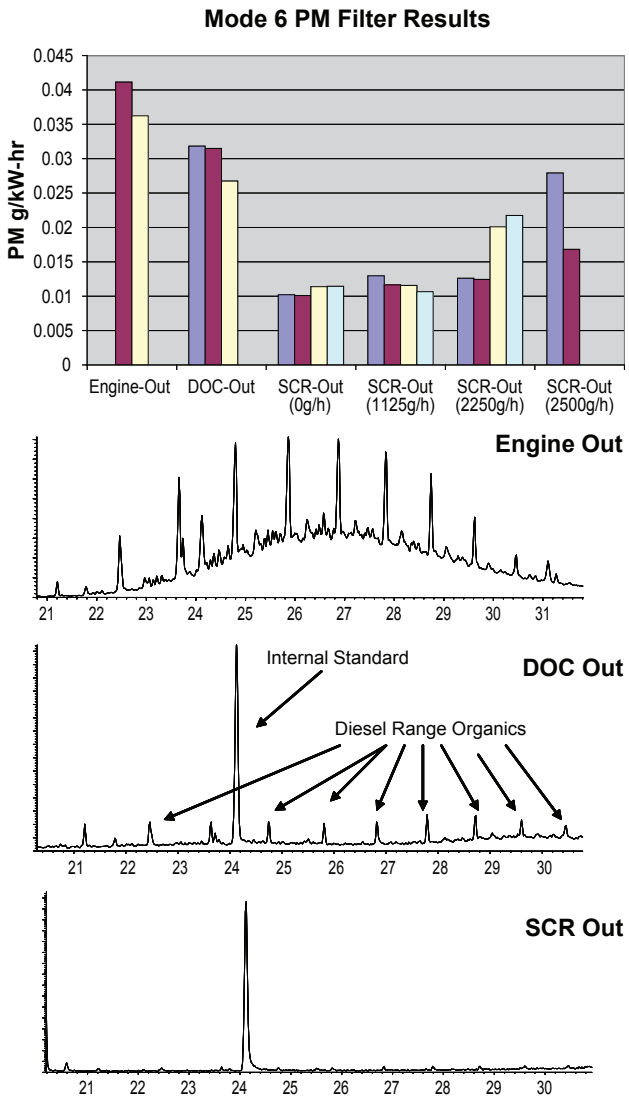


FIGURE 4. Brake Specific PM Emissions and Chemistry During the Application of Urea to the SCR Catalyst

Conclusions

- The combination of high rail pressure and urea-SCR was effective at lowering PM and NOx emissions from an off-highway diesel engine to within Tier 4 and interim Tier 4 levels, respectively. This approach is considered to have better fuel efficiency compared to reformer-based systems
- Total PM mass for Modes 1, 3, and 7 decreased gradually with increasing rail pressure; however, for Mode 6, the mass actually increased with high rail pressure.
- The SOF of the particulates was high. For modes 1, 3, and 6 the SOF increased initially, reached a peak value, and then decreased with increasing rail pressure.

II.B.10 Discovery of New NOx Reduction Catalysts for CIDI Engines Using Combinatorial Techniques

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Subcontractors:
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- Accelrys, Inc, San Diego, CA

Objectives

Develop new NOx selective catalytic reduction (SCR) catalysts that can operate in the lean exhaust of diesel or lean gasoline engines. These catalysts can:

- Utilize the onboard fuel as the reductant (i.e., hydrocarbon-SCR, HC-SCR).
- Have NOx conversion activities in excess of 80%.
- Span the operating range (e.g.; temperature and flow rate) for these lean engines.
- Have sufficient durability and resistance to poisoning to meet the 120k standard.

Accomplishments

- Tested over 5,600 materials for NOx reduction potential since the initiation of the project and testing of materials with simulated diesel fuel is the standard.
- Twenty full-size catalysts have been coated to use for engine studies.
- Conversions of 92% (Highway Cycle), 76% (US06 Cycle) and 60% (Federal Test Procedure, FTP) have been measured (V6 common rail diesel).
- Sulfur poisoning has been evaluated and regeneration strategies have been identified using both reactor studies and engine evaluations.
- Laboratory thermal aging studies have been completed.
- Phosphorus poisoning studies have been initiated.
- Discovery testing with a simulated gasoline fuel has been started.

Future Directions

- Use the discovery system to refine the downselected catalysts to make them production viable.
- Use the discovery system to evaluate materials for gasoline applications using simulated gasoline fuel.
- Dyno evaluate the downselected catalysts to identify control strategies that satisfy the emission control standards, resist or regenerate from poisoning and coking.
- Develop a production feasibility analysis for one of these catalyst systems.
- Produce the final report and conclude the project.

Introduction

This GM project was initiated on August 16, 2002. Its goal is to develop new NOx reduction catalysts for lean combustion systems such as both light- and heavy-duty diesels and for stratified charge gasoline engines. These new catalysts are needed to enable these engines to meet the Tier II NOx standards for the North American markets that are being phased in over the time period between 2007 and 2010.

Approach

Selective catalytic reduction (SCR) with reductants from the fuel (HC-SCR) is the technology that is the focus of development of the new catalytic materials. The approach is to use high throughput technology to develop the new materials (Engelhard, now a division of BASF), informatics to mine the data arising from the fast throughput experimentation (Accelrys and GM) and classic reactor evaluation to determine the suitability of the new materials for automotive applications (GM and BASF).

Results

To date at BASF, over 5,600 new materials have been evaluated on the discovery system since the initiation of the project. To date the results from this approach have identified at least two catalysts for

coatings that have been downselected for detailed analysis that would identify if these coatings might have the potential for engine applications. Issues considered in these analyses include effects of poisoning (sulfur and phosphorus poisoning), propensity to coke, thermal aging and engine control strategies that would allow a diesel powertrain to satisfy emission standards. These studies have included reactor studies with a simulated diesel fuel (67 vol% n-dodecane and 33 vol% m-xylene), coating and canning of the materials on full size monolith bricks and engine testing of these catalysts.

The catalyst/dyno setup is shown in Figure 1. This design includes a DOC to clean up the engine-out hydrocarbons and a dosing system for controlled addition of hydrocarbon to the SCR catalysts. The mixer is added to ensure full vaporization of the fuel before the HC-SCR catalyst.

This dyno test system (V6 common rail diesel) has been used to evaluate the effects of hydrocarbon dosing (carbon to nitrogen ratios, C/N), oxygen concentrations, space velocities and transient effects in the engine environment. Instantaneous NOx conversions measured (2005) over the US06 Cycle (Figure 2) shows conversions consistent with the high conversions observed from the laboratory reactor experiments. Subsequent engine studies using the same dyno setup with a larger catalyst volume have measured conversions of 92% (Highway Fuel Economy Test, HWFET), 76% (US06) and 60% (Federal Test Procedure, FTP).

Thermal aging of the same catalytic coating as was used in the engine test were performed (Figure 3). For air aging the sample is held at the specified temperature (650°C) for varying times in air with 10% water vapor added to gases. The air aging at 16 hours is the standard aging used for all the discovery samples. As can be seen from the figure there is little loss in activity for the sample. The redox aging cycle between rich and lean feeds is more representative of the aging that would occur for the stoichiometric three-way catalyst. This aging cycle typically causes exotherms within the catalyst. These exotherms can often exceed the inlet gas temperature by several hundred degrees. Consequently, redox aging can expose the catalyst to temperature variations that exceed the temperatures the catalyst "sees" with air aging. As can be seen in the figure the redox aging does cause a greater loss in activity than air aging; however, with a gas temperature

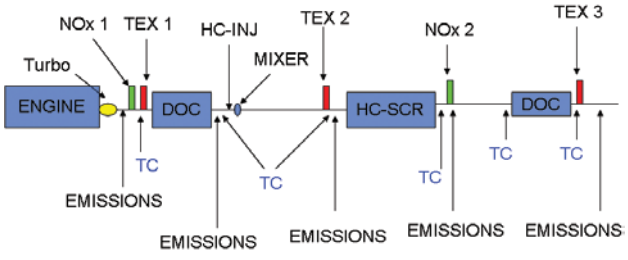


FIGURE 1. Schematic shows the test cell design for measurement of emission reduction technology using the full-size HC-SCR converters. TEX indicates species detectors for the emissions at various points within the aftertreatment system. HC-INJ indicates a system for controlled injection of hydrocarbons into the exhaust stream.

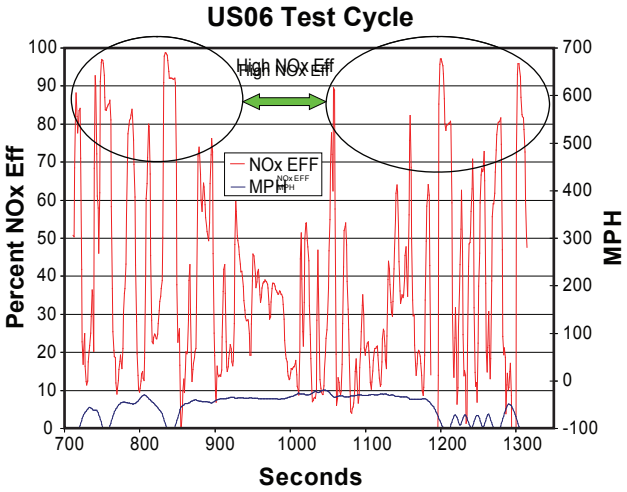


FIGURE 2. Graph of the instantaneous NOx conversion for this HC-SCR dyno measurement over a part of the US06 test cycle. For presentation convenience, the miles per hour in the test cell is multiplied by -100 to move it off the graph of the NOx conversion.

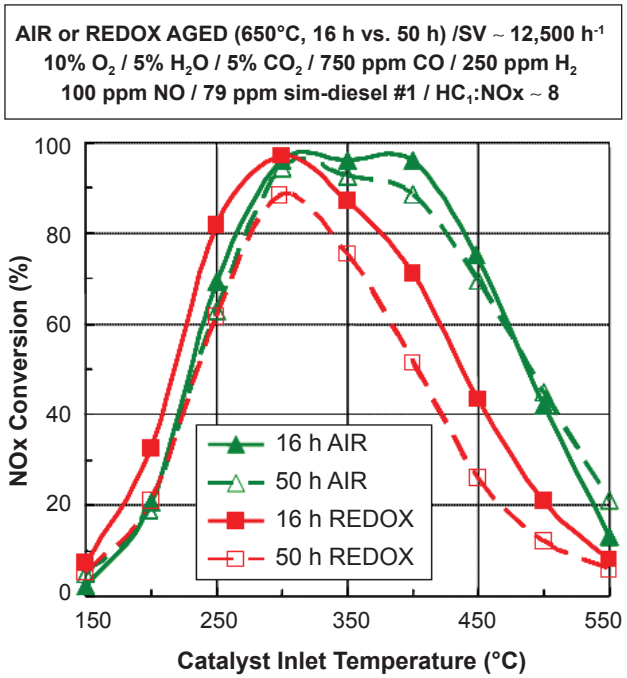


FIGURE 3. Comparison of the activity of monolith samples after aging. The air aging at 16 hours is the standard aging used for all the discovery samples. Redox aging cycles between rich and lean feeds.

of 650°C it does not cause much more damage. Other aging data does show that these catalysts are quite sensitive to temperature, and higher aging temperatures cause significantly more damage. However, 650°C is a common upper limit to the exhaust temperatures of today's modern diesels.

Sulfur in modern diesel fuels has been significantly reduced. We have evaluated the effects of sulfur poisoning on the downselected catalyst coating used in the engine tests. A range of regeneration conditions were examined. This particular catalyst sample was sulfated and desulfated multiple times over approximately three months. Optimum exhaust gas conditions were developed for desulfation. The activity of the catalyst was evaluated at the beginning of that phase of the project. These catalysts similar to all the catalysts in this project were aged at 650°C in steam for 16 hours. At the end of that extensive study the activity of the desulfated catalyst was measured and compared with the initial activity (see Figure 4). There was some small loss of overall activity; however these results do show that this catalyst for coating can be regenerated from sulfation and is relatively stable to multiple regenerations.

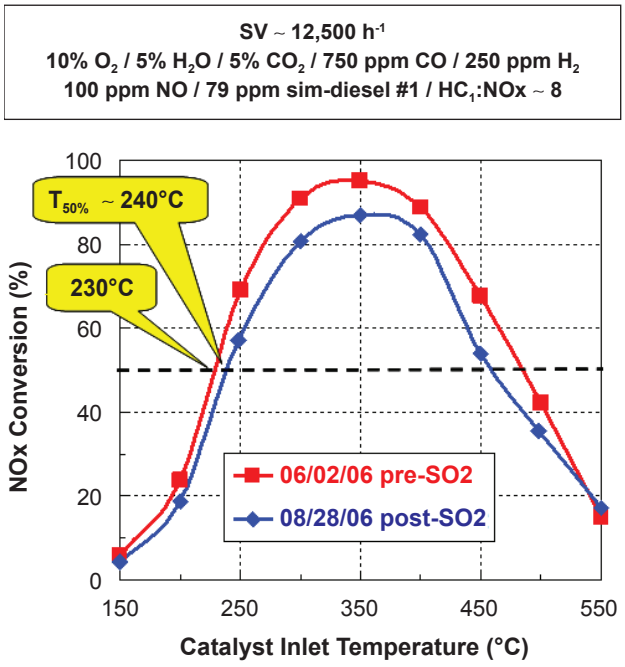


FIGURE 4. Comparison of the activity of a monolith sample after sulfur poisoning and regeneration. This sample was used to test a range of regeneration strategies. There is very little loss of activity from these tests.

Conclusions

The encouraging conversion results on the dyno test stand to a large degree have moved this project from new materials discovery for diesel NOx reduction into a product development phase. Much of the discovery work during the latter portions of FY 2006 was used to develop additives to address issues that could arise in applying this technology. Some of the discovery work has been applied to discovering active catalytic materials for lean gasoline NOx reduction.

Evaluation of the effects of sulfur poisoning, coking, phosphorous poisoning and thermal aging at this point do not seem to be a durability barrier for the use of these materials in automotive applications.

This project is planned to complete in calendar 2007 so that refinements in the active catalytic materials will assist in developing the feasibility analysis planned for the end of the project.

Special Recognitions & Awards/Patents Issued

1. Five records of invention were filed based on work from this project during this year.

II.B.11 Efficient Emissions Control for Multi-Mode Lean DI Engines

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DOE Technology Development Manager:
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Objectives

- Examine benefits of HC emissions from low-temperature combustion to support hydrocarbon selective catalytic reduction (HC-SCR).
- Investigate unusual engine control approaches to enhance catalyst performance.
- Assess potential for combining aftertreatment technologies (such as SCR with lean-NOx trap, LNT) to provide aftertreatment solution for multiple operational modes (e.g., low-temperature combustion [LTC] vs. conventional diesel combustion).

Accomplishments

- Modified LNT regeneration strategies to generate engine-out hydrogen and other reformate products under net-lean conditions.
  - Individual cylinder control provides up to 0.8% hydrogen with over 1% CO, and 3,000 ppm cracked HCs with 9% oxygen in exhaust.
- Evaluated commercial HC-SCR catalysts on engine.

Future Directions

Evaluate commercial HC-SCR catalysts (Pt, Cu, and Ag), and Pacific Northwest National Laboratory (PNNL) HC-SCR catalyst

- Bench reactor experiments
  - Promotional effect of hydrogen
  - Temperature sweep
  - Investigate CO or HC masking
- Engine-based study
  - Conventional diesel combustion
  - High Efficiency Clean Combustion (HECC) modes
  - Late-cycle post injection or in-pipe injection
  - Individual cylinder control

Introduction

New combustion regimes are being investigated as a means to improve the efficiency of diesel engines. 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. Additionally, new combustion regimes are sought that will result in improvements in brake specific fuel consumption (BSFC). While these regimes will be implemented whenever possible in future production engines, it is expected that diesels will still run in the more conventional modes at certain operating conditions. The wide range of operating conditions provides a challenging environment for the aftertreatment system. Multi-mode operation of the engine will almost certainly require a multi-mode aftertreatment system. This project aims to leverage existing combustion and aftertreatment R&D at ORNL, collaborating with industry partners to develop and characterize advanced catalysts to fill this need. While lean-NOx trap and urea-SCR technology show great promise for reducing NOx under conventional diesel combustion conditions, the lighter load, low NOx regimes may require different catalyst technology. Treatment of the HC and CO emissions during low temperature combustion is of concern even when engine-out NOx is low enough to not require further treatment. Because of the relatively high HC to NOx ratio in LTC modes, HC-SCR may be an attractive option to augment the LNT or urea-SCR 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 modest activity. Experiments to date have shown that LTC can result in an order of magnitude reduction in NOx, with PM emissions and BSFC comparable to levels at "factory" calibrations. Under these combustion modes, HC emissions have been speciated, and a wide range of reactive compounds have been found, including light alkenes, oxygenates, and other compounds known to be effective HC-SCR reductants. As these HC emissions must be treated, it is logical to use them to reduce NOx rather than simply oxidizing them. When operating in traditional combustion regimes, the HC requirements of the aftertreatment system might be fulfilled by injecting additional fuel by a number of means, including in-cylinder injection. The

ongoing LNT studies at ORNL (described separately within this annual progress report) have developed strategies for periodic rich operation (necessary for LNT regeneration). Variations of these strategies were developed (under this "Multimode Catalysis" project) to investigate reformate production under net lean conditions. Results of these experiments will be discussed in the Results section. Commercial HC-SCR catalysts have been obtained from a Manufacturer of Emission Controls Association (MECA) partner and were evaluated under a variety of conditions in FY 2006 using a slipstream for screening 2-inch diameter catalyst cores.

Strategies developed for LNT regeneration have included a late-cycle post injection (80 degrees after top dead center, or Post80), and a delayed extended main (DEM) strategy in which the main injection pulse is extended into the rich regime and retarded to offset any torque increase associated with overfueling. These strategies have been well characterized under the auspices of the related LNT project, and the results have been published [1]. The regeneration strategies study showed that while the reductant levels from the DEM strategy decreased with increasing air:fuel ratio (AFR), only the HC level changed significantly with leaner AFR for the Post80 strategy. That is, the carbon monoxide (CO) and hydrogen (H_2) peaks were relatively constant across the rich AFR sweep for Post80.

Another reported application of reformate is to enhance HC-SCR catalyst function [2-4]. Researchers have shown reformate, or more specifically H_2, to significantly improve NO conversion over Ag/Al_2O_3 catalysts across a wide temperature range. Additionally, H_2 has been shown to offset performance losses of HC-SCR catalysts associated with increased space velocity and sulfur presence. The presence of H_2 in lean exhaust can also serve to accelerate catalyst light-off [5-7].

These LNT strategies were exercised at several lean AFRs to examine whether the H_2 production trend could be extended into the lean regime. Hydrogen was produced in the lean regime close to stoichiometry, but dropped off quickly as AFR was increased. Individual cylinder control was then explored to generate higher levels of reformate under net lean conditions. The strategy commands one cylinder rich, while the other three cylinders remain lean. To preclude engine imbalance and perhaps premature engine wear, each cylinder is programmed to run rich for only 400 milliseconds (ms), although this parameter is adjustable. For example, cylinder 1 runs rich for 400 ms while cylinders 2-4 run lean. When cylinder 1 transitions back to lean operation, cylinder 3 (the next cylinder in firing order) transitions into the rich regime. This control strategy is referred to as ICDEM (Individual Cylinder Delayed Extended Main). Results of these experiments were reported last year [8]. A preliminary catalyst experiment was also conducted using a slipstream of the richest ICDEM strategy through a 2-inch core of a Pt/Al_2O_3 HC-SCR catalyst, highlighting the potential benefit of such a strategy to enhance catalyst light-off [9].

Experiments this year again used the 2-inch core engine exhaust slipstream for evaluating catalysts, as shown in Figure 1. The combination of sample pumps induced a flow of 43 liters per minute (lpm), for a space velocity of 30,000 hr^{-1}. Thermocouples were deployed at the inlet, core, and outlet of the catalyst sample. Both the Pt/Al_2O_3 sample described previously [9], and a Ag/Al_2O_3 sample from the same MECA supplier were evaluated in this setup.

Results

Based on the published results that show a remarkable improvement in NOx reduction at low temperatures for Ag/Al_2O_3 with the addition of H_2 [2-4], the objective was to investigate the benefits of reformate on HC-SCR catalyst performance. The initial experiments were conducted at an engine condition that produced catalyst inlet temperatures in the 200-240°C range. Individual cylinder control was used to run both DEM and Post80 (P80) strategies on one cylinder at a time, denoted ICDEM and ICP80, respectively. The ICDEM produced the most hydrogen and allowed a study of the promotional effect of H_2 on the NOx reduction. The ICP80 produced mostly HCs, and was considered more of a conventional HC-SCR strategy. A third set of experiments used ICP80 at a higher engine load, to increase exhaust temperature. In order to maintain a similar level of NOx, some EGR (exhaust gas recirculation) was used at this higher load. These experiments are denoted ICP80 w/EGR in the figures that follow. Figures 2-4 show the engine-out concentration of the reductants produced by each strategy as a function of the fuel injection pulsewidth of the excess fuel. This parameter is the duration of the post injection event (at 80 degrees after top dead center), or the additional pulsewidth added to the normal main

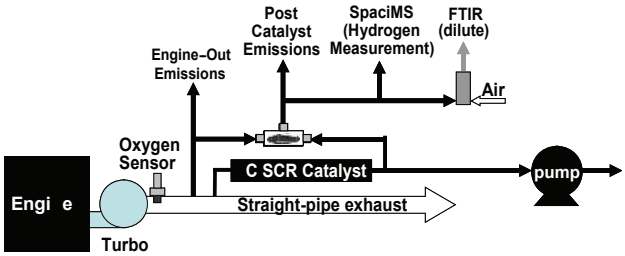


FIGURE 1. Experimental Schematic Showing Slipstream Approach used for Evaluating Catalyst Cores

injection for ICDEM. Note in Figure 2 that the ICDEM produces the most engine-out hydrogen, while Figure 4 shows that ICP80 produces the most hydrocarbons. The NOx level for all experiments was on the order of 500 ppm (parts per million). The ICDEM and ICP80 experiments had 10-12% oxygen in the exhaust. The higher load and use of EGR for the ICP80 w/EGR experiments resulted in about 6% oxygen in the exhaust.

The HC:NOx ratio is shown in Figure 5 as a function of pulsewidth for each strategy for reference purposes. The remaining figures in this report will use HC:NOx ratio for the x-axis. The best NOx conversion noted was approaching 30% for the Pt/Al_2O_3 using the ICP80 strategy at a HC:NOx ratio of 9, as shown in Figure 6. The figure also shows that this catalyst effectively treats the HC and CO emissions. Figure 7 shows the same information for the Pt/Al_2O_3 catalyst with the ICDEM strategy. There does not appear to be any promotional effect of the hydrogen on this catalyst. While the H_2 and CO are consumed, the HC conversion is below 90% and the NOx conversion is below 20%. Reasons for this drop in performance under this condition are presently unclear. In particular, at similar HC:NOx ratios, the NOx conversion is only about half for ICDEM versus ICP80 for this catalyst.

Figure 8 shows the performance of the Ag/Al_2O_3 catalyst with the ICDEM strategy. As noted earlier,

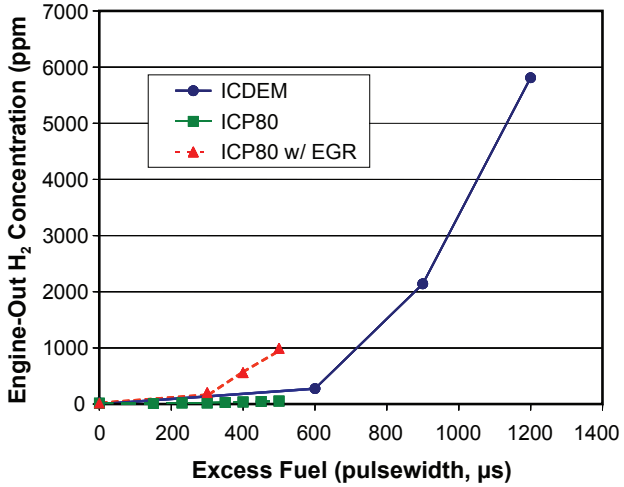


FIGURE 2. Engine-Out Hydrogen Concentration as a Function of Excess Fuel Pulsewidth

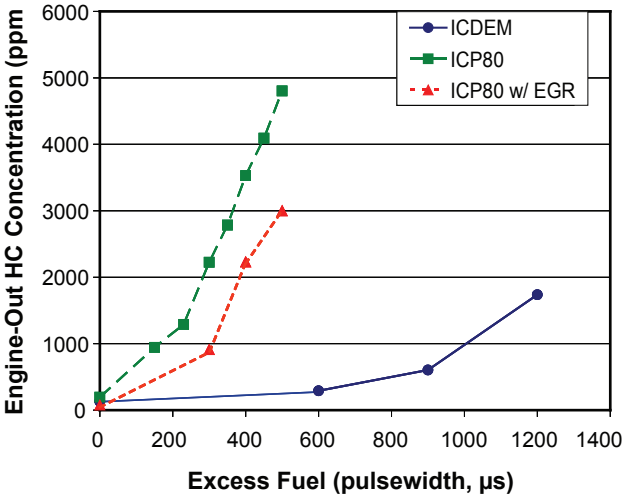


FIGURE 4. Engine-Out HC Concentration as a Function of Excess Fuel Pulsewidth

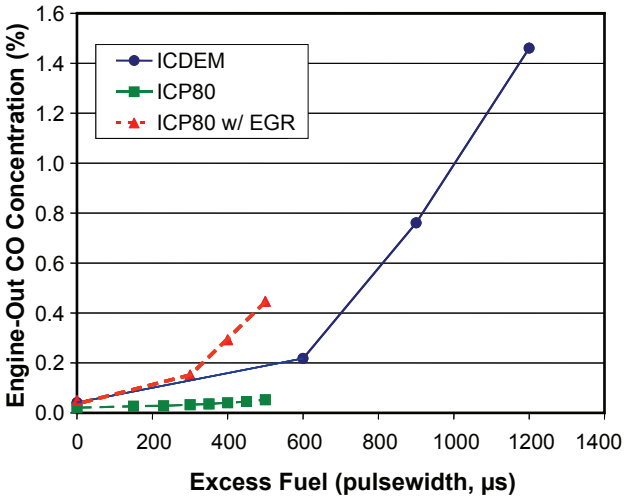


FIGURE 3. Engine-Out CO Concentration as a Function of Excess Fuel Pulsewidth

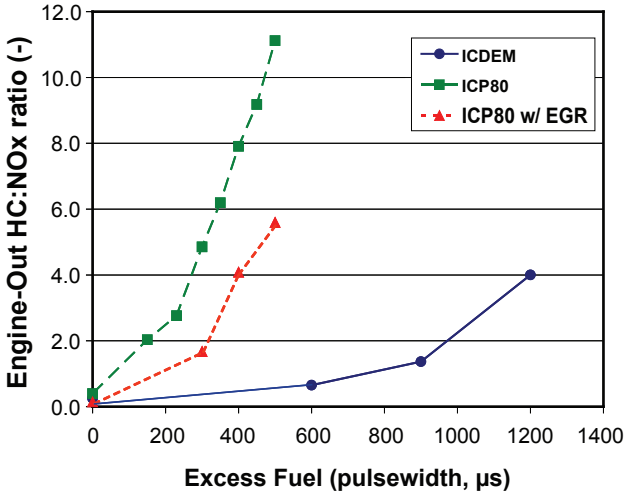


FIGURE 5. Engine-Out HC:NOx Ratio as a Function of Excess Fuel Pulsewidth

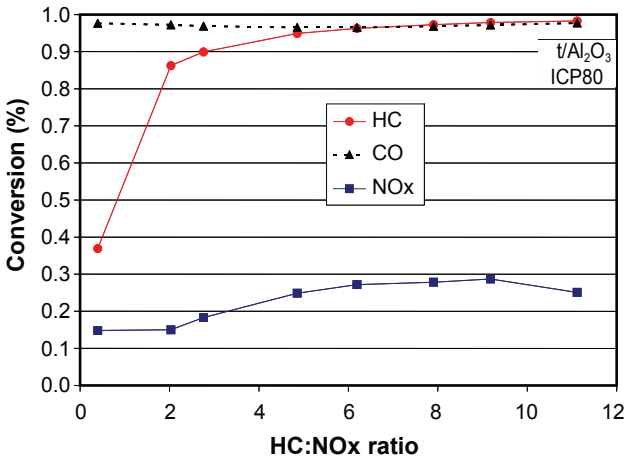


FIGURE 6. Conversion Efficiency Versus HC:NOx Ratio for Pt/Al_2O_3 Catalyst Using ICP80 Strategy

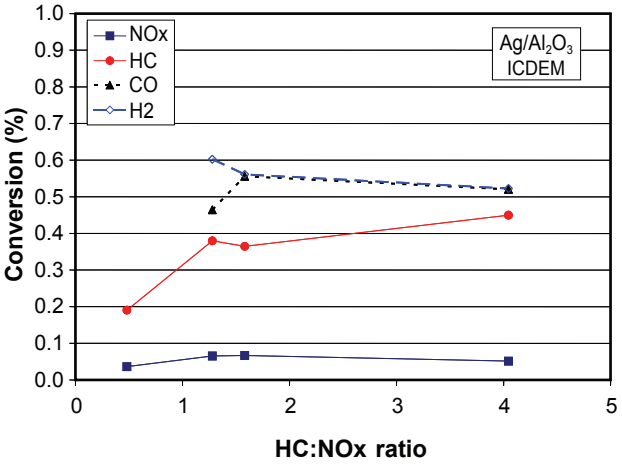


FIGURE 8. Conversion Efficiency Versus HC:NOx Ratio for Ag/Al_2O_3 Catalyst Using ICDEM Strategy

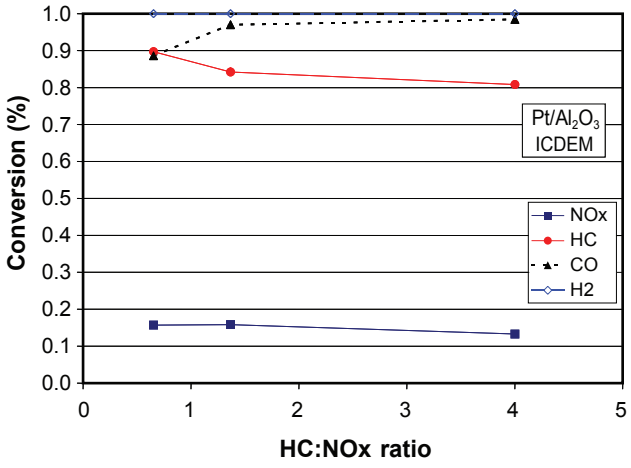


FIGURE 7. Conversion Efficiency Versus HC:NOx Ratio for Pt/Al_2O_3 Catalyst Using ICDEM Strategy

bench-scale experiments have shown Ag/Al_2O_3 catalysts to display remarkable improvements in NOx conversion when small amounts of hydrogen are added to the feed [4], so the results in Figure 8 were not anticipated. As the figure shows, the exhaust feed from the ICDEM strategy netted less than 10% NOx conversion and less than 50% HC conversion. Hydrogen and CO conversion were also very poor.

While there does not appear to be any promotional effect of the hydrogen on this Ag/Al_2O_3 catalyst for the ICDEM case, results for the ICP80 were even worse, with comparable NOx conversion and almost undetectable changes in CO or HC. In order to raise the catalyst inlet temperature, experiments were conducted with ICP80 at a higher load, with EGR to trim the engine-out NOx to a comparable level. As shown in Figures 3 and 4, the higher load and use of EGR results in comparable HC emissions and higher CO emissions. The higher temperature did promote conversion of 10-20% of the CO and HC, but NOx conversion was again negligible, in the 5-8% range. Reasons for the poor performance of this catalyst are unclear, but there are several hypotheses:

- Hydrocarbon Masking. The referenced Ag/Al_2O_3 experiments were conducted on flow reactor benches with bottled gas feed [2-4]. Perhaps the nature of real engine exhaust hydrocarbon species and particulate matter are "masking" active catalyst sites.
- CO Inhibition. Engine-out CO concentration is about three times that of the engine-out hydrogen. The CO may be chemisorbed onto the active metal sites; the chemisorbed CO may prevent H_2 and other gas species from interacting with the active sites and thereby inhibiting the activity of the catalyst.
- Catalyst Loading/Formulation. Details regarding the loading or formulation of the MECA-supplied Ag/Al_2O_3 catalyst are not known. Bench reactor experiments with this catalyst will help elucidate whether "real" exhaust was inhibiting the promotional effect of the hydrogen documented in the literature [2-4].

Follow-on experiments will be complemented by flow reactor bench evaluations. Comparing results in the "ideal" gas bench environment to those from further engine experiments will elucidate the possible functional mechanisms. Furthermore, additional catalyst formulations will be requested from MECA suppliers.

Conclusions

Strategies previously developed for in-cylinder regeneration of LNTs have been modified to allow production of H_2 and other reformate products (e.g., CO, light HCs) under net-lean exhaust conditions by overfueling individual cylinders. These strategies were used to provide reductant to HC-SCR catalysts in slipstream experiments on core samples of two MECA-supplied catalysts. Notable conclusions are the following:

- A commercial Pt/Al_2O_3 HC-SCR catalyst was shown to effectively remove HC, CO, and hydrogen from low-temperature (<240°C) diesel exhaust gas. Maximum observed NOx conversion approached 30% with a HC:NOx ratio in the 7-10 range.
- In-cylinder production of hydrogen with the ICDEM strategy does not appear to enhance low temperature performance of the Pt/Al_2O_3 catalyst under quasi-steady conditions.
- An Ag/Al_2O_3 HC-SCR catalyst was found to provide poor NOx, HC, CO, and H_2 conversion for either the ICDEM or ICP80. Follow-on experiments will attempt to discern the contradictions between bench and engine experiments.

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8. FY 2005 Progress Report for Advanced Combustion Engine Technologies, Energy Efficiency and Renewable Energy, Office of FreedomCAR and Vehicle Technologies, "Energy Efficient Emission Control for Multi-Mode Lean DI Engines," pp. 201-205, January 2006.

9. Brian West, Shean Huff, James Parks, Matt Swartz, and Ron Graves, "In-Cylinder Production of Hydrogen During Net-Lean Diesel Operation," Society of Automotive Engineers Paper No. 2006-01-0212, April 2006.

FY 2006 Publications/Presentations

1. Brian West, Shean Huff, James Parks, Matt Swartz, and Ron Graves, "In-Cylinder Production of Hydrogen During Net-Lean Diesel Operation," Society of Automotive Engineers Paper No. 2006-01-0212, April 2006. (Oral presentation at SAE Congress)

2. Brian West, Shean Huff, James Parks, Matt Swartz, and Ron Graves, "In-Cylinder Production of Hydrogen During Net-Lean Diesel Operation," Invited speaker to Diesel Crosscut Team Meeting, Detroit Michigan, November 2005.

Special Recognitions & Awards/Patents Issued

1. Provisional Patent filed, "Advanced Engine Management for Control of Exhaust Species," Ron Graves, Brian West, Shean Huff, and James Parks, 3/30/2006.

II.B.12 NOx Control for High Power Density Hydrogen Engine

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Objectives

- Demonstrate applicability of compression ignition direct injection (CIDI) aftertreatment systems for H_2 internal combustion engine (ICE) applications
  - Lean NOx traps (LNTs), urea (NH_3) selective catalytic reduction (SCR), H_2 SCR
- Determine what key catalytic chemistry is affected by carbon-free exhaust
  - Impacts modeling parameters; both H_2 ICE models and CIDI models
  - Reactor sizing, precious metal cost, and engine operation

Approach

- Initial experimentation on powder catalysts
- Evaluate promising candidates on bench-scale reactor with washcoated cores
  - LNT catalyst: Umicore High Temperature European LNT for SIDI
    - CLEERS LNT focus group reference material
  - Urea (NH_3) SCR catalyst: Iron (Fe) and zeolite-based
    - CLEERS SCR focus group reference material
- Generate data specific for modeling requirements
  - PSAT submodels
  - CLEERS global kinetics model

Accomplishments

- Completed powder catalyst evaluation
  - LNT, urea (NH_3) SCR, and H_2 SCR
  - Down-selected LNT and urea (NH_3) SCR for bench-core reactor
- Results presented at Ford H_2 ICE meeting in March 2006
- Evaluated LNT catalyst performance on ORNL bench-core reactor
  - Two reductant concentrations; 300-500°C evaluation
  - Direct comparison to conventional exhaust (with CO and CO_2)
  - Excellent overall performance–70-100% NOx conversion
  - N_2 selectivity and performance better with H_2 than CIDI exhaust
    - Up to 90% less NH_3 (undesirable by-product) formation
    - 11-33% improvement in NOx conversion

Future Directions

- With remaining funds from FY 2006, we will evaluate SCR catalysts with waschcoated cores
  - Investigate NO:NO_2 ratio
    - Ratio impacts global reactions
    - 1:1 is ideal ratio for fastest reaction path
  - Determine byproduct formation dependence
    - Vary NH_3:NOx ratio
  - Vary temperature from 300-600°C
- With any remaining funds, or if project is funded in FY 2007, the following expanded evaluation will be performed:
  - Evaluate space velocity requirements for H_2 ICE LNT and NH_3-SCR
  - Characterize effect of periodic high NOx dose
    - NOx concentration can reach 0.8-1.0% at $\Phi = 0.8$
    - NH_3-SCR and LNT

Introduction

An increasing national focus on moving towards a hydrogen economy calls for hydrogen-enabled internal combustion engines as a near-term transition technology. While there is potential for these engines to reduce carbon emissions from vehicles, NOx emissions are still problematic [1], and control of NOx emissions with aftertreatment will most likely be required. Oak Ridge National Laboratory's support to the systems analysis program has for several years focused on providing

data for important engine and emissions control related systems for use in larger systems-analysis models that estimate the fuel economy and emissions potential of multiple vehicle configurations. This area is a unique strength of ORNL and is the area in which ORNL can contribute the most to the FreedomCAR and Vehicle Technologies Program. ORNL's involvement with the fuels, engines, and emissions control research areas put ORNL in a unique position to bring input from these areas to the Systems Analysis Program.

Approach

Since little work has been performed in the area of lean NOx reduction for hydrogen ICEs, it is not clear which NOx reduction strategy is best suited to meet the emissions requirements. It is expected that one of the systems being studied for CIDI engines, i.e. lean NOx traps, urea SCR, or H_2 SCR catalysts will be required for hydrogen ICEs. The ORNL team will investigate these strategies with bench flow reactors under typical operating conditions to determine which is best-suited to hydrogen-fueled vehicles. The catalyst or trap materials and cores for the experimental work will be sought from major suppliers through informal collaborations. Additionally, ORNL can formulate catalyst samples (model catalysts) for bench-scale work as needed.

Urea SCR depends on the decomposition of urea into ammonia (NH_3) to reduce NOx in oxidative conditions. Current models of urea SCR catalysts in CIDI exhaust conditions will need to be evaluated and modified for lean-burn hydrogen engines. H_2 SCR and NOx adsorber catalysts can make use of on-board fuel (H_2) to reduce NOx. Successful expansion of current CIDI models of these catalysts for hydrogen applications will require in-depth investigation of the interaction of hydrogen with the catalysts under lean-burn hydrogen engine exhaust conditions, specifically with respect to how the chemistry varies from CIDI. NOx adsorber catalysts are expected to adsorb NOx in a similar fashion to CIDI applications, but NOx reduction ("regeneration") with pure hydrogen fuel will be a dynamic chemical and thermal process that will require thorough evaluation and study for efficient and safe catalyst operation.

Results

The Umicore high-temperature LNT catalyst was evaluated for NOx conversion, N_2 selectivity, and reductant reactivity at a space velocity of 30k h^{-1}. Two reductant concentrations and two exhaust conditions were used while studying the LNT chemistry from 300 to 500°C. The high reductant concentration introduced during the rich phase is 3.1 times the required reductant to reduce the NOx fed to the reactor during the lean phase; the low reductant is 1.1 times the required amount. The exact concentrations for all gases are displayed in Table 1. NO and NO_2 are measured using a chemiluminescence detector (CLD), CO, CO_2, NH_3, N_2O, and H_2O are measured using a Fourier transform infrared (FTIR) instrument with a gas cell attachment, and intra-catalyst measurements of H_2 are made with a spatially resolved capillary inlet mass spectrometer (Spaci-MS).

Excellent NOx conversion was observed for the high reductant concentration at all temperatures and for both the conventional CIDI and the H_2 ICE exhaust conditions; the results are summarized in Figure 1a. The most interesting result from this comparison is the 70% NOx conversion observed with conventional exhaust at 500°C. Compared to the 100% reduction observed with H_2 ICE conditions this is a considerable decrease in activity. Figure 2 shows that the NOx conversion is limited by the regeneration chemistry, as there is a very large amount of NOx released that is not converted. This result suggests that CO is considerably less effective than H_2 at reducing NOx, and thus H_2 ICE has a better regeneration environment for LNT aftertreatment. N_2 selectivity, i.e. the percentage of stored NOx that is converted to N_2, is also a key concern with LNTs. N_2O and NH_3 are by-products that have been observed in conventional CIDI exhaust, and in general they are undesirable. Figure 3a shows the percentage of stored NOx that is converted to both NH_3 and N_2O as measured by FTIR; the remainder is presumed to form N_2. H_2 ICEs have significantly less byproduct formation than CIDI exhaust at 300 and 500°C, especially with respect to NH_3. This suggests that precise reductant

TABLE 1. Gas concentrations used in for the LNT evaluation in the bench-core reactor.

	NO	O_2	CO	H_2	CO_2	H_2O
Conventional Diesel Exhaust						
High Reductant (2.8% total)						
Lean (60s)	300 **ppm**	10%	-	-	5%	5%
Rich (5s)	-	-	1.75%	1.05%	5%	5%
Low Reductant (1.0 % total)						
Lean (60s)	**300** ppm	10%	-	-	5%	5%
Rich (5s)	-	-	0.675%	0.325%	5%	5%
H_2 ICE Exhaust						
High Reductant (2.8% total)						
Lean (60s)	**300** ppm	10%	-	-	-	5%
Rich (5s)	-	-	-	2.8%	-	5%
Low Reductant (1.0% total)						
Lean (60s)	300 ppm	10%	-	-	-	5%
Rich (5s)	-	-	-	1.0%	-	5%

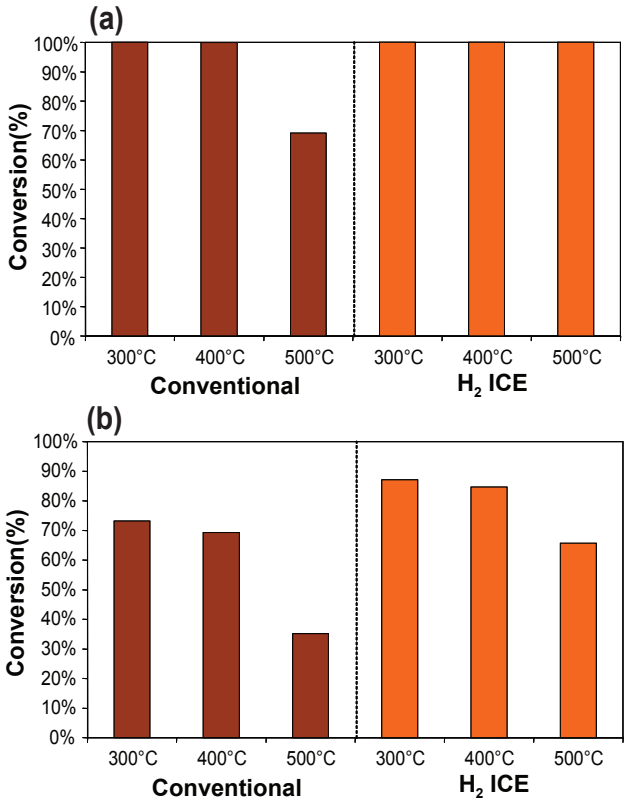


FIGURE 1. Comparison of NOx conversion for H_2 ICE and conventional CIDI exhaust using either (a) 2.8% of total reductant or (b) 1.0% of total reductant.

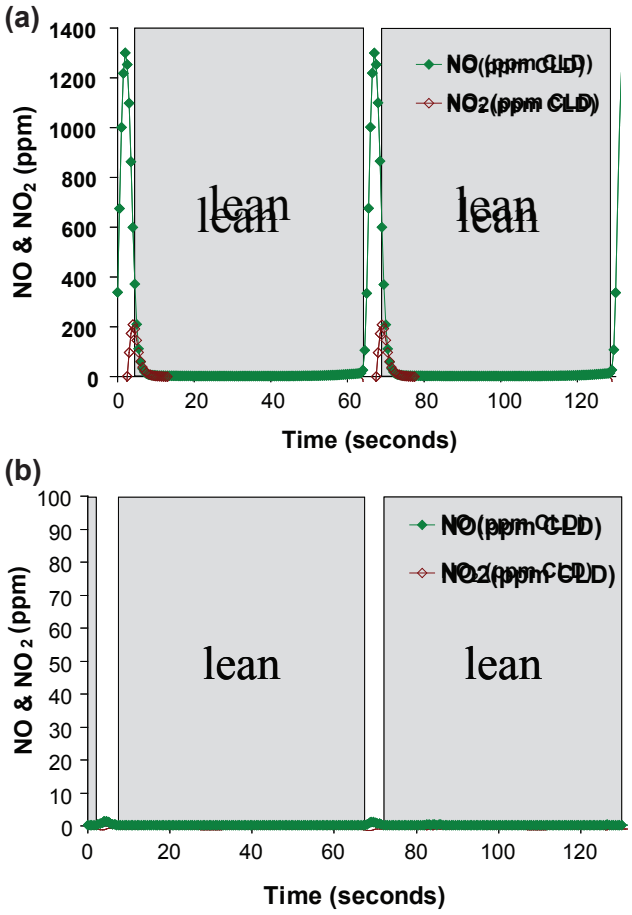


FIGURE 2. NO and NO_2 profiles at 500°C during 60 s lean and 5 s rich cycles for (a) conventional CIDI exhaust and (b) H_2 ICE exhaust.

control relative to NOx production is not as crucial for H_2 ICEs as it is for CIDI. The high reductant, intra-catalyst H_2 profiles for both conditions at 500°C are displayed in Figure 4. The key observation in these measurements is that the front quarter of the LNT is in contact with significantly more H_2 in the H_2 ICE case compared to the CIDI case. The CIDI exhaust undergoes the following water-gas-shift reaction (WGS) to produce H_2:

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (1)$$

However, this reaction is too slow to produce H_2 that is kinetically relevant to NOx reduction [2]. The result in this study further supports evidence that the CO does not have a significant contributing role in most CIDI applications, and H_2 is the most important reductant for efficient regeneration of LNTs.

When evaluating the LNT with low reductant concentrations the NOx conversion was 11-33% higher at all temperatures with H_2 ICE exhaust compared to conventional CIDI exhaust as displayed in Figure 1b. At this reductant concentration it is evident that H_2 ICE conditions increase the effective storage capacity of the LNT either from better reduction and removal of the stored NOx, or due to a competition for sites with CO_2, possibly both. Figures 5a and 5b show the NOx level at 300°C during the lean-phase is considerably higher in the CIDI case compared to H_2 ICE, which illustrates the increase in effective storage. Figures 5c and 5d show the significantly higher NOx pulse during the rich-phase which continues to illustrate the better regeneration efficiency observed with H_2ICE exhaust. Figure 3b shows that the selectivity is moderately better for the H_2 ICE case and the formation of NH_3 has been eliminated for the low reductant concentration. Intra-catalyst measurements demonstrated that all of the H_2 had reacted one-quarter of the way through the core for both cases and at all temperatures (see Figure 6). This is another very favorable result for H_2 ICE, since this suggests that smaller and less expensive reactors can be implemented to achieve 90% conversion, especially if sulfur levels are maintained at the ppb-level in the H_2 source.

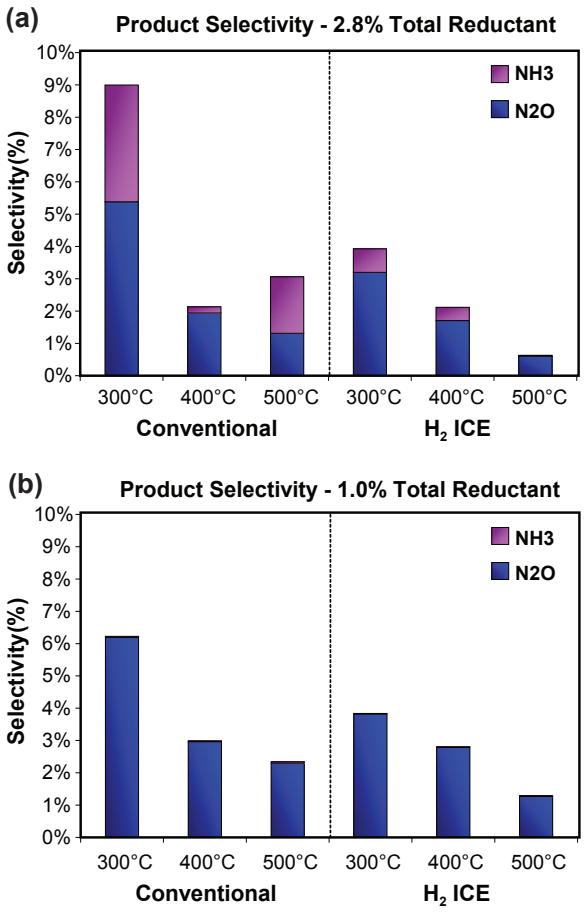


FIGURE 3. Nitrogen-based product selectivity for H_2 ICE and conventional CIDI exhaust using either (a) 2.8% of total reductant or (b) 1.0% of total reductant.

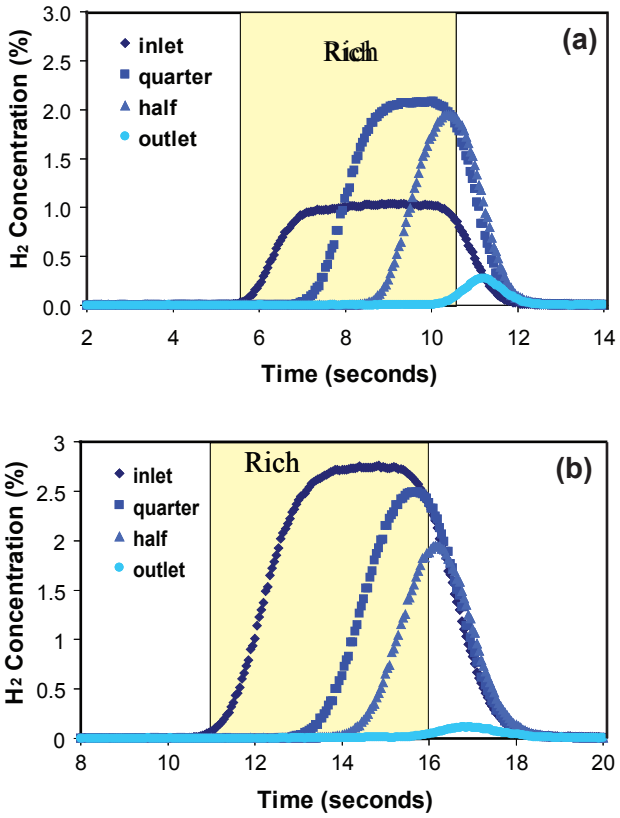


FIGURE 4. Intra-catalyst measurements of H_2 during the high reductant concentration (2.8% total reductant) experiments at 500°C for (a) conventional CIDI exhaust and (b) H_2 ICE exhaust.

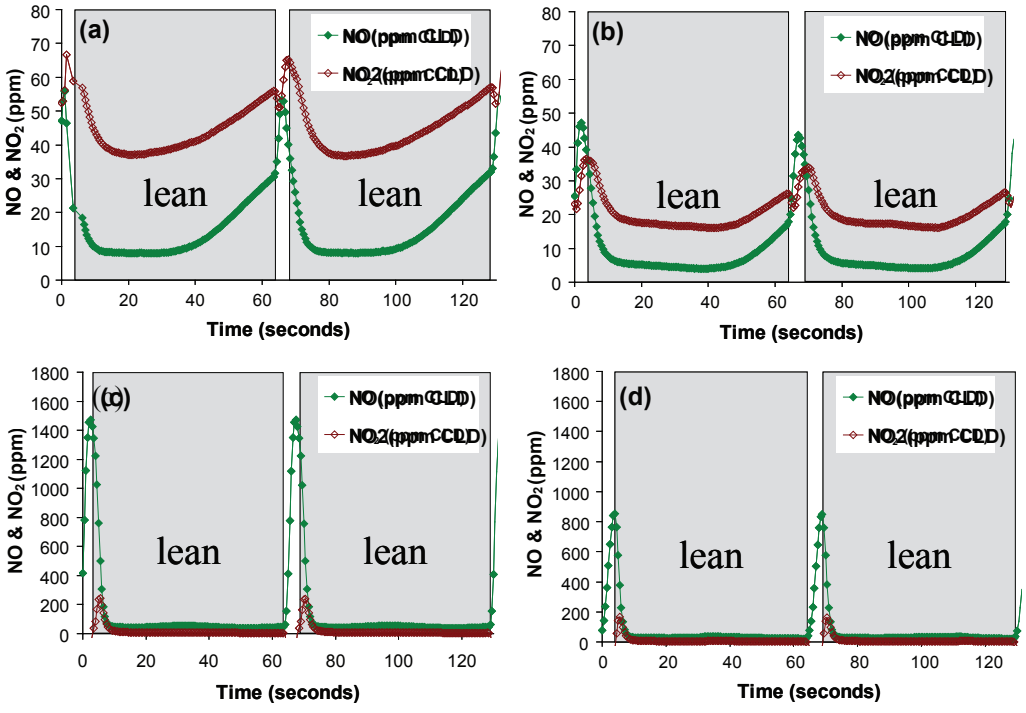


FIGURE 5. NO and NO_2 profiles at 300°C during 60s lean and 5s rich cycles for (a) conventional diesel exhaust and (b) H_2 ICE exhaust; similar profiles are also shown at 500°C for (c) conventional CIDI and (d) H_2 ICE exhaust.

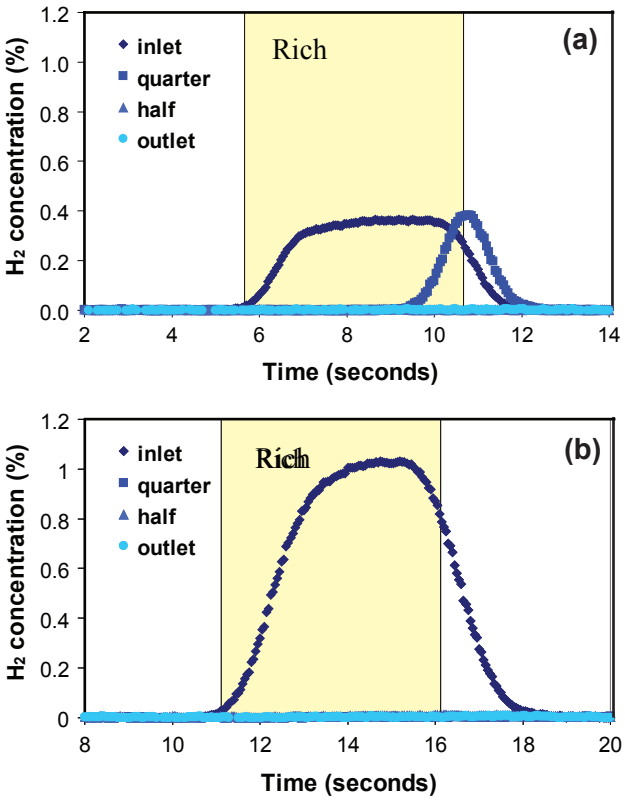


FIGURE 6. Intra-catalyst measurements of H_2 during the low reductant concentration (1.0% total reductant) experiments at 500°C for (a) conventional CIDI exhaust and (b) H_2 ICE exhaust.

Conclusions

- LNTs are a viable solution for H_2 ICE NOx aftertreatment
  - NOx conversion always higher than conventional diesel exhaust
    - Results suggest conventional CIDI exhaust is limited due to insufficient H_2
  - Field application will still depend on sulfur
    - level of H_2 source
    - Lube-oil consumption rate
- H_2-ICE based LNTs demonstrate better N_2 selectivity than CIDI applications
  - N_2O moderately lower
  - NH_3 significantly lower
  - Precise reductant control not as crucial for H_2 ICE
    - Less NH_3 slip with excess reductant
    - Dependence on accurate NOx map less critical than with diesel
    - Effort also improves understanding of LNTs with conventional diesel exhaust

FY 2006 Publications/Presentations

1. T.J. Toops, "H_2 Internal Combustion Engine NO_x Aftertreatment", H_2 ICE meeting at Ford, December 8, 2006, Dearborn, MI.

2. T.J. Toops, J.A. Pihl, "H_2 Internal Combustion Engine Research: Evaluation of NO_x Aftertreatment Systems", Advanced Combustion and Emissions Control Meeting, November 9, 2006, Southfield, MI.

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II.B.13 Cross-Cut Lean Exhaust Emission Reduction Simulation (CLEERS)

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Kenneth Howden

The following report is for two separate activities included under CLEERS:

- Administrative Support (Stuart Daw and Vitaly Prikhodko)
- Joint Development of Benchmark Kinetics (Stuart Daw, Kalyana Chakravarthy, Todd Toops, Jae-Soon Choi, Jim Parks, Josh Pihl, and Vitaly Prikhodko)

Objectives

Administrative Support

Provide coordination of the CLEERS activity for the Diesel Cross-Cut Team in accomplishing the following:

- Promote development of improved computational tools for simulating realistic full-system performance of lean-burn engines and the associated emissions control systems.
- 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 R&D needs and priorities.

Joint Development of Benchmark Kinetics

- 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.
- Provide benchmark laboratory measurements of NOx reduction chemistry and reaction rates.
- Coordinate laboratory measurements of lean-NOx trap (LNT) and selective catalytic reduction (SCR) materials with ongoing test-stand/vehicle studies in the National Transportation Research Center (NTRC) facility.
- Develop and validate global chemistry and (low-order) models for LNT and SCR kinetics.

Accomplishments

Administrative Support

- Continued co-leading the CLEERS Planning Committee.
- Assisted in facilitating the SCR, LNT, and diesel particulate filter (DPF) Focus Group telecons with strong domestic and international participation.
- Continued co-leading LNT Focus Group and dissemination of standard LNT materials protocol.
- Continued identification of key technical priorities from CLEERS community.
- Provided regular update reports to DOE Diesel Crosscut Team.
- Held 9th CLEERS workshop at University of Michigan, Dearborn on May 2-4.
- Maintained website functionalities, security, and data to facilitate web meetings and serve Focus Group interactions.

Joint Development of Benchmark Kinetics

- Continued testing and validation of the LNT material characterization protocol in conjunction with the LNT Focus Group, SNL, PNNL and collaborating suppliers.
- Continued benchmarking of Umicore commercial reference LNT material in LNT standard protocol.
- Continued in-depth study of the global kinetics of LNT regeneration, with specific emphasis on formation of byproduct N_2O and NH_3, effective fuel penalty, and potential coupling of LNT with SCR.
- Continued refinement of instrumentation on the ORNL bench-flow reactor to enhance capabilities for highly resolved measurements of key species (e.g., O_2 and NH_3).
- Initiated DRIFTS measurements of Umicore reference catalyst to study relationship of S poisoning to multiple storage sites.

Future Directions

Administrative Support

- Continue co-leading 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.
- 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 10th CLEERS workshop in the spring of 2007.
- Continue maintenance and expansion of CLEERS website.
- Continue providing regular update reports to the DOE Diesel Crosscut team.

Joint Development of Benchmark Kinetics

- Continue expansion of the capabilities of the ORNL bench-flow reactor.
- Continue development and demonstration of methods for utilizing LNT protocol data to generate global reaction kinetics and simulate device-scale performance.
- Continue characterization of Umicore LNT reference material at multiple scales and transmit results to the LNT Focus Group as they become available.
- Update and post revised global LNT models with input from SNL, literature, and ORNL experimental data as these become available.
- Continue identification of synergies between LNT NH_3 generation kinetics and NH_3-SCR as a potential alternative to urea-SCR NOx control.
- Coordinate bench reactor studies of the impact of sulfation and desulfation on LNT durability and kinetics.

Introduction

Improved catalytic emissions controls will be essential for utilizing high efficiency lean-burn engines without jeopardizing the attainment of the U.S. Environmental Protection Agency (EPA) emission standards scheduled to take effect in 2007 and again 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 (Crosscut Lean Exhaust Emissions Reduction Simulation) was initiated to promote development of improved computational tools and data for simulating realistic full-system performance of lean-burn engines and the associated emissions control systems. While CLEERS does not directly support the development of extensive full-emissions-system performance simulation codes, it does provide explicit support for the following activities:

- Public workshops on key emissions control topics;
- Collaborative interactions among Crosscut Team members, emissions control suppliers, universities, and national laboratories under specially organized topical focus groups;
- Development of experimental data, analytical procedures, and computational tools that are directly useful for understanding component performance and the behavior and durability of catalytic materials;
- Development of consistent frameworks for sharing information about emissions control technologies; and
- Development of explicit recommendations to DOE and the DOE Crosscut Team regarding the most critical emissions control R&D needs and priorities.

ORNL is currently involved in two separate DOE-funded tasks that support CLEERS:

- Overall administrative support; and
- Joint development of benchmark LNT kinetics with SNL and PNNL.

Previous work on micro-scale catalyst modeling for performance and durability has been terminated due to funding reductions.

In the administrative task, ORNL staff members coordinate the CLEERS Planning Committee, the CLEERS Focus groups, the public workshops, and the CLEERS website (www.cleers.org). The joint kinetics development task involves collaboration among ORNL, SNL, and PNNL to produce key kinetics information needed for predicting the performance of LNTs both individually and integrated with catalyzed particulate filters and ammonia-based selective catalytic reduction. 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. The collaboration is structured to build on the strengths of each lab and leverages against other DOE-funded activities to maximize benefits.

Approach

Administrative Support

In FY 2006 ORNL continued acting as the lead coordinator of the overall functions of the CLEERS Planning Committee and Focus Groups. Stuart Daw of ORNL is responsible for providing general assistance to each of the Focus Groups and is a co-leader (with Dick Blint of GM) of the LNT Focus Group. George Muntean and Darrell Herling from PNNL are co-leaders of the DPF and SCR Focus groups, respectively, and report on their activities elsewhere. ORNL organizes and implements the public workshops under guidance from the Focus Groups and Planning Committee, providing both technical and secretarial support. The CLEERS website is maintained (under direction of Sreekanth Pannala) on an ORNL server accessible via the internet. Both public and restricted areas have been set up on this website to facilitate distribution of technical information, workshop information and presentations, and interactive web meetings. Stuart Daw provides assistance to Dick Blint (GM) in presenting periodic status updates and summary reports to the Crosscut Team. Both Stuart and Vitaly at ORNL respond to general requests and inquiries about CLEERS from the public and technical community.

Joint Development of Benchmark Kinetics

ORNL's responsibility in this activity is to set up and conduct experimental measurements of LNT chemistry and reaction rates that will help to define the critical physical characteristics of LNT materials responsible for determining practical performance (i.e., NOx emissions reduction and energy efficiency). In this function, ORNL utilizes reference non-competitive adsorber materials in the ORNL bench-flow and DRIFTS reactors. Where possible, these bench measurements are also supplemented with other specialized measurement capabilities such as high-resolution microscopy at the ORNL High Temperature Materials Laboratory (HTML). ORNL maintains regular interactions with PNNL and SNL and the industry collaborators through the LNT Focus Group in order to maximize the value of the data generated and provide feedback that can be considered in planning future experiments. Where possible, laboratory results are compared with and analyzed in the context of test-stand/vehicle LNT measurements generated in parallel projects at ORNL's NTRC facility. For assistance in interpreting trends, ORNL utilizes simplified computer LNT codes that can be used to evaluate the laboratory and test stand data. Results are published in peer-reviewed journals, presented in public meetings, and/or posted on the CLEERS website.

Results

Administrative Support

The ninth CLEERS workshop was held May 2-4 at the Dearborn campus of the University of Michigan. As with the previous workshop, there were more than 110 registrants, including many researchers from emissions controls suppliers, universities (both foreign and domestic), software vendors, and consultants. All three emissions control technology areas (LNTs, DPFs, and SCR) were highlighted as indicated in the technical program and presentations available on the website (www.cleers.org). More detailed summaries of the workshop discussions were also provided to the Diesel Crosscut Team in subsequent CLEERS updates. Key observations coming from the workshop included the following:

- There have been exciting new developments in the integration of LNTs with NH_3-based SCR. In some instances, the utilization of LNTs to generate NH_3 may reduce or eliminate the need for urea injection.
- Major progress has been made in defining a detailed kinetic mechanism for LNT regeneration, including the generation of NH_3, for a realistic commercial catalyst.
- More needs to be done to develop refined kinetic models of urea-SCR including the effects of NH_3 storage and hydrocarbon poisoning.
- More information about the modeling of pre-catalyst mixing devices for urea-SCR is needed.
- Oxidation catalysts are assuming increasingly important roles in integrated emissions control systems, and additional studies of the kinetics are needed for these new contexts.
- Integrated system performance (including combinations of SCR, LNT, and DPF) is now a high priority.

The LNT, SCR, and DPF Focus Groups have continued regular phone/web meetings throughout the year, and summary reports of the meetings have been provided to group members and the Diesel Crosscut Team. As in previous years, meeting topics have included reviews of experimental data donated by members, technical presentations by outside invited experts (e.g., from non-member universities), and discussions of technical needs and priorities among the Crosscut member companies. After much discussion, it has been decided that we will implement a trial change in the Focus Group meeting format such that the three individual meetings held each month will be reduced a single combined meeting. Responsibility for meeting coordination will alternate among the three individual LNT/SCR/DPF Focus Groups. It is believed that this

alternative meeting schedule will more effectively utilize the time commitment of the participants and also allow more effective discussions targeted on system integration issues. After a three-month trial period, the effectiveness of this new format will be re-assessed.

Technical priorities identified by the CLEERS Crosscut members have been updated in discussions among the Planning Committee and Focus Group leaders and on the basis of an anonymous survey held over the summer of 2006. The results have been summarized in a single CLEERS priorities document, which has been distributed to the Diesel Crosscut Team and which will be posted early in FY 2007 on the CLEERS website. Highlights of the updated priorities include:

- The importance of device interaction and systems integration simulation as key issues.
- Recognition that oxidation catalysts are extensively utilized in integrated systems and that additional kinetics models for these devices in a multi-component context is needed.
- Potential synergies between the chemistry of LNTs and conventional three-way catalysts.
- Increased emphasis on modeling of 3-D spatial details inside each type of device.
- Emphasis on resolving transport effects, hydrocarbon and ammonia storage, and spray modeling for urea SCR.
- Expansion of the available kinetics for particulate oxidation in DPFs to include particulates produced by more advanced engines operating in low temperature combustion modes.

Due to other commitments, Prof. Harold Kung (from Northwestern University) felt it necessary to resign from his position on the CLEERS Planning Committee. After an extensive review of potential candidates, the Crosscut Team has accepted Prof. Louise Olsson (from Chalmers University) as his replacement, and she has graciously agreed to accept the position. Her very active prior participation in CLEERS and her strong familiarity with current European aftertreatment R&D are important attributes she will be bringing to the role.

A tentative date for the next (10^{th}) CLEERS workshop has been set for May 1–3, 2007. The planned venue will again be the University of Michigan, Dearborn campus, with Prof. Tariq Shamim acting as host.

Joint Development of Benchmark Kinetics

Further improvements have been made to the ORNL bench flow reactor to allow more consistent LNT catalyst experimentation over a range of operating conditions. Specifically, a balancing system has been installed to prevent sudden pressure swings in the reactor outlet pressure during lean/rich cycling, where the composition of the inlet gas stream undergoes very rapid transitions in fractions of a second. Also, improved seals have been installed on the quartz reactor tube so that much higher temperature conditions (e.g., >1,000°C) can be studied.

Monolith length effects on LNT performance have received considerable attention this year in bench reactor studies. LNT performance changes associated with monolith length differences (at constant space velocity) have been reported anecdotally for some time, but careful studies of the causes have not been reported in the open literature. Such changes can be extremely relevant to simulations of practical LNT systems because many catalytic reactor models commonly assume that performance is controlled by residence time (i.e., the inverse of space velocity) rather than the specific dimensions (e.g., the diameter and length). Likewise, there has been an ongoing debate among the CLEERS LNT group concerning the need to specify the dimensions of the sample cores used in the standard bench protocol. So far, our experiments confirm that at least some operating conditions, monolith length and/or the internal linear gas velocity can have a significant impact on performance. Specifically, it appears that shorter monoliths exhibit higher NOx breakthrough during fast cycling when there is insufficient reductant for complete regeneration. An example of this effect as revealed in bench flow reactor measurements is illustrated in Figure 1. The reasons behind this difference appear to be related to reductant depletion by stored or gaseous oxygen and are still being investigated. But it is already clear that this effect is real and needs

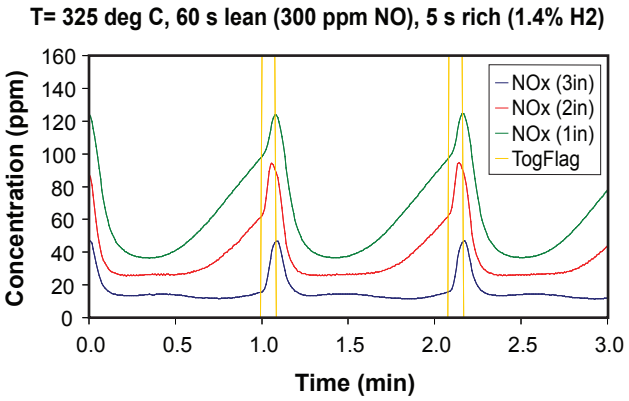


FIGURE 1. Example performance differences seen for different length monolith cores of the Umicore LNT reference catalyst under fast cycling conditions in the ORNL bench flow reactor. The yellow line indicates the beginning and end of regeneration. Even though gas flow has been adjusted in each case to keep the space velocity constant at 30,000 (1/hr), there is still greater NOx breakthrough as monolith length decreases from 3 to 2 to 1 inch.

to be properly addressed in evaluating kinetic data and simulating device performance.

Studies of the generation of N_2O and NH_3 byproducts during LNT regeneration have continued with the objective of developing an explicit and detailed kinetic mechanism for device simulation. This is particularly relevant in the context of commercial implementations of LNT-SCR combination systems, where the LNT is now used to generate NH_3 that is subsequently utilized for SCR NOx reduction. Special steady-state bench reactor experiments (under reducing conditions) have continued this year with the objective of measuring the relative reaction rates of NO with H_2 and CO to form N_2, N_2O, and NH_3 in the absence of O_2 and NOx storage reactions. Figures 2-4 illustrate the general trend observed for NH_3 and N_2O generation from NO reaction with H_2 over the Umicore catalyst as a function of temperature. Companion DRIFTS reactor studies (Figures 5 and 6) suggest that NCO (isocyanate) is an important intermediate species in NH_3 formation. As noted below, the role of isocyanate seems to be confirmed in the kinetic mechanisms developed from these bench data. The steady-state experiments have also revealed that the two main 'sinks' for NH_3 are oxidation by O_2 and NO to N_2O and decomposition to N_2 and H_2 at temperatures above 350°C.

Combining the steady-state reducing condition trends with observations from cycling experiments suggests the transient regeneration scenario depicted in Figure 7. Here we observe that at locations downstream from the propagating reductant front there is little or no NH_3 because any that is formed is rapidly oxidized. Near the center of the reductant front, NOx reduction to N_2 and NH_3 compete with each other as NOx is rapidly released from storage sites. However, upstream of the reductant front, NH_3 continues to be generated by the reduction of NOx from 'slow' release storage sites. Thus NH_3 only becomes visible at the reactor exit when the reductant front has completely passed through and regeneration is mostly complete. We speculate that increasing the population of 'slow' NOx storage sites

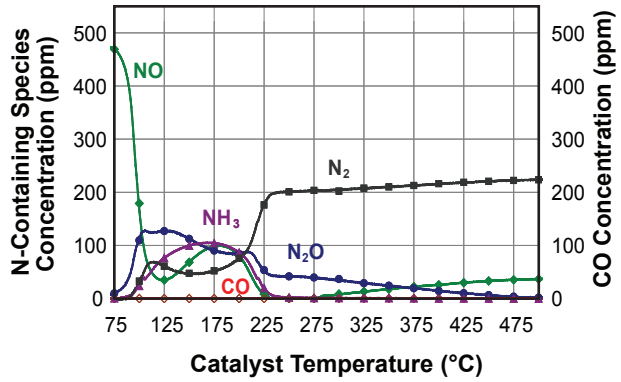


FIGURE 2. Pseudo-steady-state bench reactor conversion of N species and CO with a feed ratio of 1:1 NO/H_2 in water vapor, CO_2, and N_2 as temperature is ramped at 5°C/min.

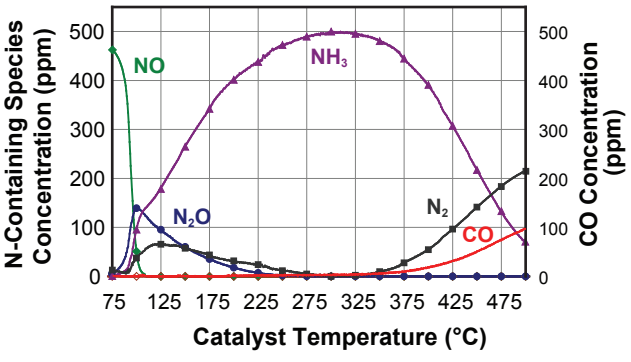


FIGURE 3. Pseudo-steady-state bench reactor conversion of N species and CO with a feed ratio of 1:2.5 NO/H_2 in water vapor, CO_2, and N_2 as temperature is ramped at 5°C/min. Note the higher NH_3 production compared to Figure 2.

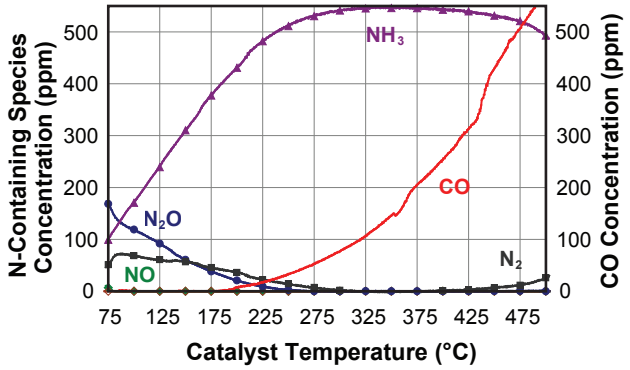


FIGURE 4. Pseudo-steady-state bench reactor conversion of N species and CO with a feed ratio of 1:10 NO/H_2 in water vapor, CO_2, and N_2 as temperature is ramped at 5°C/min. At such high H_2 concentrations, NH_3 generation dominates even at high temperature.

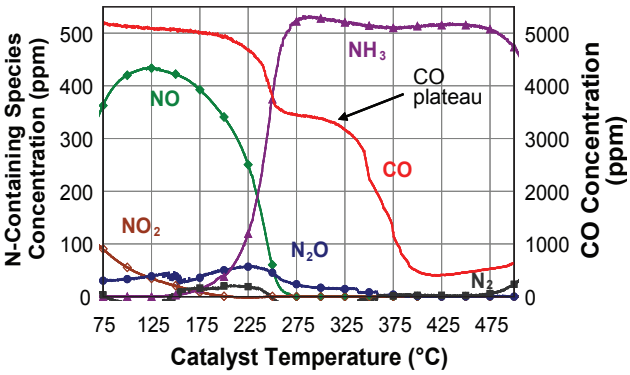


FIGURE 5. Pseudo-steady bench reactor conversion measurements for 1:10 NO_2/CO in water vapor, CO_2, and N_2 as temperature is ramped at 5°C/min. The second CO plateau above 250°C correlates with the rise of NH_3.

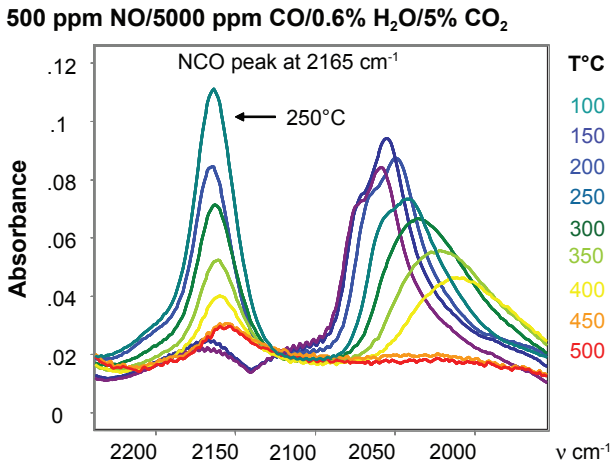


FIGURE 6. DRIFTS spectra illustrating evidence for NCO hydrolysis as prominent source for NH_3 generation. Here the feed gas is NO and CO in water vapor, CO_2 and N_2. At the same temperature that NH_3 formation jumps in the bench flow experiment, the DRIFTS measurement indicates a sharp decrease in NCO on the catalyst surface.

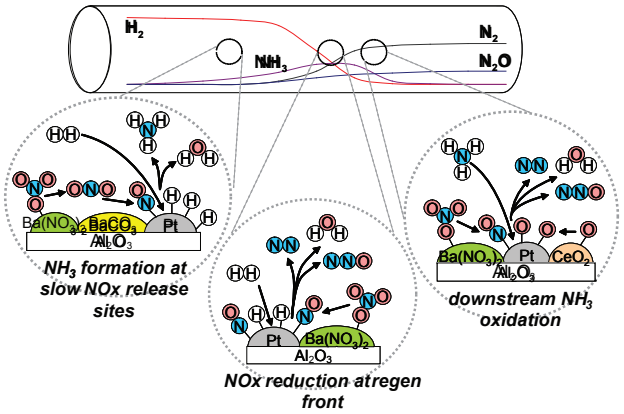


FIGURE 7. Proposed scenario for the stages involved in LNT regeneration as the reductant front progresses axially down the monolith.

might lead to enhanced NH_3 generation for situations where the latter is the desired result.

The above steady-state data are now being collaboratively studied by SNL and ORNL to develop a detailed kinetic mechanism for reducing conditions that is consistent with the observations. So far, this effort has been successful in developing a relatively compact mechanism that does a remarkably good job reproducing both the steady-state and transient features described above. An example of this good fit produced by this mechanism for steady-state reduction is illustrated in Figure 8. Highlights of the mechanism developed to date include:

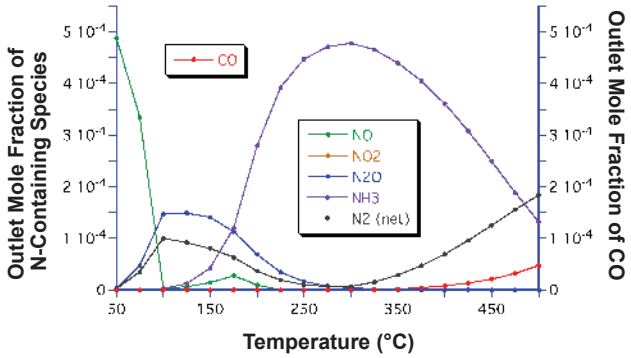


FIGURE 8. Predicted steady-state conversion for 1:2.5 NO/H_2 in water vapor, CO_2, and N_2 as a function of temperature based on the recently developed regeneration kinetic mechanism. Compare with Figure 3.

- Twenty three thermodynamically consistent surface reactions (all reversible);
- Elementary mass-action kinetics with no altered reaction orders or coverage dependent activation energies; and
- Important roles for both isocyanate formation and water-gas-shift reactions.

Additional details on this mechanism are reported in the SNL annual report. Current LNT modeling studies are focused on coupling this mechanism with a corresponding lean-phase mechanism that can be utilized to capture the main features of fast LNT cycling.

Initial studies of LNT sulfation and desulfation have utilized a Ba-based model catalyst in the DRIFTS reactor. At 200°C, initially formed sulfur groups appear to form that do not impact NOx storage sites until the samples have been further heated. Heating to 500°C drives the sulfates from their "observer" sites to active storage sites. Sulfation also impacts the active Pt surface area. At 300°C, the level of stored nitrates decrease readily with SO_2 in the feed stream; and additional heating is not necessary to impact storage. At 400°C, the effect of the SO_2 is most pronounced in the bulk-phase, where nitrates are readily decreasing. At all temperatures, CO adsorption on Pt diminishes with increasing sulfation, indicating loss of active Pt sites. When SO_2 is removed from the gas-phase these sites are recovered.

Conclusions

Administrative Support

Approximately 120 representatives from automotive and engine manufacturers, emissions controls suppliers, universities, and national laboratories attended the ninth international CLEERS workshop on May 2–4 at the University of Michigan, Dearborn campus. The

complete technical program, meeting summary, and most of the presentations are available on the website (www.cleers.org). Important new developments in emissions controls simulation and shifts in R&D priorities were identified, leading to subsequent discussions among the CLEERS Planning Committee, the LNT, DPF, and SCR Focus Groups, and the DOE Diesel Crosscut Team. These discussions are expected to be reflected in adjustments in national lab R&D in FY 2007. The next CLEERS workshop is planned for May 1–3, 2007.

The LNT, SCR, and DPF Focus Groups have continued regular phone/web meetings throughout the year with considerable international participation. The meeting topics have included reviews of experimental data donated by members, technical presentations by outside invited experts (e.g., from non-member universities), and discussions of technical needs and priorities among the Crosscut member companies. A trial change of the monthly meeting format will be implemented starting this October for a period of three months. During this period, all three groups will participate in a single joint monthly meeting.

An updated list of CLEERS R&D priorities has been developed and approved by the DOE Diesel Crosscut Team. The updated list includes an increased emphasis on emissions control device interaction and system integration and more extensive modeling of details in oxidation, DPF, and urea-SCR catalysts.

Joint Development of Benchmark Kinetics

ORNL LNT bench reactor studies have revealed important new insights regarding monolith length effects, the detailed mechanisms of regeneration and NOx reduction (including the formation of N_2O and NH_3), and the mechanisms of catalyst sulfation and desulfation. The impact of monolith length on NOx conversion is most apparent when the amount of reductant supplied is insufficient for regeneration. Under these circumstances, shorter monoliths suffer a significant penalty in NOx conversion efficiency and thus an increased potential fuel penalty. Generation of large quantities of NH_3 typically is associated with over regeneration (i.e., excess reductant). A relatively compact but detailed kinetic mechanism has been developed for regeneration based on the bench reactor measurements for the Umicore reference LNT catalyst.

Sulfur poisoning of LNT catalyst appears to occur in two stages, the first of which has minimal impact on NOx storage sites. The second sulfation stage is much more irreversible and is promoted by higher temperatures.

The above insights are currently being incorporated into improved LNT kinetic mechanisms, experimental characterization procedures and device simulation models. Future plans include the investigation of combined LNT-SCR device simulation.

Publications/Presentations

1. J.-S. Choi, W.P. Partridge, W.S. Epling, N.W. Currier, and T.M. Yonushonis, "Intra-channel evolution of carbon monoxide and its implication on the regeneration of a monolithic $Pt/K/Al_2O_3$ NOx storage-reduction catalyst, "Southeastern Catalysis Society Fall Symposium, Asheville, North Carolina, September 25–26, 2005.

2. J.A. Pihl, "Byproduct formation during regeneration of Lean NOx Traps," Master's Thesis, University of Wisconsin, November 2005.

3. J. Pihl and Todd Toops, "DRIFTS Studies of Lean NOx Trap Sulfation and Desulfation," 9th CLEERS Workshop, May 2–4, 2006, www.cleers.org.

4. J.-S. Choi, V. Prikhodko, K. Chakravarthy, and C.S. Daw, "Assessing Monolith Length Effect on LNT Performance," 9th CLEERS Workshop, May 2-4, 2006, www.cleers.org.

5. J. Pihl, J. Parks, T. Toops, S. Daw, and T. Root, ""Experimental studies of NH_3 and N_2O formation in lean NOx traps," 9th CLEERS Workshop, May 2–4, 2006, www.cleers.org.

6. R. Larson, K. Chakravarthy, C.S. Daw, and J. Pihl, "Modeling Kinetics of NH_3 and N_2O Formation in Lean NOx Traps," 9th CLEERS Workshop, May 2–4, 2006, www.cleers.org.

7. J.-S. Choi, W.P. Partridge, W.S. Epling, N.W. Currier, and T.M. Yonushonis, "Intra-channel evolution of carbon monoxide and its implication on the regeneration of a monolithic $Pt/K/Al_2O_3$ NOx storage-reduction catalyst," Catalysis Today, vol. 114, p. 102, 2006.

8. T. Toops, D.B. Smith, W.P. Partridge, "NOx Adsorption on $Pt/K/Al_2O_3$", *Catalysis Today*, vol. 114, p. 112, 2006.

9. Y. Ji, T.J. Toops, U.M. Graham, G. Jacobs, and M. Crocker, "A Kinetic and DRIFTS Study of Supported Pt Catalysts for NO Oxidation," *Catalysis Letters*, vol. 110, no. 1–2, pp. 29–37, August 2006.

10. J.A. Pihl, J.E. Parks II, T.J. Toops, C.S. Daw, and T.W. Root, "Product Selectivity During Regeneration of Lean NOx Trap Catalysts," SAE 2006-01-3441.

11. R.S. Larson, K. Chakravarthy, J.A. Pihl, and C.S. Daw, "Modeling of chemistry in lean NOx traps under reducing conditions," SAE 2006-01-3446.

Special Recognitions & Awards/Patents Issued

1. Special recognition for collaborative R&D under CLEERS from U.S. CAR presented to R. Blint, May 2006.

II.B.14 CLEERS DPF Modeling

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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) diesel particulate filter (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

- Developed tools for digital reconstruction of three-dimensional filter substrate microstructures from a small set of two dimensional images.
  - The use of fewer two-dimensional images dramatically decreases the time and expense involved with analyzing a new substrate, allowing additional different materials to be studied
  - Statistical metrics are used to verify the fidelity of the reconstructions
  - Reconstructions of any shape or volume can be produced
- Added soot oxidation kinetics to the micro-scale lattice-Bolzmann filter model.
  - Kinetics include separate temperature dependent rates for oxidation by NO_2 and oxygen
  - Rates can be adjusted according to the presence of soluble organic fraction (SOF) and changes in soot reactivity as it is oxidized
  - Initial parametric studies highlight the importance of catalyst placement with respect to the porous filter micro-structure
- Further developed single-channel experimental techniques.
  - Multiple filtration studies were carried out, including catalyzed and uncatalyzed Corning Duratrap RC filter material
  - Studies were conducted to differentiate the contributions of channel flow and wall flow resistance to overall pressure drop through a DPF device
- Developed techniques for observing regeneration on the surface of uncatalyzed and platinum catalyzed single channel filter samples.
- Coordinated and led monthly teleconferences for the CLEERS DPF sub-team.

Future Directions

- Extend micro-scale regeneration model to include surface catalytic reactions which convert NO to NO_2, allowing studies of phenomena such as 'NOx recycle' and optimization of catalyst loading and placement.
- Extend micro-scale regeneration model to include coupled heat transfer and oxidation exotherms, allowing studies of 'light-off' conditions during active filter regeneration.
- Conduct single channel experiments with catalyzed and uncatalyzed samples in parallel, in order to better quantify the effect of catalyst loading on regeneration behavior.

Introduction

High efficiency diesel engines provide an important short to medium-term strategy for meeting the nation's transportation needs while minimizing emissions implicated in global climate change. However, concerns over the health effects of particulate emissions from diesel engines have prompted legislation in the U.S.,

Europe, and Asia which has set challenging limits on vehicular exhaust soot concentrations. DPFs have emerged as an important enabling technology to comply with these new limits. DPFs have a negative impact on fuel efficiency because they introduce back-pressure to the exhaust system and, in the case of active regeneration systems, require energy to burn away collected soot. These factors must be minimized in order for high efficiency diesel engines to provide their maximum economic and environmental benefits.

Mechanisms taking place during filtration and regeneration at the microscopic scale of pores in filter substrates are critical to DPF performance. Many different porous substrate materials have been explored by industry, each with their own set of advantages and disadvantages. Currently, ceramic materials such as cordierite and silicon carbide are considered to be the most practical for near-term application. The way in which soot particles interact with substrate microstructures during filtration determines removal efficiency and back-pressure. Overall back-pressure can also be minimized by prompt and efficient oxidation of soot trapped in the filter, which involves pore-scale transport of heat and, in many cases, active gaseous species such as NO_2. Filtration efficiency can vary dramatically by particle size. This has important implications for human exposure to ultra-fine nanoparticles, which are suspected of posing significant health risks. The project described in this report seeks to elucidate pore-scale mechanisms involved in DPF operation through sub-scale computer simulation in order to promote more effective and reliable DPF devices which introduce a minimum negative impact on fuel economy.

Approach

A computer model has been developed to predict the nature and location of soot deposits within porous filter substrates by simulating the flight and deposition of individual soot particles. Detailed digital maps of the microscopic pores in various substrate materials are created using a novel stochastic reconstruction technique. The lattice-Boltzmann method is used to solve for the flow field of exhaust through the substrate microstructure as soot deposits form. The paths of simulated soot particles are derived from the exhaust flow field and include random Brownian motion. Simulations with various DPF substrates, including cordierite and silicon carbide, show how the substrate microstructures affect filtration performance. The micro-scale model has recently been extended to include the transport of active gaseous species and oxidation of accumulated soot. Parametric studies were conducted to examine the effect of substrate microstructure on net rates of soot consumption.

Experimental methods have been developed to observe the loading and regeneration of external surfaces of individual channels, allowing meaningful comparisons to model predictions. Techniques have also been developed to measure fundamental parameters, such as filter wall permeability and channel flow resistance, which are necessary for accurate modeling of DPF performance at the device scale. Visible and infrared video cameras were used to observe loaded surfaces of filter samples during regeneration experiments in an effort to quantify the effect of catalysts on the initiation of 'light-off' during active regeneration events and to gain insight into pore scale phenomena which might promote faster and more efficient oxidation of collected soot.

Results

Pursuant to the overarching goal of the CLEERS project to promote improved device scale modeling of diesel after-treatment technologies, Pacific Northwest National Laboratory (PNNL) has continued to coordinate monthly teleconferences in order to discuss current CLEERS DPF research with various stakeholders, including OEMs, universities, and other national laboratories. Representation by industry and academia has been consistently good, and presentations by various special speakers have sparked helpful and informative discussions on a variety of topics. One benefit of hosting the monthly meeting has been the opportunity to receive continual feedback on the direction of specific CLEERS research activities at PNNL.

Over the course of FY 2006, tools were developed for faster and more flexible characterization of substrate microstructures. Detailed modeling of pore-scale phenomena requires accurate, high resolution characterization of the three-dimensional structure of porous filter substrates. Three-dimensional digital geometries were previously obtained using scanning electron microscopy of repeatedly polished substrate samples. This resulted in a series of two-dimensional grayscale micrographs. The 2-D images had to be precisely aligned, and the 3-D volume was then reconstructed by interpolation. Reconstructing a volume of any thickness required a large number of polishing steps. This procedure, while in principle allowing exact reconstruction of a given volume, had several drawbacks. The multiple polishing and microscopy steps made it relatively expensive and time-consuming to characterize new substrates. Also, subsequent analyses were constrained to the size and shape of the exact substrate volume examined.

To overcome these difficulties, a stochastic reconstruction technique was developed whereby a given substrate could be characterized from a small set of micrographs, all of which may be obtained during

a single scanning electron microscopy (SEM) session. Computer algorithms scan through the digitized 2-D images and tabulate statistical properties of the porous structure, including local porosity and chord length distributions. Local porosity must be accounted for because the porosity of some substrates (e.g. cordierite) has been observed to vary across the thickness of a filter wall. Chord length distributions are a statistical metric which have been widely used in the reconstruction of porous materials such as soils and rocks [1]. Chord length distributions contain information about pore size, shape, and connectivity.

A stochastic algorithm is then used to generate a 3-D reconstruction of the porous material by randomly placing a collection of solid grain shapes. The same statistical metrics are measured for the reconstructed volume, and the reconstruction process is iterated until there is satisfactory agreement between the reconstructed volume and the 2-D images. In this way, a volume of any size or shape can be generated which matches the observed structural characteristics of a given substrate. Using this technique, the microstructures of several current commercial substrate materials were reconstructed, including Corning Duratrap RC and Ibidin silicon carbide. Figure 1 shows the chord length distributions from original micrographs of a cordierite sample and those from a corresponding reconstruction. A somewhat similar approach has been taken to reconstruct DPF microstructures in proprietary modeling software [2, 3].

The shape and location of soot deposits in a filter substrate's microstructure are important not only for predicting filtration performance of various filter materials, but also for predicting regeneration behavior and perhaps other important phenomena like ash accumulation. Precious metal catalysts convert NO to NO_2, which is important for oxidation of soot in many filter regeneration strategies. How these gaseous species move from catalyst to soot within the 3-D flow field may be an important factor in getting the most benefit from a given catalyst loading. Pore-scale simulations of individual soot particle motion and deposition during loading were carried out in order to predict the location and morphology of soot deposits. These simulations have been carried out for several common DPF substrate materials, including cordierite and silicon carbide. Figures 2 and 3 show a small section of reconstructed cordierite filter wall before and after loading with soot. Figure 4 shows corresponding pressure drop predictions as a function of total soot loading. Figure 5 shows predicted depth of soot penetration into a silicon

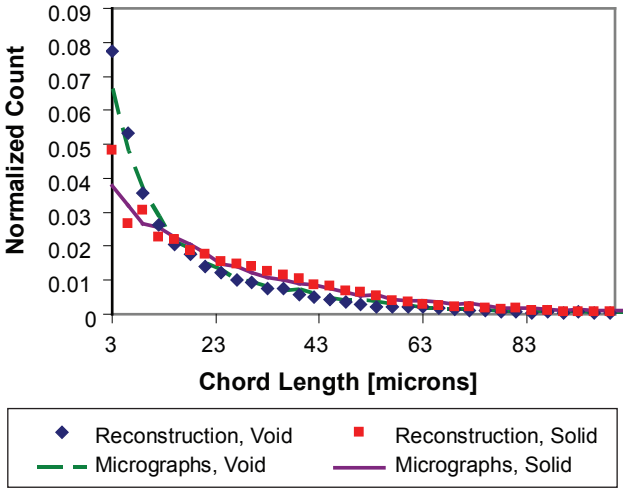


FIGURE 1. Chord Length Distributions from Cordierite Micrographs and 3-D Reconstruction

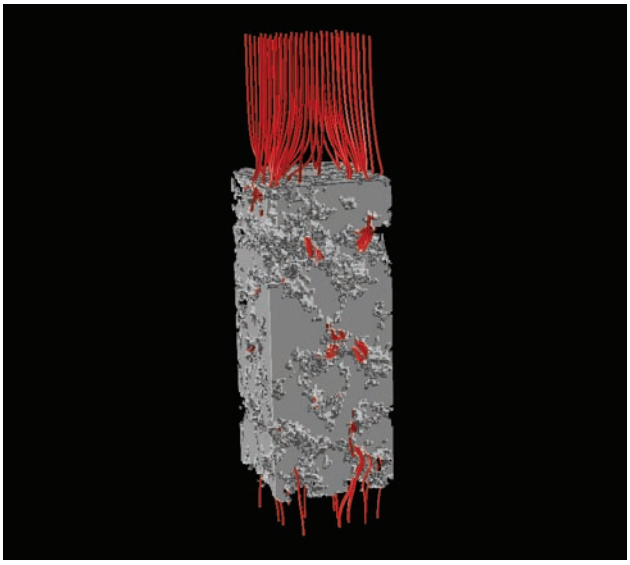


FIGURE 2. Volume of Reconstructed Cordierite before Loading with Soot

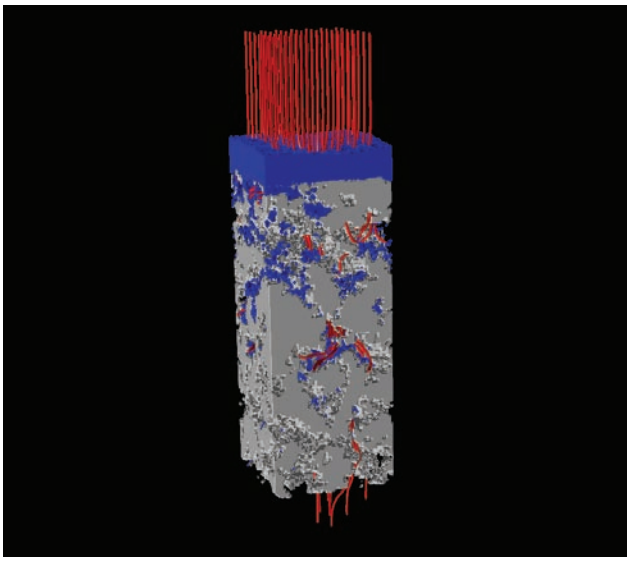


FIGURE 3. Volume of Reconstructed Cordierite after Loading with Soot

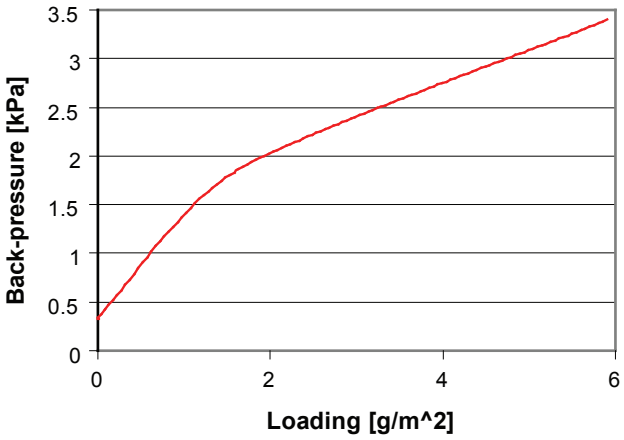


FIGURE 4. Predicted Pressure Drop across a Cordierite Filter Wall as a Function of Loading

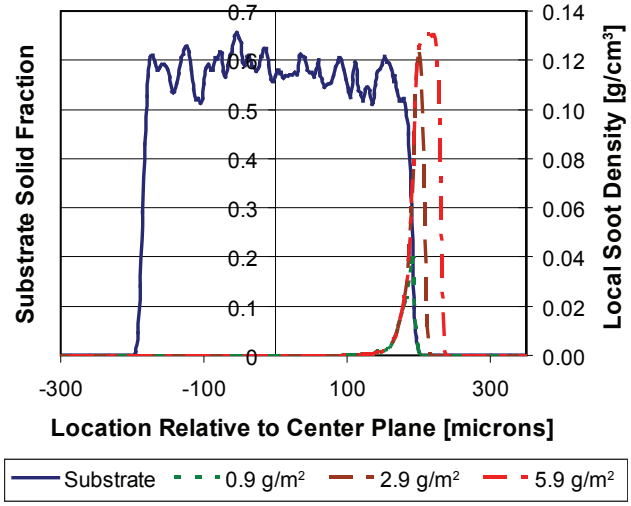


FIGURE 5. Predicted Penetration of Soot into Filter Wall during Loading

carbide filter wall at three different total loadings. The solid line, representing local substrate solid fraction, corresponds to the scale in the center, and the dashed lines, representing local soot density, correspond to the scale on the right side.

Recently published soot oxidation chemistry was also incorporated into the pore-scale filter model in FY 2006. The correlation employed was published by Messerer and associates in the Journal Carbon [4]. It includes temperature dependent terms for both NO_2 and O_2 oxidation as well as changes in the oxidation rates as the soot is consumed. Initial parametric studies using these kinetic relationships were conducted by introducing NO_2 at a fixed rate in three locations: upstream of the loaded filter, at the loaded filter surface, and on the back side of the filter wall (which would represent a worst case for catalyst location). Oxidation rates for the first two cases were similar, but

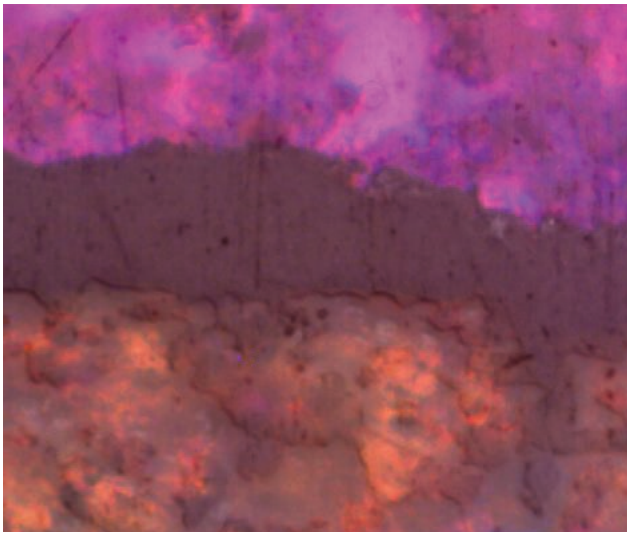


FIGURE 6. Thin Section Image of a Loaded Duratrap RC Filter Wall

were reduced almost by a factor of four in the third case. These results indicate that some NO_2 can migrate upstream from catalytic sites within the filter wall, but that the porous microstructure of the filter wall can be a significant barrier to transport of active gaseous species during regeneration.

Single channel loading experiments were carried out for a number of substrates, and the associated techniques were further refined over the course of FY 2006. Other experimental work focused on three areas:

1. Improving visualization techniques for soot within the substrate using a thin section technique. This method involves the use of vapor adhesives to stabilize soot deposits, allowing preparation of thin sections which can be examined using visible light refractometry (Figure 6). This work could allow direct observation of soot penetration into filter walls and is documented in detail in a forthcoming publication (SAE draft - publication 4).
2. Isolating individual contributions to overall pressure drop in DPF devices. Experimental techniques have been developed to directly measure the pressure drop across individual channel walls and pressure drop due to flow along DPF channels. These contributions to overall pressure drop are intertwined in most test data, and methods for measuring them separately could dramatically improve DPF models at all scales.
3. Developing a parallel measurement apparatus that allows testing of two single channel samples under identical exhaust conditions. This technique can be used to observe pressure drop and thermal changes in catalyzed and un-catalyzed single channel samples during loading and regeneration, allowing quantitative observation of catalytic action during soot oxidation.

Conclusions

- Stochastic reconstruction techniques may be used to economically generate three-dimensional geometries for simulation of pore scale phenomena in DPF substrates.
- Penetration of soot into filter walls of DPFs is dependent upon substrate pore geometry, and can be qualitatively predicted using micro-scale modeling.
- The degree of soot penetration into filter walls and the interaction between deposits and the substrate micro-structure can have a significant impact on overall back-pressure.
- Active gaseous species like NO_2 can migrate upstream through the porous substrate to take part in soot oxidation reactions.
- The porous substrate microstructure nevertheless constitutes an significant barrier to transport of gaseous species from catalytic locations within the filter wall.
- New experimental techniques have provided insights into soot stabilization and visualization, and into phenomena contributing to the total pressure drop across DPF devices.

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II.B.15 Innovative Emission Control Device Renewal

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Subcontractors:
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- Michigan Technological University

Objectives

The objective of this project is the development of a diesel particulate filter (DPF) regeneration technique that minimizes:

- Impact on engine operation
- Power consumption
- Cost

Accomplishments

- Developed a microwave heating technique that uniformly heats the DPF, and eliminates parasitic soot absorption.
- A number of materials have been evaluated as possible microwave absorbing candidates.
- Lab demonstration of microwave regeneration of a soot-loaded DPF.
- A range of different spot configurations have been modeled for their effectiveness in initiating and propagating soot oxidation.
- A proprietary microwave absorbing configuration has been designed and patent applications have been filed.
- Engine control strategies for microwave assisted regeneration have been identified.
- The DPF was successfully regenerated on a vehicle using the alternative heating strategy.
- The soot ignition and energy deposition techniques developed from the microwave work have been applied to investigate alternative heater concepts.

Future Directions

The future direction of the project will examine an alternative regeneration technique which builds off the knowledge gained from the microwave regeneration work, and may provide an economy benefit over it.

Introduction

The goal of this project is to leverage the exotherm of soot oxidation during DPF regeneration in order to regenerate the DPF with a minimum amount of added energy. Instead of heating the entire DPF to the soot oxidation temperature, only selected spots are heated to the oxidation temperature of the soot. The resulting oxidation wave is allowed to propagate throughout the length of the DPF. To accomplish this, an effective heat source must be identified to start the PM oxidation process. This heater must be energy efficient, and be compatible with the typical vehicle electrical architecture. Furthermore, an engine control strategy must be developed to optimize the performance of this type of regeneration. The current project activities address each of these needs.

Approach

This project aims to develop a new approach to regenerate particulate filters in compression-ignition, direct injection (CIDI) diesel engines. This project has investigated the technology of spot heating within a DPF using various techniques in order to ignite the soot and leverage the heat from the soot oxidation to propagate a complete regeneration of the DPF. This project has investigated:

- A range of microwave active materials for both activity and stability in the DPF environment.
- A series of spot configurations within the DPF to identify those with the highest efficiency in soot ignition.
- Modeling has been used to predict the efficiency of spots to absorb energy.
- Modeling has also been used to predict the optimum spot positioning to ignite and propagate the soot oxidation with the minimum energy input.
- An alternative heating approach was also investigated to evaluate competitive heating technologies.

Results

An effective heating strategy must be developed to start the soot ignition. Microwave heating was evaluated by HRL Laboratories. A wide range of diesel exhaust compatible materials were evaluated for their microwave absorption properties and Curie temperature (the temperature where the material no longer absorbs the magnetic field component of the microwave source). The materials were typically in the form of a ceramic coating and included silicon carbide, indium tin oxide, nickel oxide, and iron or lithium-based ferrites. The figures of merit for the materials examined were the following:

1. Stable under diesel engine exhaust conditions.
2. Able to be heated with microwaves at 2.45 GHz to the soot ignition temperature.
3. For configurations relying on magnetic absorption, the material has a high Curie temperature.

To avoid parasitic absorption of microwaves by the soot in the DPF, set-up configurations were devised that confined heating to the front region of the trap. Using this configuration, lab experiments demonstrated 75% regeneration efficiency with respect to soot removal under controlled air flow conditions. Further work is required to reduce power consumption and to increase the compatibility of the microwave system with automotive designs.

An alternative strategy to microwave heating was also developed that concentrated the thermal energy to the front of the DPF to start particulate ignition. The alternative approach was applied to a vehicle to evaluate the effectiveness of this system

By only heating the front of the DPF, a much smaller amount of energy is used to ignite the particulate matter compared to raising the temperature of the entire DPF. This technique relies on leveraging the particulate oxidation energy to continue the soot burning as a flame front travels down the DPF channel (see Figure 1).

This approach has been demonstrated on a running diesel truck with a heavily loaded DPF. The DPF was then cut into 1" segments to analyze the effectiveness of this regeneration approach (see Figure 2).

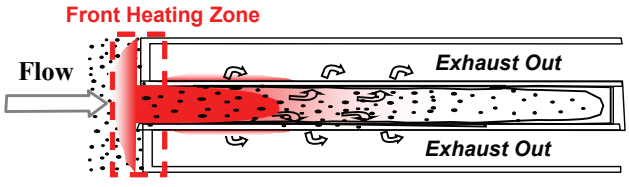


FIGURE 1. Front-Ignited DPF Regeneration

Figure 2 illustrates that nearly 85% on the soot was removed during this regeneration cycle. This outcome was also predicted by our DPF model as illustrated in Figure 3. Soot oxidation on the front face creates a propagating wave that was simulated using the DPF regeneration model developed by Michigan Technological Institute (MTU). Figure 3 is an example of one of these simulations. Figure 3 shows the evolution of the temperature in a DPF from the addition of heat. The different colored lines represent the temperature and soot levels at a specific point in time as the flame front propagates down the length of the DPF.

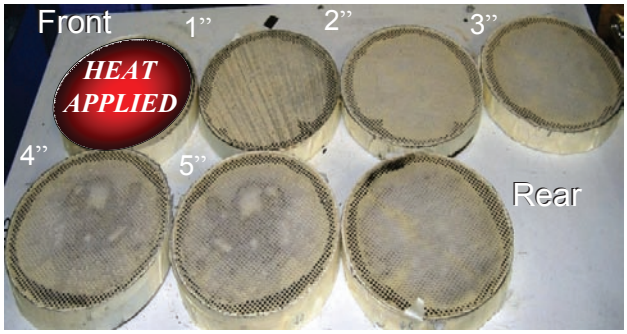


FIGURE 2. Segmented DPF After Regeneration

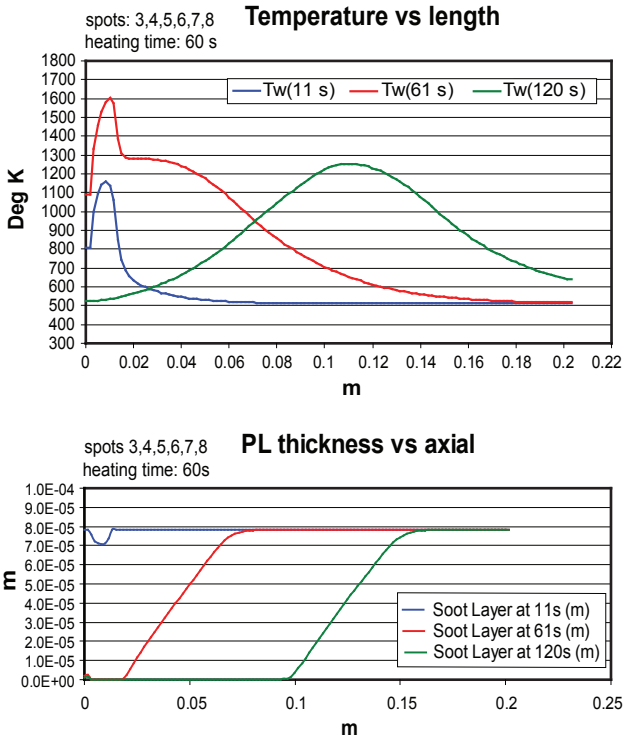


FIGURE 3. DPF Model Regeneration Results

Presently we are evaluating this selective heating regeneration technique on cordierite DPFs where substrate durability is an issue. Several heating designs and engine control strategies are being developed to address the substrate durability concerns.

Conclusions

The goal of this project was to develop a very robust and energy efficient approach to regenerate a DPF. Experimental results with the current heating and control strategy has been effective in reducing the fuel penalty required to regenerate a particulate filter. Additional benefits include: reduced tailpipe temperatures during regeneration, shorter regeneration times, and overall higher regeneration efficiencies. Several experimental regenerations have been successful and the technique looks increasingly promising.

II.C.1 Variable Valve Actuation

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Objectives

- Develop an optimal, cost-effective, diesel variable valve actuation (VVA) system for advanced low temperature diesel combustion processes.
- Build and demonstrate a mechanism for the diesel variable valve actuation system.

Accomplishments

- Received engine model and requirements and prepared mechanism design layout.
- Initiated and completed literature study to further the comprehension of advanced mode diesel combustion (AMDC)/VVA requirements.
- Initiated and completed detailed engine selection matrix.
- Completed benchmarking study on competing technologies.
- Determined resultant mechanism valve profiles and worked with OEM to identify differences.
- Prepared system requirements document based upon all available data.
- Developed production type carrier for ease of engine assembly and application to other engines.
- Identified design interferences with original equipment manufacturer (OEM) engine and proposed possible solutions.
- Submitted provisional patents covering the VVA mechanism.

Introduction

The project objective is to develop and demonstrate an optimal, cost-effective diesel variable valve actuation (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 enable expanding 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 in reducing the penalty in fuel consumption related to extremely low emission standards.

Delphi Corporation has major manufacturing and product development and applied R&D expertise in the valve train area. Historical R&D experience includes the development of fully variable electro-hydraulic valve train on research engines as well as several generations of mechanical VVA for gasoline systems.

Approach

Delphi utilized a milestone approach in the development of the VVA mechanism including:

- Identify preliminary functional requirements
- Identification of the target engine
- Building the engine model
- Calibration of the engine model
- Definition of representative points in the drive cycle
- Literature study and competitive analysis
- Develop detailed VVA functional requirements
- Identification of optimal valve lift profiles to maximize fuel economy
- Identification of required mechanism analysis tools
- Selection of the candidate VVA system

Results

Significant focus for FY 2006 was placed on the establishment of an evaluation matrix of the current state-of-the-art of VVA technologies and systems that may be applicable to AMDC technology. During this year Delphi completed the engine evaluation matrix and selected the diesel engine to be used for Phase 1 and Phase 2 of the project. After evaluating more than 25 engines based upon the criteria developed by the design team, the engine was selected.

As part of the research effort during FY 2006, significant literature studies were completed in order to determine preliminary requirements required for engine selection. More than 100 research papers were studied and summarized to verify that the approach is viable.

The Delphi literature study indicates three potential valve motion solutions which include: variable lift, variable duration at fixed lift, and a combination of variable lift and duration as indicated in Figure 1.

	Intake	Exhaust	
I	Cont. VVA, w/o Phaser	Conventional valve train	System complexity
II	Cont. VVA, w/ Phaser	Conventional valve train	
III	Cont. VVA, w/o Phaser	2-step VVA, w/ Phaser	
IV	Cont. VVA, w/ Phaser	2-step VVA, w/ Phaser	
V	Cont. VVA, w/o Phaser	Cont. VVA, w/o Phaser	
VI	Cont. VVA, w/o Phaser	Cont. VVA, w/ Phaser	
VII	Cont. VVA, w/ Phaser	Cont. VVA, w/ Phaser	

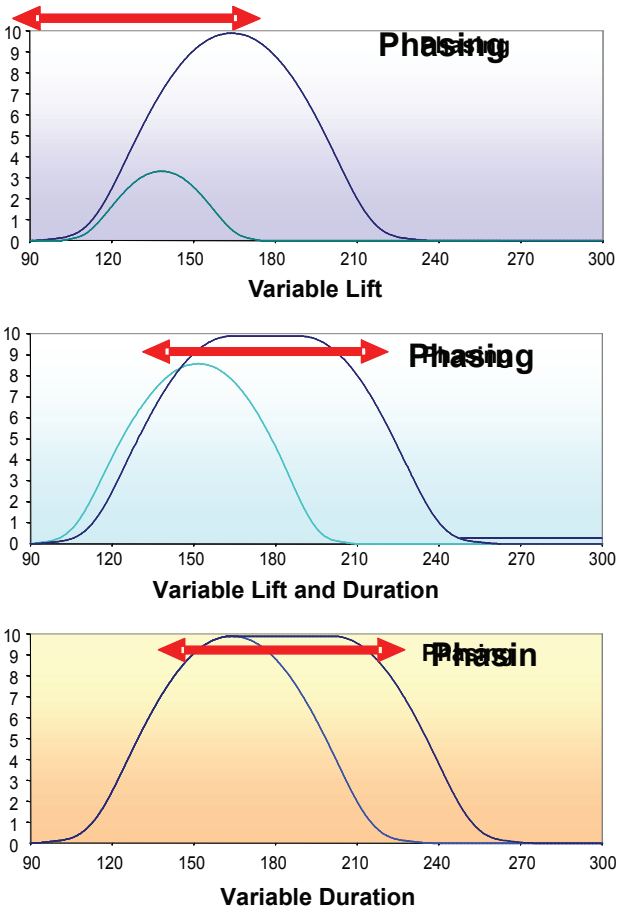


FIGURE 1. Potential Valve Motion Solutions

Lift profiles specific to the engine have been determined by Delphi and the OEM based upon significant dynamometer testing. These profiles are being used to develop the variable valve mechanism.

The engine selection matrix was populated and the candidate engine selected based upon an internal weighting system. Certain factors such as valve train type and availability of controller software were considered critical to the success of the project and thus were valued highly. Valve trains were classified into five main types as shown in Figure 2. Type 2 and Type 3 valve trains are preferred due to flexibility and ease in packaging.

More than 25 engines were evaluated based upon the specific criteria developed for the VVA project. During this period three separate meetings were held with the selected OEM to determine system specifications and verify the applicability of the Delphi mechanism to the OEM engine application. The OEM supplied desired lift profiles determined from more than two years of engine dynamometer testing. This data has enabled Delphi to quickly develop an actuation system that meets the requirements of this project.

The VVA mechanism is part of a programmable valve train system for an internal combustion engine. Control of the VVA will be from a powertrain control module (PCM) through the actuator, via the VVA control shaft. The actuator will be controlled by a pulse width modulated (PWM) drive signal in response to a positional command. A throttle position sensor (TPS) style potentiometer shall be mounted on one end of the control shaft. The sensor will be used for feedback to the closed loop PID-type positional control software in the PCM.

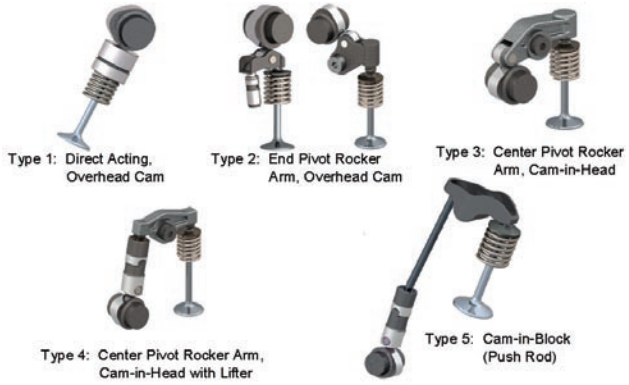


FIGURE 2. Valve Train Types

Conclusions and Future Directions

- Phase I VVA objectives have been met.
- Evaluate new dual cam designs that will address all engine performance requirements.
- Develop detailed packaging designs on the engine that address injector interference, cylinder head height and width, cradle bearing cap penetration into the cylinder head and other packaging issues.
- Complete baseline valve train kinematic/dynamic analysis for both intake and exhaust valve train.
- Set up cylinder head model.
- Build VVA hardware.
- Demonstrate and document VVA mechanism.

Special Recognitions & Awards/Patents Issued

Provisional patents submitted:

1. System for Continuously Varying Engine Valve Duration
2. Continuously Variable Valve Actuation System

II.C.2 Low-Cost Fast-Response Actuator for Variable Compression Ratio Engines

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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 control system.
- Installation of existing VCR engine in mule vehicle.
- Test the VCR actuator system in a mule vehicle & 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 is currently being built for bench testing the hydraulic actuator system.

Future Directions

- Optimize the actuator control system.
- Installation of existing VCR engine in mule vehicle.
- Test the VCR actuator system in a mule vehicle & demonstrate low-cost, fast-response and mass production practicality.

Introduction

Several VCR mechanism concepts have been advanced since U.S. Patent Number 5,819,702 was issued to Charles Mendler in 1998 and SAAB disclosed its VCR engine [1,2,3,4,5,6,7,8]. Since then research conducted by the U.S. Department of Energy, the European Commission – Research, automobile manufacturers, and engine engineering firms have found that fuel economy can be improved by about 30% with VCR, boosting and engine down-sizing [3,4,9,10]. Analysis conducted by Envera in 2004 indicates VCR can provide fuel economy gains larger than 30% through optimized conventional combustion and/or homogeneous charge compression ignition (HCCI). GM and others estimate that HCCI combustion offers the potential for improving gasoline fuel economy by about 25% [11]. Down-sizing and HCCI technologies can be combined for very significant gains in fuel economy.

With respect to large trucks, future 2010 on-highway and 2014 Tier 4b regulations mandate ultra-low NOx and PM emissions. VCR technology enables improved control and performance of HCCI combustion diesel engines. VCR HCCI engines hold potential for significantly reducing emissions and improving efficiency from these diesel engines.

The first high-performance Envera VCR mechanism was built for the former Partnership for a New Generation of Vehicles (PNGV) program. The engine attained efficiency goals and continues to be used for research at Oak Ridge National Laboratory (ORNL). The engine is now going into its 6th year of service, a testament to the engines robustness and durability.

A peak engine efficiency of 35% was required for attaining the 80 mile per gallon PNGV fuel economy target. The ability to attain peak engine efficiency over 38% in a production VCR engine was demonstrated by Envera in November 2002 [12].

Equally significant, computer modeling conducted in 2004 by Envera for DOE/ORNL showed high efficiency for the gasoline VCR engine at light power levels [13]. High efficiency at light power levels is required for attaining high fuel economy because vehicles are operated at these light power levels most of the time. The computer modeling indicated that the gasoline VCR engine with conventional spark-ignition (SI) combustion can attain an efficiency of 25.6% at 2 bar bmep and 2,000 rpm. Recent analysis by Envera

indicates an efficiency of 28.3% may be attainable for the SI gasoline VCR engine at 2 bar bmep and 2,000 rpm. For comparison, DOE reported in May 2006 a compression ignition direct injection (CIDI) engine efficiency of 27% at 2 bar bmep and 1,500 rpm [14]. The production Mercedes A170 common-rail CIDI turbo-Diesel attains a fuel efficiency of about 24.1% at 2 bar bmep and 2,000 rpm.

The data indicates that spark ignition (SI) gasoline VCR engines can attain about the same light-load efficiency as CIDI Diesel engines of equal displacement. This high-efficiency SI VCR combustion technology can be combined with down-sizing for very significant gains in fuel economy. These SI engines can also be operated on alternative fuels such as ethanol and butanol derived from switch grass, and can attain low tail-pipe emission levels using proven catalytic converter technology.

It is quite possible that VCR could also raise the efficiency of the CIDI engine. Envera built a VCR Mercedes A170 for ORNL and successfully tested the engine in 2006. It is anticipated that ORNL will use the engine for research in the areas of HCCI combustion; conventional combustion efficiency optimization, and alternative fuels. CIDI engines can be down-sized, but to a smaller degree than gasoline engines because they have a lower maximum engine speed and require higher air flow to minimize emissions.

Several VCR mechanisms have now been proposed and prototyped with U.S. and European Government funding in addition to funding from automotive and diesel manufacturers and engine research firms. The Envera VCR mechanism remains a leading production candidate. The latest generation Envera VCR mechanisms is about 75% lighter than first generation PNGV hardware, can be packaged inside the oil pan of existing engine blocks, and has robust valve chain and power take-off systems.

The current DOE/NETL/Envera effort is directed towards reducing 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 super 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.

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 NETL program 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:

2,000 rpm	4 bar bmep	Low CR
2,000 rpm	4 bar bmep	Mid CR
2,000 rpm	12 bar bmep	Mid CR
6,000 rpm	4 bar bmep	Mid CR
6,000 rpm	12 bar bmep	Mid CR

Results

The 2,000 rpm, 12 bar bmep condition causes the highest loading on the hydraulic system. Figure 1 shows a maximum hydraulic pressure inside the hydraulic cylinder of about 2,250 psi. At higher engine speeds the loads are reversing and peak loads smaller due to the inertial effects of the piston.

As can be seen in Figure 1, the hydraulic cylinder pressure is under 400 psi for 2/3^{rds} of the crank angle rotation.

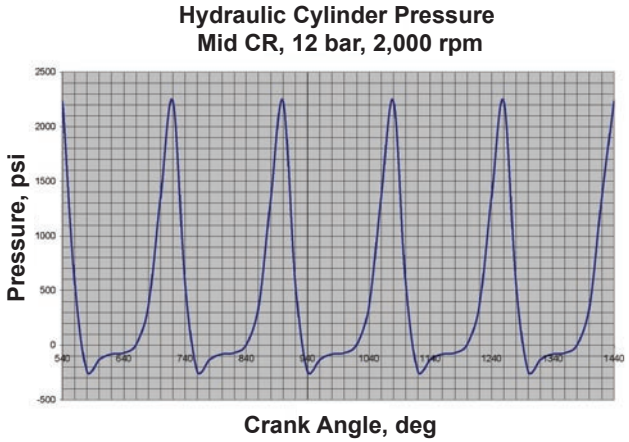


FIGURE 1. Base case hydraulic cylinder pressure vs. crank angle at mid compression ratio. Peak hydraulic cylinder pressure is approximately 2,250 psi.

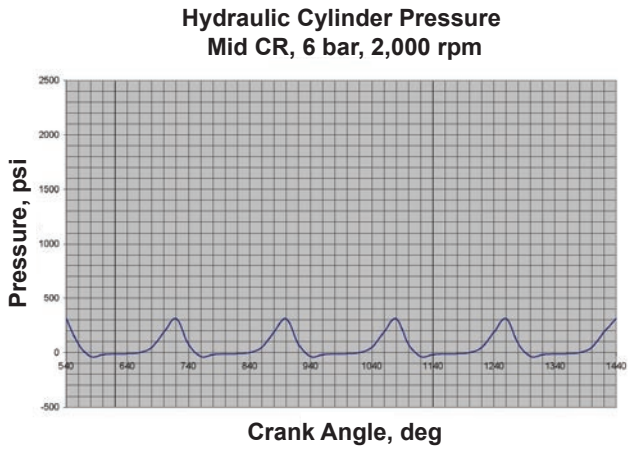


FIGURE 2. Optimized system hydraulic cylinder pressure vs. crank angle at mid compression ratio. Peak hydraulic cylinder pressure is approximately 314 psi.

The analysis showed a peak hydraulic pressure larger than desirable, but the lower range pressures generally reasonable. 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. Figure 2 shows the estimated hydraulic cylinder pressure of the newly optimized hydraulic system.

A test rig was designed for evaluating actuator system response under load. The system is currently being assembled. Testing will take place at the end of the current project's Phase I.

Conclusion

- 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.
- Down-sized gasoline VCR engines having optimized combustion can provide very large fuel economy benefits, and attain low tail-pipe emission levels using proven catalytic converter technology. The SI VCR engine can be operated on alternative fuels such as ethanol and butanol derived from switch grass.

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III. HEAVY TRUCK ENGINE

III.1 Heavy-Duty Truck Engine Program

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Objectives

- Program Phase I goal - demonstrate 45% brake thermal efficiency from a heavy-duty diesel engine capable of meeting 2002 U.S. Environmental Protection Agency (EPA) legislated emissions requirements.
- Program Phase IIA goal - demonstrate 45% brake thermal efficiency from a heavy-duty diesel engine capable of meeting 2007 U.S. EPA legislated emissions requirements.
- Program Phase IIB goal - demonstrate 50% brake thermal efficiency from a heavy-duty diesel engine capable of meeting 2010 U.S. EPA legislated emissions requirements.

Accomplishments

- Phase I goal successfully completed. Demonstrated 45% brake thermal efficiency from a heavy-duty diesel engine (Cummins' ISX) while meeting 2002 U.S. EPA legislated emissions requirements in Q2 of 2002.
- Phase IIA goal successfully completed. Demonstrated 45% brake thermal efficiency from a heavy-duty diesel engine (Cummins' ISX) while meeting 2007 U.S. EPA legislated emissions requirements in Q2 of 2004.
- Phase IIB goal successfully completed. Demonstrated 50% brake thermal efficiency from a heavy-duty diesel engine (Cummins' ISX) while meeting 2010 U.S. EPA legislated emissions requirements in Q2 of 2006.

Future Directions

The Heavy-Duty Truck Engine Program at Cummins Inc. concluded at the end of FY 2006. The program fostered significant technological development of heavy-duty diesel engines and associated aftertreatment systems while maintaining a high level of fuel efficiency. This work will continue under new programs in pursuit of greater efficiency with further emissions benefits. Most notably:

- Continue the pursuit of combustion optimization towards efficient, low emission performance under the High Efficiency Clean Combustion Program.
- Pursue utilization of waste heat energy to benefit efficiency through the Exhaust Energy Recovery Program.

Introduction

The Heavy-Duty Truck Engine Program at Cummins Inc. was initiated in 2000. The Program's main goal was to drive heavy-duty diesel engine technology toward greater efficiency in the face of significant emissions reduction requirements. At the program's outset, emissions of nitrous oxides (NOx) were federally mandated to be no more than 6 gm per bhp-hr (brake specific NOx or BSNOx) and emission of dry particulate matter was limited to no more than 1 gm per bhp-hr (brake specific dry particulate matter or BSDPM). Typical engine efficiency at the program outset was approximately 44%. The Program's final demonstration goal set an emissions limit of 0.2 gm BSNOx and 0.1 gm BSDPM (2010 U.S. EPA legislated emissions) while achieving 50% efficiency from the engine system. This final program demonstration goal represented a 97% reduction in BSNOx emissions and a 90% reduction in BSDPM emissions while simultaneously demonstrating engine efficiency improvement by 14%.

During the program, the architecture of the Cummins ISX heavy-duty diesel engine was extensively revised. Most notably, high pressure, cooled exhaust gas recirculation (EGR) was introduced as a means to reduce BSNOx emissions. This technology was proven and successfully put into production where it has realized simultaneous benefits in efficiency and emission reduction. Particulate filtration aftertreatment technology was developed and is planned for production to meet 2007 emissions regulations. Fuel injection technology was advanced during the Program with high pressure, common rail fuel systems being successfully applied to achieve program demonstrations. Variable valvetrain (VVT) technology was examined for its benefits to efficient combustion and aftertreatment thermal management. Waste heat recovery methods

were explored and successfully applied to achieve the Program's high efficiency demonstration.

Approach

Cummins' approach to the Program objectives emphasized analysis-led-design in nearly all aspects of the research. An emphasis was placed on modeling and simulation results to lead the way into feasible solutions.

For the deliverable in each phase, a configuration matrix study was conducted to determine appropriate, feasible solutions. Engine system solutions included air handling schemes, control system approaches, and aftertreatment system combinations. Based on extensive model/simulation data, previous testing experience, or verifiable supplier's information, a best-choice solution set of system components was selected. A variety of laboratory tests were conducted to verify performance and to tune system functions. Model predictions were verified and models were refined as necessary. Often, different portions of systems were pre-tested independently to quantify their behavior so their data could be analyzed in a model-based simulation before combined test cell testing was conducted. Concurrent to laboratory testing and tuning, a vehicle system demonstration was planned and prepared for. Once satisfactory test cell system performance was verified, vehicle demonstrations were conducted.

Data, experience, and information gained throughout the research exercise was applied wherever possible to commercial products. Cummins honed its technical skill and ability through this Program while providing satisfactory results for 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 as well as resources.

Results

During 2006, Cummins Inc. achieved the final Program goals (Phase IIB) by focusing on combustion development and waste energy recovery. Transient performance was demonstrated in compliance with 2010 emissions. The experimental Rankine cycle waste heat recovery system, designed and specified during 2005 was assembled and operated with the ISX engine to successfully demonstrate the 50% brake thermal efficiency goal.

Major Accomplishments in 2006

Demonstrated 2010 transient emissions performance from base engine architecture assuming NOx reduction aftertreatment system

Cummins Inc. investigated a number of combustion/aftertreatment system combinations to meet the 2010 on-highway emissions standards. Urea-based selective catalytic reduction (SCR) and NOx adsorber technology were considered in combination with many different base engine architectures to reach the program goals. Significant in-cylinder combustion optimization was conducted to minimize the need for aftertreatment cost and complexity. Cummins Inc. demonstrated the ability to reach the required program emissions levels under transient conditions across the engine operating map.

Demonstrated performance of an Organic Rankine Cycle (ORC) Waste Heat Recovery (WHR) system

ORC waste heat recovery system components were received during 2006 and assembled with an ISX engine capable of meeting 2010 emissions performance. The laboratory system for maximizing engine system brake thermal efficiency extracted heat energy from the engine's jacket water, compressed fresh air stream, main exhaust gas stream and EGR. The working fluid in the system was heated to boiling and superheated in this process. The temperature of the working fluid was approximately 460°F as it was passed into an expansion turbine/generator that converted the fluid's thermal energy and momentum into electricity. Generated electric power was measured in addition to the engine's brake power. Engine BSNOx emissions were assumed reduced through the application of urea-based SCR operating at 85% effectiveness. Engine BSDPM emissions were assumed reduced through the application of particulate filtration operating at 90% effectiveness.

The assembled system was designed to achieve peak operating efficiency at a torque peak operating condition for the base engine. This operating point afforded the Rankine cycle with the highest temperature waste heat available. At this condition the following operation was recorded:

Engine Load	378 hp
Engine Speed	1200 rpm
Engine Fuel Consumption	121 lbm/hr
Rankine Cycle Recovered Power	42.5 kWe (57 hp)
Combined Cycle Power	435 hp
Combined Cycle Brake Thermal Efficiency	50%

Conclusions

During FY 2006, Cummins successfully demonstrated systems against the Phase IIB goal. This was the last phase of the Program. We may conclude from this final program demonstration that:

- Compliance to 2010 U.S. EPA legislated emissions under transient cycle operation is feasible with the ISX engine using advanced combustion techniques
- A high level of base engine efficiency is possible and may be driven even higher through the application of a Rankine cycle WHR system

The Heavy-Duty Truck Engine Program at Cummins Inc. fostered the successful development of significantly advanced technology for heavy-duty diesel engines. A high level of fuel efficiency has been maintained while achieving dramatic reductions in engine emissions. These results will in many cases be carried forward to benefit the end-user and the environment. The work was the result of a great many talented individuals who were supported through the program by the Cooperative Agreement. Cummins Inc. looks forward to a continued successful relationship with the Department of Energy in new, efficiency-focused development programs.

FY 2006 Publications/Presentations

1. 'Achieving High Efficiency at 2010 Emissions' – 2006 Diesel Engine Emissions Reduction (DEER) Conference, Christopher R. Nelson.

III.2 Heavy Truck Engine Project (Heavy Truck Clean Diesel, HTCD)

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Objectives

- Demonstrate the technologies required to improve fuel efficiency and comply with the 2007 & 2010 (0.2 g/bhp-hr NOx, 0.01 g/bhp-hr PM) on-highway emission standards for heavy duty trucks.
- Thermal efficiency improvement from a baseline of 43% to 50% is targeted.

Accomplishments

- A diesel engine system capable of 50% thermal efficiency while meeting 2010 on-highway truck emissions levels was identified using simulation. The simulation work was conducted using Caterpillar's in-house cycle simulation code. The resulting system includes the following high efficiency components that are currently being developed under the HTCD project:
  - High efficiency aftertreatment
  - Reduced friction piston rings
  - Reduced flow restrictions
  - Reduced heat rejection components
  - High efficiency air systems
  - Turbo-compound system
  - Compact high efficiency cooling system
  - Optimized combustion system
    - A high pressure injection system
    - Variable intake valve actuation
    - Increased cylinder pressure limits
    - Increased compression ratio
- A demonstration engine capable of reaching high efficiency while meeting the 2010 on-highway truck emission regulations was built and tested. To date, the engine has been built with all the high efficiency components listed above except for the reduced heat rejection components and without one of the three high efficiency air system components. The test results for the engine showed the engine reached a peak efficiency of 47.5%. At the 2010 emissions levels, the efficiency achieved was 47%. This represents an improvement of 10-12% over the baseline engine.

Future Directions

This cooperative research project will conclude at the end of 2006. The Caterpillar team will utilize best-in-class design practices, advanced modeling techniques, single-cylinder engine testing and multi-cylinder engine testing to advance the technology to build on the major advances made in FY 2006. The focus going forward will be on transfer of the technology developed in the project to production. Technology development continues in the following key areas:

- Caterpillar will continue to focus on developing supporting engine systems to facilitate full-load homogeneous charge compression ignition (HCCI) on a multiple-cylinder engines. Fuel efficiency, cost and manufacturability will also be areas of focus. As noted above, this work has been shifted to the high efficiency clean combustion (HECC) cooperative research project
- Caterpillar will continue to focus on efficient NOx aftertreatment. The team will also focus on fuel efficiency, packaging and cost. Additional DOE funding would be valuable in developing highly efficient aftertreatment which allows the engine to be optimally calibrated.
- Caterpillar will continue to focus on the waste heat recovery. This work will continue on the EWHR (exhaust waste heat recovery) cooperative research project. The focus will continue to be on improving the thermal efficiency by 10% through improved waste heat recovery.
- Caterpillar will continue to focus on thermal efficiency improvements. This work will be shifted to the HECC cooperative research project. The focus will be on identification of a path to reach 55% overall thermal efficiency.

Introduction

Increasingly stringent air quality standards have driven the need for cleaner internal combustion engines. Many emissions reduction technologies adversely affect fuel consumption (and subsequently U.S. dependence on foreign oil). This project seeks to find technology paths and fuel economy building blocks, which allow a more favorable trade-off between fuel economy and emissions. This favorable trade-off will decrease the fuel used and the associated foreign oil dependency, reduce owning and operating costs, and still allow compliance with the more stringent emissions regulation. This heavy truck engine cooperative research agreement provides the framework to research, develop and demonstrate methods to provide better fuel economy.

Approach

The development team is utilizing a multi-discipline approach to address these complex technical challenges. The development team has a unique mix of technical experts from the fields of controls, combustion fundamentals, aftertreatment, engine design, engine development, and manufacturing. The team is concurrently improving analytical tools to model and better understand the fundamentals of combustion and aftertreatment while delivering novel hardware to the test stand to validate the models, improve our understanding, and advance the technology. The unique team with over 70 years of experience delivering successful compression ignition engine technology to the marketplace is utilizing best in class design practices, advanced combustion, aftertreatment and engine system modeling techniques, rapid control strategy development tools, single-cylinder engine testing, and multi-cylinder engine testing. In the initial stages of the project, the approach is to focus on many higher risk technology developments. As additional information and knowledge is gained on the technologies, work then shifts to final development of chosen concepts and then finally to technology demonstrations. This will lead in turn into Caterpillar's New Product Introduction projects.

This project focuses on developing multiple paths for meeting 2007 and 2010 emissions while striving for 50% thermal efficiency. The procedure used is to conduct research on multiple paths and to develop multiple fuel economy building blocks to enable a down-select to the most promising system for future production engines.

- Multiple emissions paths are being considered for meeting the 2010 emission requirements. HCCI systems and NOx aftertreatment systems are being explored to accomplish the 2010 emission requirements. The HCCI portion of this project is under continued development in the HECC cooperative research agreement.
- Aftertreatment is being developed and evaluated to meet 2010 emission requirements. Technology areas that are being explored are aftertreatment system modeling, PM aftertreatment, and NOx Aftertreatment. Membrane technology was evaluated earlier in this project.
- Thermal efficiency improvements are being developed including novel approaches in the areas of reduced engine friction, improving airflow through the engine, improving brake specific fuel consumption/emissions trade-offs through developing advanced fuel systems and combustion system optimization.

Results

As stated above, Caterpillar has made significant progress in developing fuel-efficient solutions that will support the emissions standards. Figure 1 shows a schematic for the 50% overall thermal efficiency system capable of 2010 on-highway emissions levels. The system incorporates high efficiency aftertreatment to allow optimal calibration of the engine. The system also includes reduced friction from the pistons, rings, and liners. The system also reduces pumping losses through the use of a better breathing head and improved manifolds. The system also includes air system improvements to the series turbochargers and a turbocompound unit. There is an intercooler added between the compression stages. Finally, an optimization of the combustion system was performed including compression ratio, peak cylinder pressure, and valve timings. Figure 2 shows the contributions of the building blocks to reach 50% overall thermal efficiency.

The system was built and tested in 2006. The system was designed to be packaged in a Class 8 truck as seen in Figure 3. The results to date show the ability to

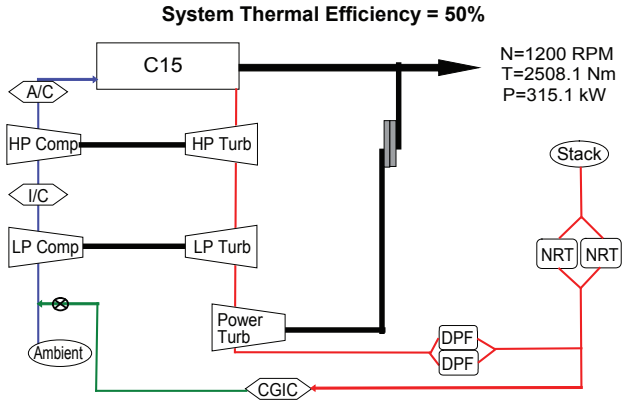


FIGURE 1. Schematic of 50% Thermal Efficiency Engine System

achieve a peak efficiency of 47.5%. The system achieved 47% overall thermal efficiency at 2010 on-highway emissions levels.

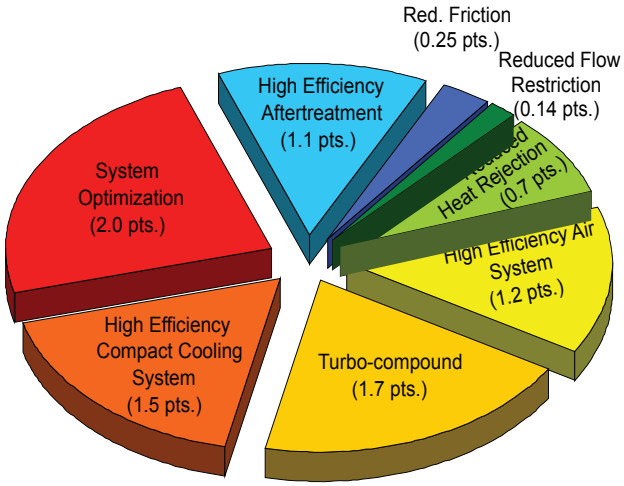


FIGURE 2. Contribution of 50% Thermal Efficiency Building Blocks

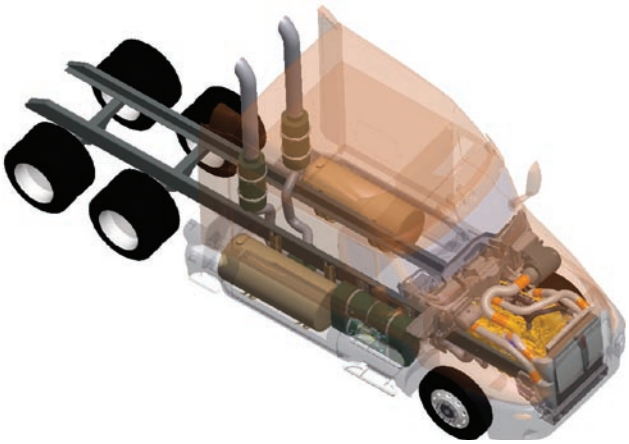


FIGURE 3. Design for 50% Engine Within Existing Class 8 Chassis

Conclusions

Through this project, Caterpillar has developed technology building blocks and integrated them into a system that will improve fuel economy from baseline production engines while meeting more stringent emissions regulations. Caterpillar has aggressively developed multiple technology paths for efficiently meeting the challenges of 2010 on-highway engine emission levels. The HCCI development reported in previous annual reports has resulted in world-class power density and significant technical progress against each of the key technical challenges. The progress has clearly positioned this advanced combustion technology as a potentially viable approach to meeting the future regulatory and commercial requirements of the marketplace. The development on NOx aftertreatment concepts has shown the potential of this technology to help meet the 2010 challenges. The fuel economy building blocks demonstrated as part of this project have resulted in world class efficiency levels at the 2010 on-highway emissions levels. In summary, the technologies developed in this DOE/Caterpillar cooperative research agreement have the potential to significantly reduce the nation's dependence on foreign oil and improve the trade balance.

FY 2006 Presentations

1. Milam, D., Donaldson, G., Easley, W., Bond, M., Roozenboom S., Brucker, J., Hittle, C., and Coon, N., "Demonstration of a 50% Thermal Efficient Diesel Engine - Including HTCD Program Overview," DOE DEER Conference, Detroit, MI, Aug. 2006.

III.3 Heavy-Duty Engine Technology for High Thermal Efficiency at EPA 2010 Emissions Regulations

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Objectives

- Develop, implement and validate an integrated experimental and analytical roadmap in support of the Phase 2B thermal efficiency and emissions goals of the collaborative Department of Energy (DOE)-Detroit Diesel NZ-50 (Near-Zero Emissions at 50% Thermal Efficiency) heavy-truck project.
- Demonstrate advanced engine component, sub-system and system technologies, feasible for subsequent product development and eventual commercialization, which are capable of achieving a brake thermal efficiency of 50% at Environmental Protection Agency (EPA) 2010 emissions regulations.
- Demonstrate the effectiveness of NZ-50 technologies to meet the stretch project goal of 7%-10% over-the-road fuel economy improvement, over and above the already aggressive project objective of 50% thermal efficiency at a single operating condition.
- Demonstrate the effectiveness of NZ-50 technologies to meet the stretch project goal of EPA 2010 emissions over transients (e.g. the Federal Test Procedure cycle, FTP), over and above the project objective of EPA 2010 emissions at a single operating condition.

Accomplishments

- Demonstrated integrated experimental and analytical technologies capable of achieving 50.2% thermal efficiency at EPA 2010 emissions regulation at a single operating condition in a multi-cylinder engine configuration, thus meeting a key FY 2006 and overall NZ-50 project objective.
- Experimentally demonstrated a brake thermal efficiency of 48.4% at EPA 2010 emissions regulations level at a single operating condition in a multi-cylinder engine test-bed environment. An additional 1.8%-point thermal efficiency improvement was demonstrated via analytical evaluation of potential engine system enhancements including reduced pumping losses, adaptive breathing cycles and reduced parasitic losses.
- Experimentally demonstrated greater than 45% thermal efficiency at several over-the-road representative operating conditions, thus demonstrating the potential to achieve 8.2% improvement in over-the-road vehicle fuel economy for a Class 8 heavy-duty tractor equipped with NZ-50 Phase 2B engine technologies (stretch project goal).
- Developed and experimentally demonstrated a multiple-mode, low emissions combustion concept to reduce engine-out emissions below EPA 2007 regulated levels over both steady-state and transient operation, while substantially mitigating the deterioration in brake fuel consumption typically associated with such advanced combustion processes.
- Experimentally demonstrated EPA 2010 emissions over steady-state and transient operation (FTP and over-the-road), enabled by the multiple-mode, low emissions combustion concept (stretch project goal).
- Developed and enhanced forward engineering methodologies for engine system technology development, enabled by advanced analytical tools. Utilized this technology development approach to develop and validate the NZ-50 technical roadmap.
- Developed model-based control algorithms for advanced combustion and integrated engine-aftertreatment system control to enable optimal 2010 and post-2010 system performance over transient over-the-road operation.
- Identified and partially mitigated the challenges and risk factors associated with application and viability of some of the NZ-50 sub-system enhancements and advanced technologies necessary to realize the emissions and thermal efficiency gains.

Future Directions

- Successfully wrap up the remaining technical activities of the current budget period, including the consolidation and refinement of the demonstrated

thermal efficiency milestone and the development of the integrated controls system. A technical report to document the salient aspects of the project through Phase 2B is also being prepared.

- Identify elements of a conceptual roadmap to achieve further improvement in thermal efficiency, with emphasis on over-the-road fuel economy.
- Utilizing the results of this system-based NZ-50 project, identify the foundation for the next generation of sub-system technology concepts (e.g. combustion and exhaust energy recovery) for further improvement in thermal efficiency.

Introduction

During the second half of last century, the brake thermal efficiency of heavy-duty diesel engines increased substantially, enabled by improvements in sub-system technologies and the introduction of electronic controls. Since the beginning of this decade, the regulations that mandate allowable nitric oxides and particulate matter emissions from diesel engines have also become increasingly stringent. Without external influences, such as collaborative government-industry programs, the increasingly stringent emissions regulations would have resulted in significant deterioration in thermal efficiency (Figure 1). This can be attributed to the increase in complexity of diesel engine and aftertreatment technology and yet extremely short technology introduction lifecycles of about three years. Collaborative government and industry programs have played a significant role in mitigating this anticipated thermal efficiency deterioration and are having a net favorable impact on commercial technology by allowing the development of higher risk but potentially higher reward technologies. Such programs are conducted at an advanced engineering level and substantial time and effort is still required through subsequent, industry-led product development cycles for eventual commercialization. Nevertheless, these programs lay a strong technical foundation for such a product development phase to be undertaken.

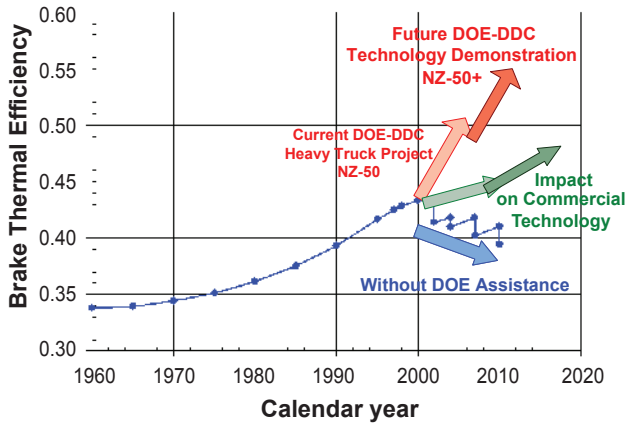


FIGURE 1. Heavy-Duty Thermal Efficiency Trend

An example of such a collaborative effort is the DOE-Detroit Diesel NZ-50 project, a multi-year effort initiated in CY 2000 with a key objective of demonstrating 50% thermal efficiency at EPA 2010 emissions regulations at a single operation condition. This primary objective was successfully met during FY 2006. In addition, the thermal efficiency benefit obtained at a single operating condition was extended to several representative over-the-road operating conditions thus demonstrating over 8% increase in fuel economy with NZ-50 technologies. Also, tailpipe-out emissions compliant with EPA 2010 regulations have been demonstrated over steady-state and transient operation (FTP and over-the-road), enabled by a multiple-mode, low emissions combustion concept developed as part of the NZ-50 project.

Approach

The technological complexity of today's state-of-the-art and the future diesel powertrain requires a system-based development approach. This system-based development approach inherently requires an integrated experimental and analytical technology development methodology. During the last few years, Detroit Diesel has developed and validated such an integrated technology development methodology. Analytical tools, ranging from 0-D for controls development, 1-D for system optimization and 3-D for detailed component development, are an integral part of this approach. Such tools are typically utilized to develop and evaluate technical concepts, while deriving their boundary conditions from "real-world" vehicle and system operating conditions thus increasing the possible opportunities for eventual commercial viability. The analytical results are complemented by sub-component and component testing in a bench and/or fixture test-bed environment. Promising concepts are down-selected and then integrated in steady-state test-beds that validate the results of the analysis and "simulate" operation of a transient test-bed. In turn, transient test-beds are utilized to validate the findings of steady-state testing and to simulate vehicle operation, thereby completing one development cycle and laying the foundation for subsequent development iterations.

Detroit Diesel's integrated experimental and analytical system-based development approach was utilized to optimize the combustion processes to meet the project objectives of thermal efficiency and emissions. A multiple-mode, low emissions combustion concept was developed and validated over steady-state and transient conditions. Enabling specifications

of the other engine sub-systems such as the fuel injection sub-system and the air/EGR sub-system were identified via analysis and pre-prototype testing of combustion concepts. Analysis was also utilized to develop and optimize the enabling sub-systems and to define the design of prototype hardware. In some cases, pre-prototype test cell hardware was combined with in-house rapid prototyping controls strategies to provide the desired flexibility in fuel injection system characteristics. The core engine system was integrated with basic NOx and particulate matter (PM) aftertreatment to enable meeting the EPA 2010 emissions regulations and to achieve the project thermal efficiency objectives. The entire system was then integrated within an overall model-based controls environment that works with multiple input and multiple output signals, while cooperatively managing the often conflicting requirements of individual sub-system via hierarchical functions.

Results

The most significant accomplishment during FY 2006 was the demonstration of technologies to achieve greater than 50% thermal efficiency at a single operating condition. A brake thermal efficiency of 48.4% was demonstrated through aggressive experimental tests and a brake thermal efficiency of 50.2% was achieved by combining hardware experiments with advanced analytical simulations. The integrated experimental and analytical approach incorporates promising pre-developed technologies that could be expected to ultimately mature into production-viable solutions, with the appropriate time and resources allocated to them. Figure 2 shows the technical roadmap of the progress in thermal efficiency and emissions during the various phases of the program.

Figure 3 illustrates the primary technical building blocks of the thermal efficiency demonstration effort, including advances in in-cylinder combustion, fuel injection system, exhaust recovery, air system and parasitic load reduction. For part of the technical demonstration effort, the peak cylinder pressure was driven to the vicinity of 250 bar by overstressing the current production engine core (block, head and bearing system) into an operating regime of major mechanical concern and very limited life expectation. Substantial advanced material and design technology insertion will be required to enable the application of the very aggressive demonstration settings in a reliable and cost-effective production setting.

One example of the technical building blocks that were evaluated during the course of the project is adaptive engine breathing technologies. A cycle simulation based analytical model was utilized to optimize intake and exhaust valve events to improve thermal efficiency by reducing pumping losses. Figure 4 shows the improvement in fuel economy over several engine operating conditions. The application of this adaptive breathing technology was also extended to assess its potential for thermal efficiency improvement and for thermal management of aftertreatment devices during transient operating conditions.

A multiple-mode, low emissions combustion concept was developed and successfully validated over several steady-state and transient conditions. Figure 5 shows the cumulative engine-out NOx and PM emissions over the transient FTP cycle for the baseline combustion process representative of prototype EPA '07 combustion versus the low emissions combustion process. The low emissions combustion process demonstrates the potential to reduce NOx by 20% without any PM trade-off. For this case, the fuel

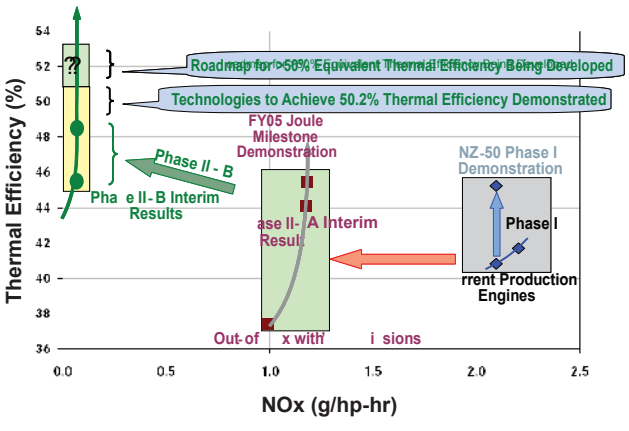


FIGURE 2. NZ-50 Thermal Efficiency Status – Integrated Experimental and Analytical Results

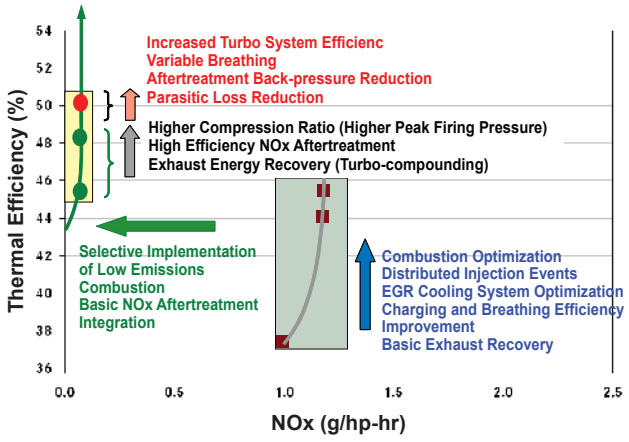


FIGURE 3. NZ-50 Thermal Efficiency Roadmap – Key Technical Building Blocks

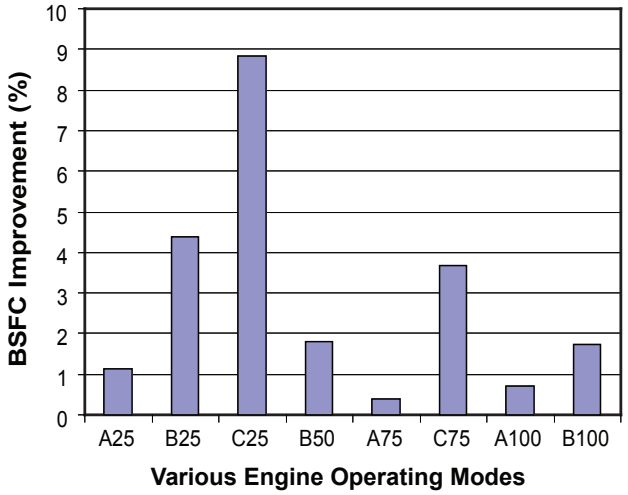


FIGURE 4. Potential of Adaptive Breathing Optimization for Thermal Efficiency Improvement

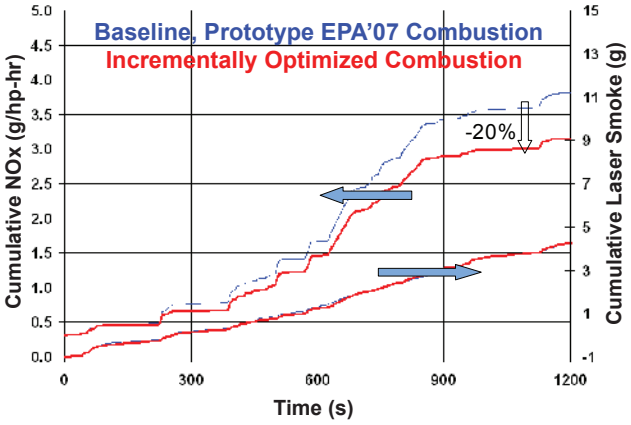


FIGURE 5. Selective Implementation of Low Emissions Combustion over Transient Hot FTP Cycle – Experimental Multi-cylinder Results

economy penalty that is typically associated with low emissions combustion processes was substantially mitigated. In another similar development effort, an advanced combustion process was developed to reduce the engine-out PM over a transient cycle by about 20% without increasing NOx.

These low emissions combustion concepts to incrementally reduce the engine-out NOx and PM emissions provided the foundation for the demonstration of EPA 2010 tailpipe-out emissions standards over the transient emissions cycle, thus fulfilling another stretch target of the project. Figure 6 shows the roadmap for the achievement of transient EPA 2010 tailpipe-out emissions through selective implementation of low emissions combustion to reduce engine-out NOx, integration of model-based controls and overall system optimization. Once again, model-based controls played

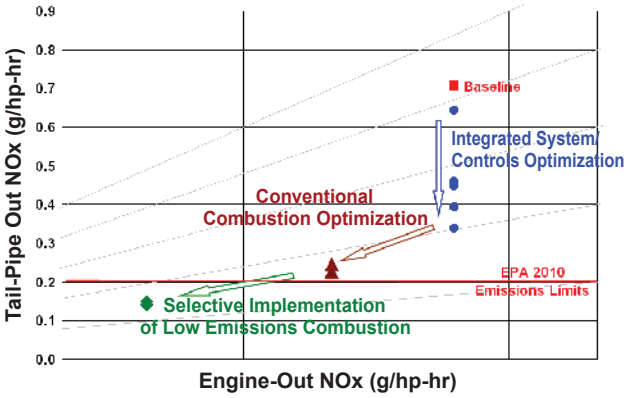


FIGURE 6. Transient Emissions Reduction Roadmap – Experimental Multi-cylinder Results

a critical role for effective integration and optimum performance of the advanced sub-systems. Emerging concepts of more pervasive model-based controls with increasing robustness and on-board optimizing functions are expected to enhance seamless transition between operating modes as well as ensuring optimum performance of the total engine and aftertreatment system.

Conclusions

- Demonstrated integrated experimental and analytical technologies capable of achieving 50.2% thermal efficiency at EPA 2010 emissions regulation at a single operating condition in a multi-cylinder engine configuration, thus meeting a key FY 2006 and overall NZ-50 project objective.
- Experimentally demonstrated a brake thermal efficiency of 48.4% at EPA 2010 emissions regulations level at a single operating condition in a multi-cylinder engine test-bed environment. An additional 1.8% thermal efficiency improvement was demonstrated via analytical evaluation of potential engine system enhancements including reduced pumping losses, adaptive breathing cycles and reduced parasitic losses.
- Experimentally demonstrated greater than 45% thermal efficiency at several over-the-road representative operating conditions, thus demonstrating the potential to achieve 8.2% improvement in over-the-road vehicle fuel economy for a Class 8 heavy-duty tractor equipped with NZ-50 Phase 2B engine technologies (stretch project goal).
- Developed and experimentally demonstrated a multiple-mode, low emissions combustion concept to reduce engine-out emissions below EPA 2007 regulated levels over both steady-state and transient operation, while substantially mitigating the

deterioration in brake fuel consumption typically associated with such advanced combustion processes.

- Experimentally demonstrated EPA 2010 emissions over steady-state and transient operation (FTP and over-the-road), enabled by the multiple-mode, low emissions combustion concept (stretch project goal).

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IV. WASTE HEAT RECOVERY

IV.1 Developing Thermoelectric Technology for Automotive Waste Heat Recovery

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- RTI International, Research Triangle Park, NC
- University of South Florida, Tampa, FL
- University of Michigan, Ann Arbor, MI
- Oak Ridge National Lab, Oak Ridge, TN

Objectives

- Develop cost-effective bulk thermoelectric materials for exhaust heat recovery.
- Develop high efficiency thin-film superlattice-based modules for radiator heat recovery.
- Complete manufacturability and cost assessment of bulk and thin-film modules.
- Validate the exhaust subsystem modeling.
- Select initial thermoelectric materials for the exhaust subsystem.

Accomplishments

- Demonstrated that the thermoelectric performance of misch-metal-filled skutterudites is comparable to that of single-rare-earth-element-filled skutterudites.
- Achieved ZT = 1.3 at 800 K in nano-composite n-type skutterudites, the highest reported ZT values for n-type skutterudites.
- Synthesized, and for the first time measured transport properties of novel antifluorite compounds.
- Achieved nearly 15 Watts electric output from large superlattice-based multi-module array with an external ΔT of 100 K.
- Established high temperature bulk material thermoelectric property measurement systems, and validated properties of many materials.
- Quantified the electric power requirements associated with the 10% fuel economy improvement target for the Federal Test Procedure city and highway cycles.
- Completed cost and manufacturability assessments for bulk and thin-film modules.
- Completed the initial exhaust waste heat recovery subsystem design and performance analysis.
- Initiated the initial radiator waste heat recovery subsystem design and performance analysis.

Future Directions

- Complete the initial radiator waste heat recovery subsystem design and performance analysis.
- Analyze subsystem cost for exhaust and radiator.
- Select thermoelectric materials for exhaust and radiator subsystems.
- Develop cost-effective thermoelectric materials and modules.

Introduction

In the past year, this project has been focused on several areas: economic feasibility of automotive thermoelectric waste heat recovery; initial thermoelectric material selections for exhaust and radiator heat recovery modules; design and performance analysis of the exhaust and radiator heat recovery subsystems; and the search for high performance and cost-effective thermoelectric materials and modules.

We have made significant progress in each of these focus areas. As part of the economic feasibility study, we have completed cost and manufacturability assessments for bulk and thin-film thermoelectric devices. The project electric power targets have been established for city and highway driving cycles. Critical vehicle level information for the two driving cycles, such as temperatures, heat flow rates, air flow rates, exhaust gas chemistries, etc., were obtained to enable the design and performance analysis of exhaust and radiator thermoelectric subsystems. A vehicle platform has been identified for the purpose of this analysis. The locations and geometric envelopes of thermoelectric subsystems have also been identified and established.

The discovery part of this project has demonstrated cost-effective skutterudite materials as potential material candidates. We have also established expertise in the area of nano-structured bulk materials, as evidenced by the development of the best n-type nano-composite skutterudites. We have synthesized and performed microscopic analysis of some novel nano-structured bulk materials. The structural data help us discern the fundamental mechanisms that determine the electron and phonon transport in these materials. Novel compositions of antifluorite compounds have been investigated for the first time by us. The preliminary data show that these materials' thermoelectric properties are tunable. One of the most interesting aspects of these materials is that they are very cost-competitive when compared with other potential materials.

As part of this project, Oak Ridge National Laboratory (ORNL) has installed and tested high temperature bulk material thermoelectric property measurement systems. Samples from various sources have been tested, compared, and validated in the past year. This continues to be a critical component of our project in terms of verifying material properties and providing material properties for subsystem design and modeling. ORNL is planning on expanding their capability into thin-film measurements next year.

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 General Electric (GE). Most of the material properties are also validated at ORNL to avoid potential pitfalls. System engineers work closely with vehicle engineers at General Motors (GM) to ensure that accurate vehicle level information is used for developing subsystem models and designs. Subsystem output is then analyzed by GM for 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

Installation of ULVAC ZEM-2 System

The ULVAC ZEM-2 (M8) system was installed at ORNL on April 13, 2006, as shown in Figure 1. The initial testing showed the system met the specs, and it was quickly used to characterize bulk thermoelectric materials in this project.

Type 1: Marlow Industries Elements

Specimens from the Marlow Industries Inc. were tested using the ULVAC system. Three types of elements, undoped, n-type and p-type, were tested, and the results are shown in Figures 2 and 3. Since the thermal power and resistivity values of these commercial elements are well known, we use them as a reference standard to calibrate/validate the high temperature results. The results are reproducible and matched the literature values very well.

Type 2: GM Skutterudite Materials

Bulk specimens from GM were tested from 50ºC to 500ºC using the ULVAC system. Four compositions of misch-metal filled skutterudites were measured. Figure 4 shows the Seebeck coefficient of the GM specimen. The material was characterized at GM using the PPMS from 0 K to 300 K. The ULVAC system carried out measurements from 300 K to 800 K. The two systems show very consistent Seebeck results, and the match at room temperature is nearly perfect.

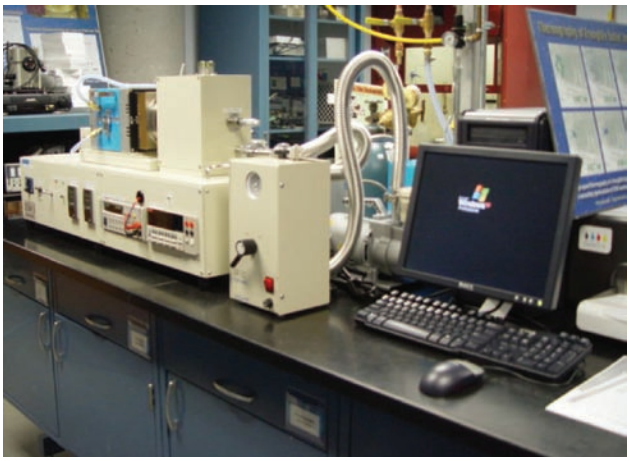


FIGURE 1. ULVAC ZEM-2 System at ORNL

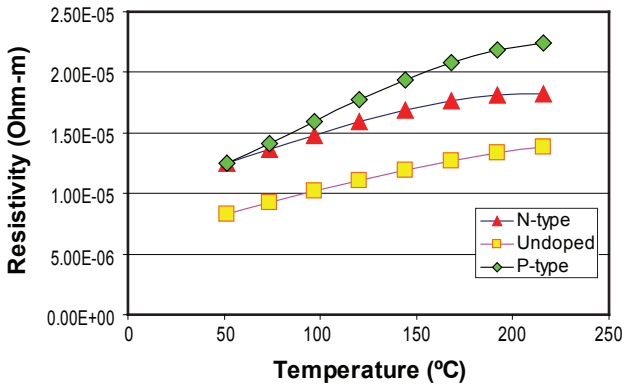


FIGURE 2. Electrical Resistivity of Marlow Elements

However, the match on electrical resistivity was not as perfect, as shown in Figure 5. A small, <5% drop was observed in the high temperature results. The specimens used in both measurements were from the same sintered rod, but cut from different locations. Considering the possible specimen-to-specimen variation in resistivity and the two completely differently measurement systems, the results are acceptably within the expected experimental error range.

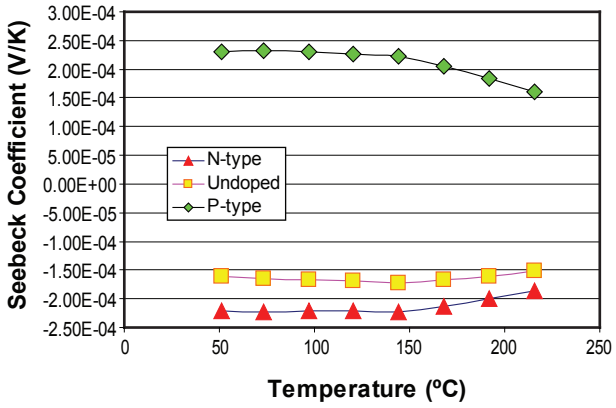


FIGURE 3. Seebeck Coefficient of Marlow Elements

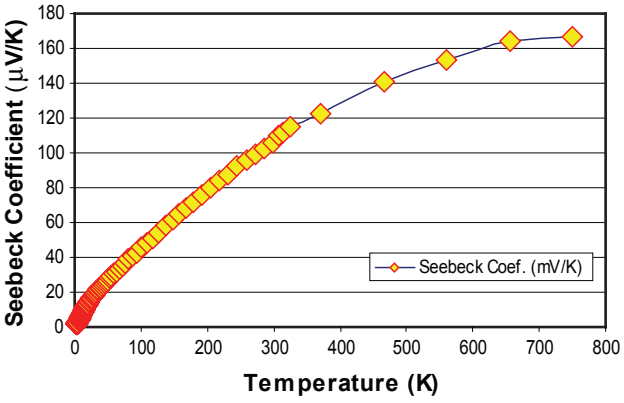


FIGURE 4. Seebeck Coefficient of GM Misch-Metal Sample

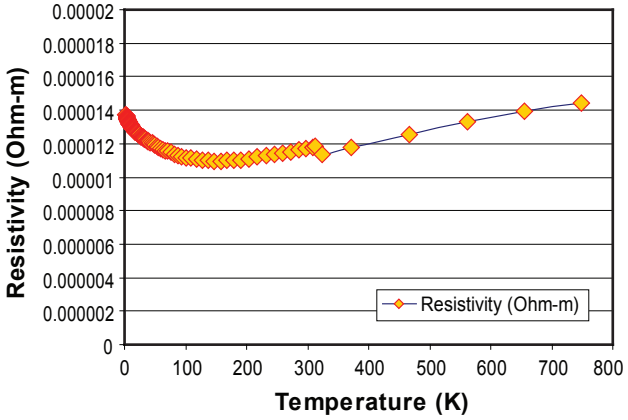


FIGURE 5. Electrical Resistivity of a GM Specimen

Type 3: Clathrates from University of South Florida

Five clathrate specimens from the University of South Florida (USF) were tested at ORNL. Figure 6 shows the electrical resistivity data obtained by the ULVAC system.

Room temperature values provided by USF and measured using the ORNL Signatone Pro4 system were also plotted. The resistivity also showed very good match among the three systems. Figure 7 shows the Seebeck results of the same specimen. The USF data matched ULVAC data nicely. Complete low temperature data available at USF also confirmed the overall match of the two systems.

Novel Clathrates

From our previous work [1] it was found that the transport properties of $Ba_8Ga_{16}Si_xGe_{30-x}$ are sensitive to the Si concentration x. Previous work under this project involved the synthesis and characterization

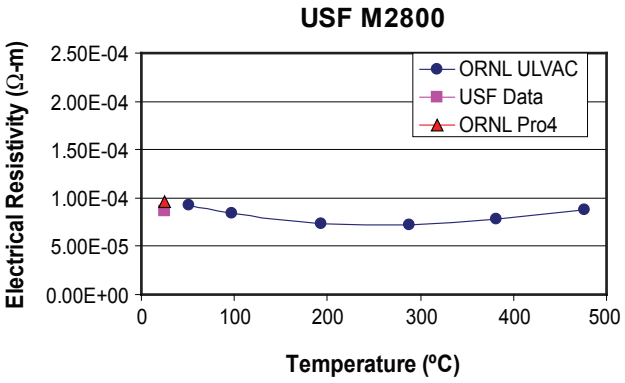


FIGURE 6. Electrical Resistivity of a University of South Florida Clathrate Specimen

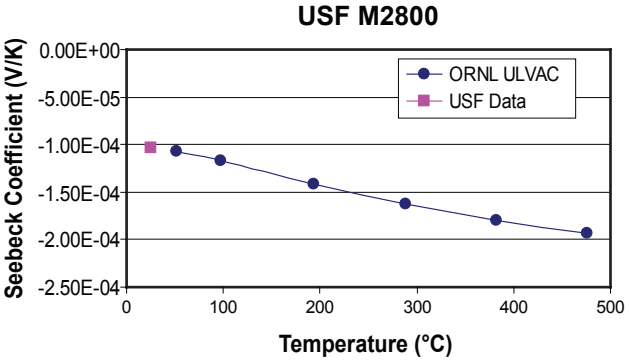


FIGURE 7. Seebeck Coefficient of a USF Clathrate Specimen

of compositions with higher Si content. The low temperature transport (12 - 300 K) was measured at USF and high temperature measurements (300 – 750 K) were conducted by Dr. Hsin Wang of the High Temperature Materials Laboratory at Oak Ridge National Laboratory. The data is shown in Figure 8. Note the excellent agreement (within experimental error) between the measurements from the different laboratories. The data also reveals that x ~ 6 may be of interest for optimization of these materials. The synthesis of more samples at x ~ 6 has begun and characterization of these specimens is currently underway.

Thin film Seebeck measurements on ceramic oxides were carried out. Initial testing suggested proper backing materials and electrical contacts are needed to establish a temperature gradient. It is expected that the ULVAC system can be used to measure Seebeck coefficient of thin films on insulating substrates. Thin film oxide materials were tested, and the results matched low temperature measurements performed at a university laboratory.

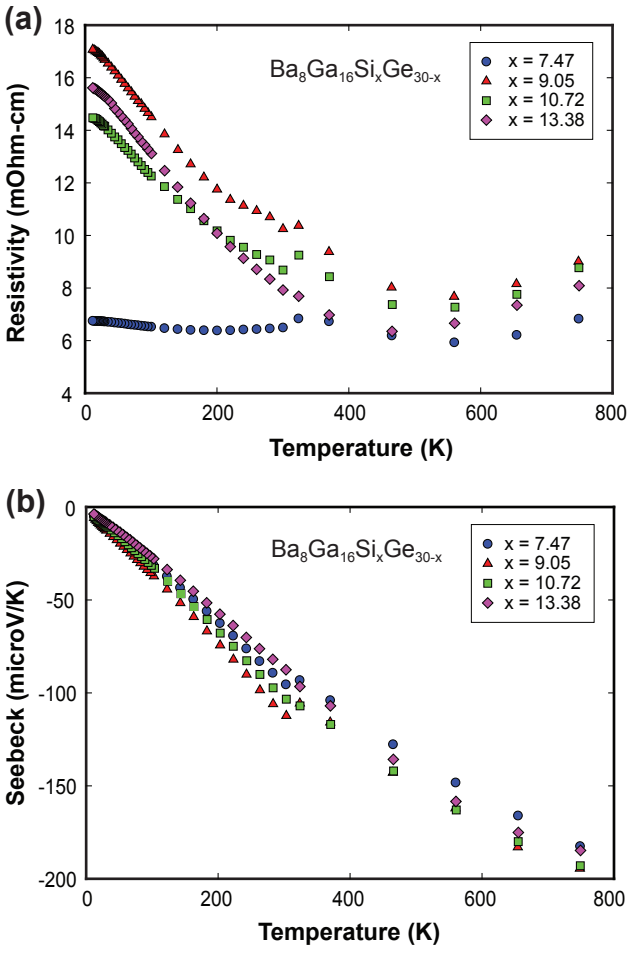


FIGURE 8. Low (<300 K) and High Temperature (>300 K) Transport Properties of $Ba_8Ga_{16}Si_xGe_{30-x}$

ORNL is in the process of acquiring the ULVAC LaserPit system. It will help to expand the measurement capability of thin film materials. In-plane thermal conductivity of many thermoelectric materials will be able to be tested at ORNL. The system is expected to arrive by the end of 2006.

Conclusions

The project has made significant progress in the areas of high efficiency cost-effective materials development, high power density thin-film superlattice-based modules, cost and manufacturability analysis for thin-film and bulk thermoelectric modules, exhaust heat recovery subsystem design and performance analysis, electric power output targets, and initial thermoelectric material selections. The next phase of our project will be focused on optimization of cost-effective bulk materials, final selection of thermoelectric materials for exhaust and radiator heat recovery devices, final design of exhaust and radiator waste heat recovery devices including estimated performance, and identification of volume capable and cost effective manufacturing processes for thermoelectric modules.

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IV.2 High-Efficiency Thermoelectric Waste Energy Recovery System for Passenger Vehicle Applications

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DOE Technology Development Manager:
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Subcontractors:
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- Visteon, Van Buren Township, MI
- Marlow Inc., Dallas, TX

Objectives

Model, design and build the key subsystem equipment to achieve fuel efficiency and emissions objectives. Key equipment includes the primary heat exchanger (PHx), thermoelectric generator module (TGM) and power control subsystem (PCS)

- Achieve 10% fuel efficiency improvement by recovery and conversion of waste heat in a passenger automotive vehicle to electric energy
- Update the system model to reflect subsystem design, build and test results
- Maintain or reduce emissions levels
- Evaluate economic viability
- Show a path to commercialization

Accomplishments

- Subsystem equipment has been modeled, designed, built and tested including:
  - Primary heat exchangers made from stainless steel that transfer exhaust gas thermal energy to the secondary loop.
  - A PCS that converts TGM output electrical power to interface with the vehicle's electrical network that has tested at >90% conversion efficiency over the range of operating conditions.
  - Twenty-watt high temperature and 750-watt low temperature thermoelectric generators have been modeled and designed and are scheduled to be built and tested by end of December 2006.
- A bumper-to-bumper vehicle performance model used to predict fuel efficiency has been developed and validated in the GT Cool model
  - Preliminary system modeling results without operating algorithm optimization showed fuel efficiency improvement ranging up to 7.7%.

Future Directions

Phase 2 activities are scheduled to conclude at the end of 2006. An acceleration plan has been proposed to the DOE to speed commercialization by improving thermoelectric element contact interfaces. The acceleration plan activities are planned to occur in Q1 2007 and include the following objectives:

- Development of improved low resistivity electrical contacts to validate weight and cost reductions needed for the target vehicle application.
- Accelerated build of a 750-watt TGM using high efficiency high temperature materials.
- Build of a table top power generator that displays real time performance, including energy conversion efficiency.

The plan accelerates the commercialization of a high temperature TGM and provides timely integration hardware early in Phase 3.

Phase 3 activities include system integration and test and are planned to begin early January 2007.

Introduction

BSST began work to develop a high efficiency thermoelectric waste energy recovery system for passenger vehicle applications in November 2004 under a cost share contract[1] awarded by the U.S. Department of Energy Freedom Car Office.

[1] Contract number DE-FC26-04NT42279

In Phase 1, the team created a system architecture, developed a system model to predict performance and established system and subsystem design requirements. Phase 2 will be completed in December, 2006 in which key subsystem components will be built and tested and the system model updated to provide a new performance prediction.

Engine exhaust gas passes through a shell and tube heat exchanger (Primary Heat Exchanger, or PHx) downstream from the catalytic converter where thermal energy is extracted and transferred to a gaseous working fluid (preliminarily designated as 75% He, 25% Xe). Wide variations in exhaust gas mass flow, which result in correspondingly wide variations in thermal flux, are managed by means of a pump which circulates the working fluid between the PHx and the TGM's hot side. The use of this working fluid loop enables optimal usage of the thermoelectric material in the TGM as well as providing a dense, minimally sized hermetic enclosure for the thermoelectric (TE) material. Heat rejection from the cold side of the TGM can be facilitated by either the vehicle's powertrain cooling system or a supplemental cold-side cooling loop. TGM electrical power is linked to the vehicle electrical bus via a load matching DC/DC converter in the Power Conditioning System (PCS). Fuel efficiency is increased by offloading the vehicle alternator by use of power generated in the TGM. The TGM is using segmented elements comprised of Skutterudites, TAGS, PbTe and BiTe.

Approach

Early in the project a key architectural decision was made to use a secondary loop to transfer exhaust gas waste heat to the thermoelectric generator (See Figure 1). The benefits of this approach include:

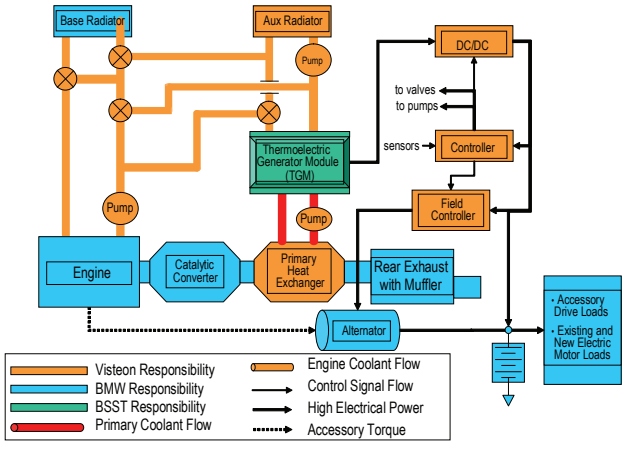


FIGURE 1. System Architecture

- Localization and hermetic packaging of thermoelectric material to mitigate potential environmental impacts
- Control of the thermal flux to the TGM through the secondary loop by means of a pump with the following important benefits:
  - Maximizing generator performance
  - Reducing thermoelectric material usage, and therefore cost

Results

The GT Cool model was integrated with the PHx, TGM and PCS models to predict system performance. The base model without the thermoelectric subsystems was validated with steady-state operating points and standard drive cycles, including FTP75 and the New European Drive Cycle (NEDC). A comparison of measured data to the simulation results for the NEDC driving cycle is shown in Figure 2.

The simulation results correspond well with the measurement results. The variations in the temperature profile have a minor influence on the power output of the TGM and are acceptable. This tool will provide accurate input parameters for the PHX/TGM subsystems from a vehicle perspective. Figure 3 shows modeling results for the TGM electrical power output.

PHX Design

Design of the PHX involved trade-offs between thermal exchange efficiency and the resulting effect on exhaust gas flow. Flow path restriction for optimization of exchange efficiency can result in exhaust back-pressures that can compromise vehicle-level fuel economy. An initial PHX prototype currently in test at Visteon is shown in Figure 4.

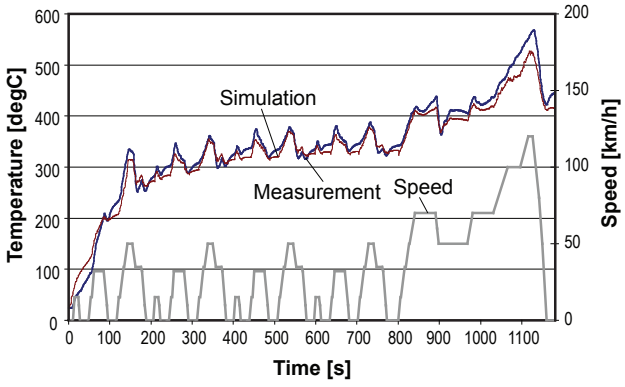


FIGURE 2. Temperature Profile of the Exhaust Gas

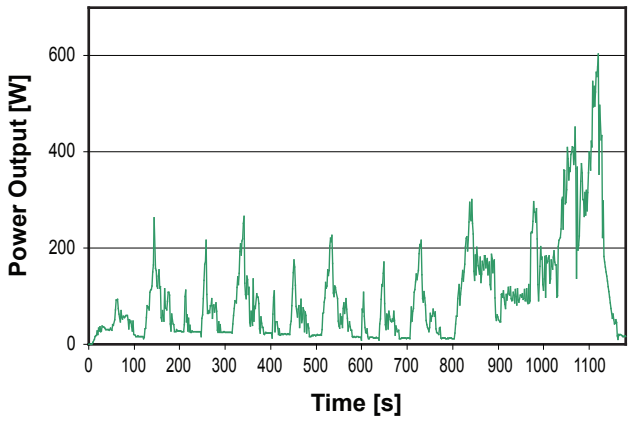


FIGURE 3. Modeling Results for TGM Electrical Power Output



FIGURE 4. Primary Heat Exchanger (PHX)

The inlet to the PHX is at lower left and includes two ports compatible with the dual pipes extending rearward from the catalytic converters. The PHX outlet section is at upper right, with a single, large port that feeds the mid-vehicle muffler.

In order to minimize direct backpressure and to maintain exhaust gas velocity for exhaust gas scavenging, the exhaust path in the tube-&-shell section is long and narrow, as opposed to being short and wide. Preliminary analyses show that, even with the use of smooth bore tubes, the PHX should be able to provide hot-side working fluid at the target temperature ranges while presenting no more than a 100 mbar incremental increase in exhaust backpressure across all operating conditions. Spiral tubes (to enhance exhaust gas contact with the interior surfaces of the tubes in the tube-&-shell heat exchanger) are an available option, should there arise a need for greater heat exchange efficiency.

Power Conditioning Subsystem

The PCS serves two functions: drawing of maximal electrical power from the TGM across a 0 V-25 V range, and conversion of TGM electrical output to supply the vehicle electrical power bus across a 12.3 V-16.5 V range. Virginia Polytechnic Institute & State University (Virginia Tech) and Visteon are developing a high-efficiency PCS for the project. The TGM acts as a Thevenin source comprised of a temperature-dependent voltage source, V_{TGM}, and source resistance, R_{TGM}. The TGM output voltage seen by the PCS is V_{in}.

A straight-forward strategy for vehicle electrical bus interaction is planned:

In conditions where the TGM/PCS cannot supply all the electrical power needed by the vehicle (e.g., cold-start), the alternator will provide electrical bus voltage regulation, under the supervision of the vehicle electrical bus controller (usually the powertrain control module, or PCM), and the PCS will act as a current source to the vehicle electrical bus. In this mode of operation, the PCS electrical output voltage floats to that established by the alternator.

In conditions where the TGM is able to supply all the electrical power needed by the vehicle, the PCS switches control modes to act as the electrical bus voltage regulator. It regulates the electrical bus voltage in a fashion that is optimal with respect to the battery at an output voltage that is slightly higher than the alternator output voltage regulation target. Under this condition, the vehicle electrical bus controller automatically and naturally shuts off the alternator as an electrical power source, thus allowing the PCS to act as the sole electrical power source for the vehicle.

The prototype Visteon PCS and test results are shown in Figure 5. Since PCS efficiencies decrease as V_{in} decreases, Visteon will implement a TGM switch network in Phase 3 that will switch the series/parallel arrangement of thermoelectric substrings in the TGM and keep V_{in} optimally high.

Thermoelectric Generator Module

A prototype device was built of six Bi_2Te_3 elements sandwiched between seven copper connectors as shown in Figure 6. Bi_2Te_3 elements were used because the tests were conducted at lower temperatures with materials that have well defined properties. These tests were conducted to better isolate problem areas in the integration of TE material into a device.

The copper connectors are placed on a liquid heat exchanger constructed from an aluminum tube. Many of the same type of liquid heat exchangers are intended to be used for the full-scale TGM device. The tube is anodized to provide electrical isolation from the copper connectors. A layer of thermal grease covers the anodized layer to help minimize thermal resistance. Two 100 W cartridge heaters provide the heat source for the device. An anodized aluminum housing encloses the heat source. Thermal grease is used as the thermal

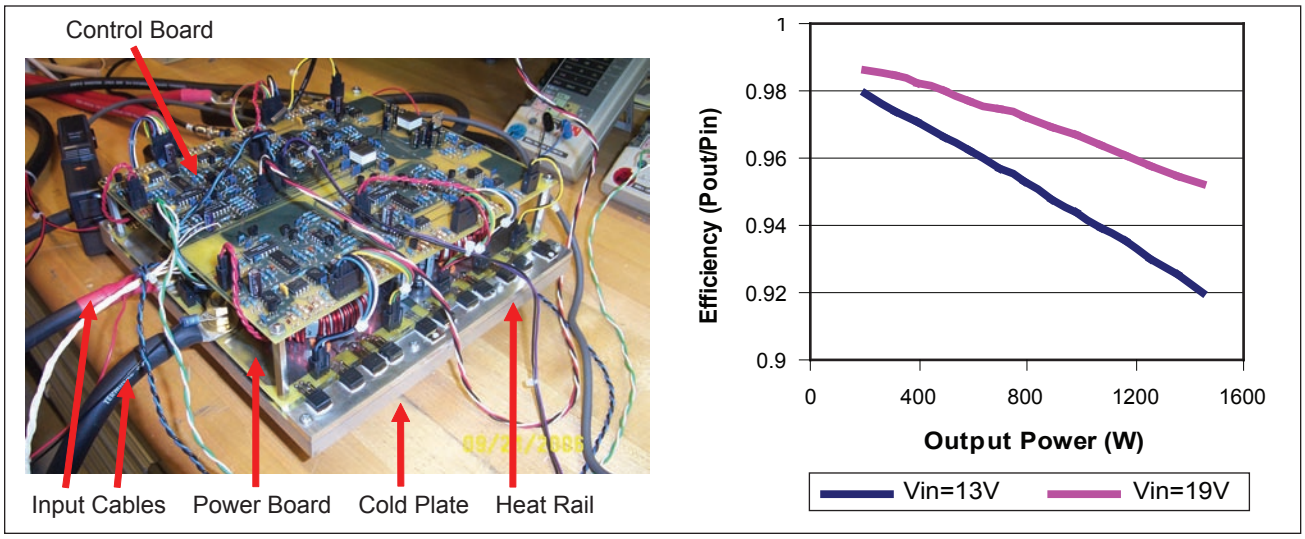


FIGURE 5. Visteon Power Converter and Test Results

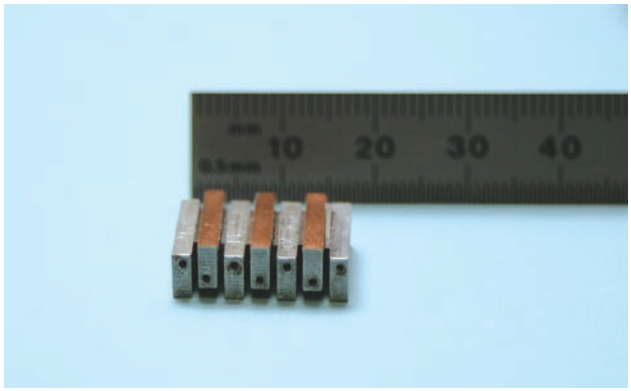


FIGURE 6. Six Bi_2Te_3 Element Device

interface material between the aluminum housing and the TE connectors. A prototype test fixture was constructed to test the device described.

Figure 7 shows power generation curves for the six individual Bi_2Te_3 elements. Using the measured data along with standard TE equations to derive current-independent temperature offsets and temperature-independent electrical interfacial resistivities, the power generation curves that were experimentally determined were duplicated numerically. The dotted lines in the graph represent the calculated power curves compared to the measured power curves represented by the solid lines. It can be seen from the figure that this method of estimation can be very accurate for all six elements.

Lessons learned from these tests on Bi_2Te_3 elements will be carried over to the tests and device design for the higher temperature materials. Interfacial resistances and temperature drops across connector interfaces should be similar for these elements.

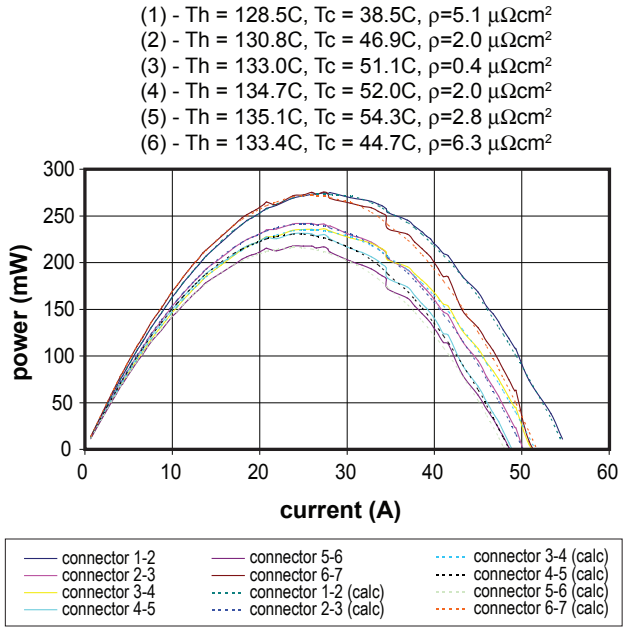


FIGURE 7. Graph Showing Power Generation Curves for Individual Bi_2Te_3 Elements

Figure 8 shows experimental results for initial testing of high temperature segmented elements. Two n-type elements were tested with dimensions and materials used listed in the figure. The same prototype fixture and device configuration to those described above were used on this test as well. Temperatures of the cold-side, hot-side heater settings and the measured TE surface temperatures are also listed in the figure. Curves are different due to the difference in element and layer thickness, as well as the slightly different temperature drops. It can be seen from the figure that the amount of power recovered increases with

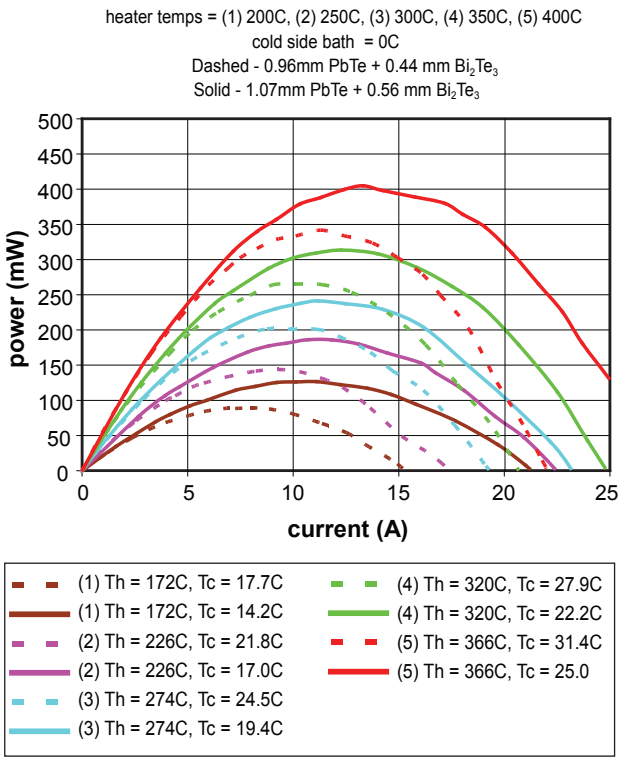


FIGURE 8. Power Generation Curves for Two N-Type Segmented Elements at Different Temperature Differences

increasing hot-side temperature. Optimal current also increases slightly with increasing temperature. Element 1 produces maximum power at 8 amperes at a hot side temperature of 172°C and at 11.3 amperes at 366°C. Further testing and analysis is necessary on these and other similar p- and n-type segmented elements to determine the same level of predictability as the tests on the Bi_2Te_3.

Using a combination of segmented elements, a fractional device will be constructed that produces 20 W of power. Once tested and analyzed, a full-scale TGM will be constructed from multiple fractional devices that will produce a nominal power output of 750 W.

Conclusions

With Phase 2 nearing completion, the design, build and test of key subsystem equipment has been accomplished (or is on track to be accomplished) per the stated objectives. An acceleration plan has been proposed to speed the commercialization of the TGM by developing improved thermoelectric material contact interfaces.

FY 2006 Publications/Presentations

1. ICT 2006
2. 2006 DEER Conference
3. 2006 DTEC Conference

IV.3 Cost-Effective Fabrication Routes for the Production of Quantum Well Structures and Recovery of Waste Heat from Heavy Duty Trucks

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Objectives

The primary objectives of Phase II were to:

- Demonstrate high ZT performance of quantum well (QW) films on Kapton® at the size required for the designed waste heat recovery generator.
- Demonstrate, as verified and accepted by an independent group of experts, using the materials proposed in the application, a demo couple consisting of both a P-leg and N-leg at greater than 5% efficiency.
- Fabricate quantum well-type materials as heterogeneous nanocomposites and report a first set of ZT measurements.

Accomplishments

A summary of the accomplishments are given as follows:

- A new thermoelectric generator (TEG) design was developed that resulted in a 6.5–7.0% fuel economy improvement, versus the earlier reported 4–4.5% (both taking into consideration benefits from the More Electric Truck [MET] design)
- A thermoelectric (TE) conversion efficiency rig was designed, fabricated, and validated using a Bi_2Te_3 couple. The design, instrumentation, operating procedures, calculation assumptions and approaches were reviewed by the Jet Propulsion Laboratory (JPL). The agreement between measured and standard data was excellent (+/- 2–7%).
- Two QW film couples were assembled using two different QW-type film compositions. Data for Seebeck coefficient, electrical resistivity, and conversion efficiency were acquired for each. The conversion efficiencies for both couples were lower than needed.
- Two routes for bulk silicon germanium nanocomposites were identified. A series of materials were prepared from each route. The materials were characterized, and TE property measurements were acquired for each material up to 400ºC. The ZT values obtained were comparable only to bulk.
- A series of bulk boron carbide nanocomposites were fabricated, characterized, and TE property measurements acquired up to 400ºC. The ZT values obtained were comparable only to bulk.

Future Directions

As of yet, the primary objectives of this period have not been met. In particular the go/no-go milestone, consisting of demonstrating either high ZT performance of quantum well (QW) films on Kapton® at the size required for the waste heat recovery generator or 5% conversion efficiency using a QW film couple consisting of both P-leg and N-leg, has gone unfulfilled. Consequently, United Technologies Research Center and the Department of Energy have decided to terminate the project as it exists. There are no open items left and no additional work has been planned.

Introduction

The trucking industry today faces several challenges related to high operating expenses due to increased fuel costs and more stringent Environmental Protection Agency (EPA) regulations. Driver comfort is also being challenged by new regulations that are restricting truck idling to certain locations. A typical truck consuming 100 units of fuel energy loses 25% in heat transfer for engine cooling and 35% in exhaust heat, leaving only 40% for useful shaft energy. To maintain a competitive advantage, automotive manufacturers as well as producers of light- and heavy-duty trucks must

deliver continuous engine efficiency improvements and reductions in emissions. DOE research suggests that electrification of heavy vehicles can improve fuel economy up to 20% in certain applications. Technologies supporting this notion are strategically important because they lower fuel consumption, decrease gaseous emissions, reduce noise, and enable substantial reduction of main engine idling. A direct thermal-to-electrical conversion system utilizing TE is one of these technologies worth supporting and is the focus of this project. The primary objective of this project is to develop a TE-based technology which improves diesel engine efficiency for heavy-duty on-highway trucks by 10%, thereby reducing the fuel economy 9.3%. During Phase I of this project, a system level analysis was carried out which yielded a TEG design with a projected fuel economy improvement of 2.2% (4–4.5% taking into consideration benefits from the MET design).

As part of Phase II, seven tasks were carried out: (1) reevaluation and modification of the existing TEG design to yield greater projected improvement in fuel economy, (2) design, fabrication and assembly of a conversion efficiency rig for the testing of QW film couples, (3) QW film fabrication, (4) QW couple assembly, (5) QW couple testing, (6) qualification of ZT testing equipment at UTRC and (7) fabrication of heterogeneous nanocomposites. Task 1 contained two subtasks – (a) reevaluation of the TEG location (b) reevaluation of the TEG cold side rejection strategy. Task 2 contained four subtasks – (a) heater design and fabrication, (b) rig instrumentation, (c) documentation of test procedure for raw data collection and (d) documentation of test procedure for the efficiency calculation. Task 3 contained three subtasks – (a) buffer layer development, (b) development of a laser annealing technique, and (c) design and fabrication of a new heater/deposition assembly. Task 4 contained three subtasks – (a) film deposition, (b) laser cutting development and (c) contact deposition development. Task 5 contained two subtasks – (a) bismuth telluride and (b) silicon germanium qualification testing. Task 6 contained two subtasks – fabrication of (a) silicon germanium and (b) boron carbide type bulk nanocomposites.

Approach

The first focus was to revise the project's TEG design to yield a greater benefit. The system level analysis carried out during Phase I of this project yielded a TEG design with a projected fuel economy improvement of 2.2% (4–4.5% taking into consideration benefits from the MET design). In an effort to achieve a higher projection for fuel economy improvement, efforts were dedicated this period to reevaluating the assumptions supporting the Phase I TEG design.

The second focus was to obtain measured values for thermal-to-electrical conversion efficiency for QW films on Kapton® at the size required for the designed waste heat recovery generator. In order to satisfy this goal, a new TE conversion efficiency test rig was needed. Efforts were therefore dedicated to design, fabricate, assemble, baseline test and document test procedures for such a rig. The test sample required for this rig was notably larger than the single, flat P-N couple demonstrated in the past by Hi-Z to give 12% conversion efficiency. The test sample also needed to be made consistent with the device design selected as part of Phase I. It was recognized that this larger test sample will have more thermal and electrical losses, when built for the first time, than the previous, single P-N couple. Consequently, a lower conversion efficiency milestone of 5% was set.

The third focus was to obtain high quality QW films on Kapton®, at the size required for the designed waste heat recovery generator, and assemble these films into a P-N couple for the purpose of conversion efficiency testing. In order to satisfy this goal, the fundamental process for fabricating QW films on Kapton® needed optimization and the process for assembling the QW films into P-N couples needed development. Efforts were therefore dedicated to achieving these goals.

The fourth focus was to evaluate, as a potential cost-reduction pathway, methods to fabricate the QW-type materials as bulk heterogeneous nanocomposites. The approach taken to achieving this goal was to first downselect one or two fabrication methods for the each of the type of nanocomposites (silicon germanium and boron carbide), develop a fabrication process by systematically varying to optimum each processing step, and produce a first set of test specimens for ZT testing.

Results

Accomplishments made included an improved TEG design yielding 4.4% fuel economy improvement (6.5–7.0% taking into consideration benefits from the MET design), a fully-functional, qualified and externally reviewed conversion efficiency rig, identification of buffer layer crystallinity as the critical parameter in achieving high quality QW films on Kapton®, development of an assembly process for the production of QW couples, conversion efficiency test results from two different fabricated film couples, fully-functional, qualified ZT testing equipment at UTRC, techniques developed for the fabrication of silicon germanium and boron carbide type nanocomposites and ZT test results from three series of fabricated nanocomposites.

After considering all system level parameters in the TEG design, the TEG was moved upstream to a hotter location in the exhaust and a dedicated cooling loop was

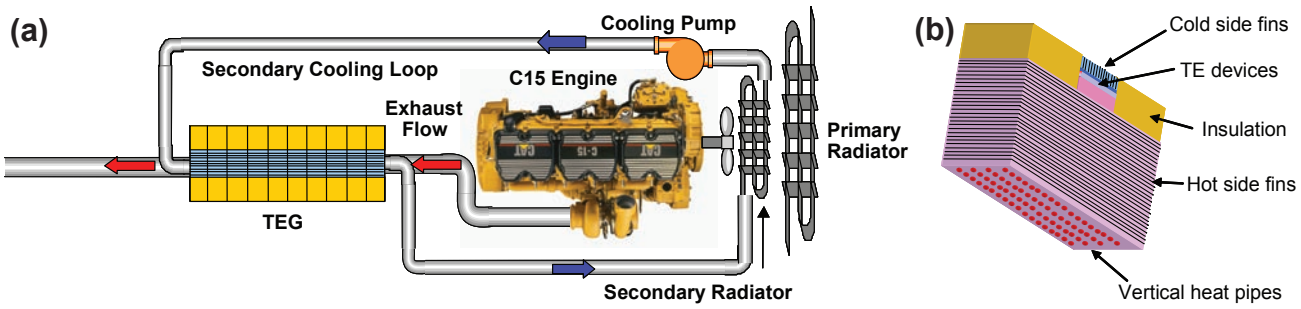


FIGURE 1. (A) System-level engine design, integrating a thermoelectric generator (TEG) for the purpose of waste heat recovery, with a Caterpillar C16 Engine. (B) Detailed design of the thermoelectric integrated heat exchanger (single segment).

included, resulted in a 4.4% fuel economy improvement (6.5–7.0% taking into consideration benefits from the MET design) as shown in Figure 1. Considering future identified improvements in heat exchanger technology (including heat exchanger materials), up to 7% fuel economy improvement is now projected as achievable (9–9.5% taking into consideration benefits from the MET design).

Figure 2 shows the conversion efficiency rig that was designed, fabricated and assembled as new this budget period, including the test sample and heater assembly. Supporting this test capability is a test procedure for the conduction of experiments (heat and current flow in plane with QW films) and collection of raw data.

Extensive instrumentation and 3-D finite element analysis was used to calculate conversion efficiency from the measured quantities. A test procedure was developed for the processing of raw data into conversion efficiency and validated against a Bi_2Te_3 test sample. The agreement between measured electric resistivity, Seebeck coefficient and conversion efficiency, and standard data, was excellent (±2–7%). The design, instrumentation, operating procedures and calculation assumptions were further reviewed by JPL and no major issues uncovered. Areas of improvement were identified and implemented to reduce uncertainties.

A process was further developed to fabricate and assemble the QW films into a P-N couple for conversion efficiency testing. The process involves three steps: (1) film deposition, (2) laser cutting, and (3) contact deposition. The films were deposited at PNNL using the larger scale sputtering machines. The films were deposited on both sides of a Kapton® substrate to a total thickness of 12 microns. The films were sectioned into approximately 12 subsections using a laser micromachining system. The films were stacked and contacts were sputtered on each end. Figure 3 illustrates how the individual films are assembled into the P-N couples, including the location for the contacts.

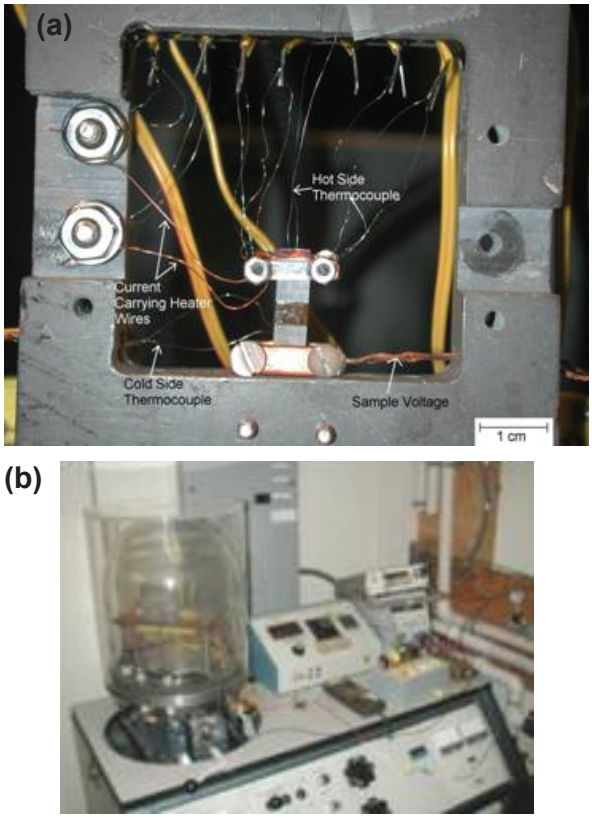


FIGURE 2. (A) Front view of the thermoelectric sample (P-N couple) clamped in the thermoelectric conversion efficiency rig. (B) Thermoelectric conversion efficiency rig positioned inside the vacuum chamber.

Figure 4 shows the first of two TE couples fabricated. The 1st couple - Kapton®/Si/$Si_{0.8}Ge_{0.2}$ - exhibited very high electrical resistivity and gave a Seebeck coefficient that was low for QW films, but consistent with bulk values. The measured conversion efficiency was very low (<1%). The 2nd couple, consisting of an alternate material (not Si/SiGe) on

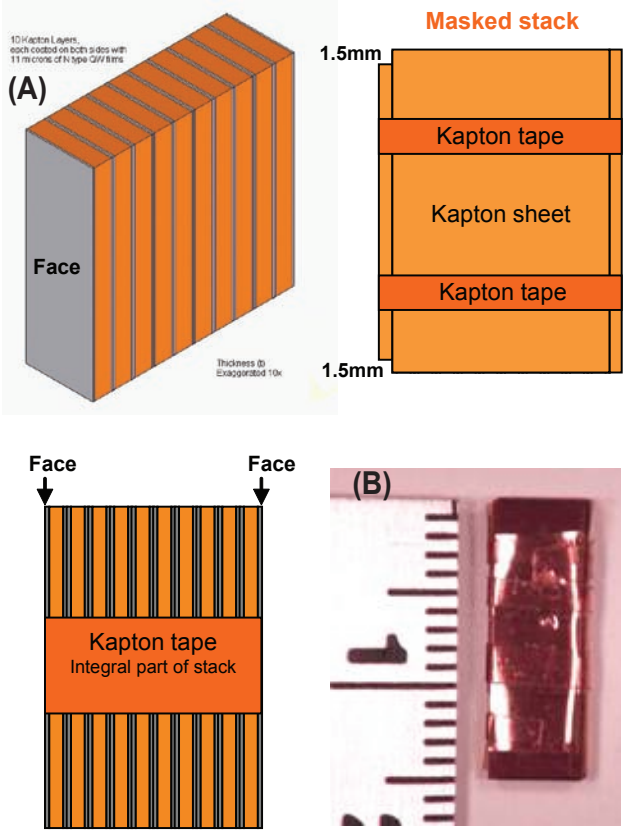


FIGURE 3. (A) Assembly and masking schematic. (B) Practice piece assembled at PNNL.

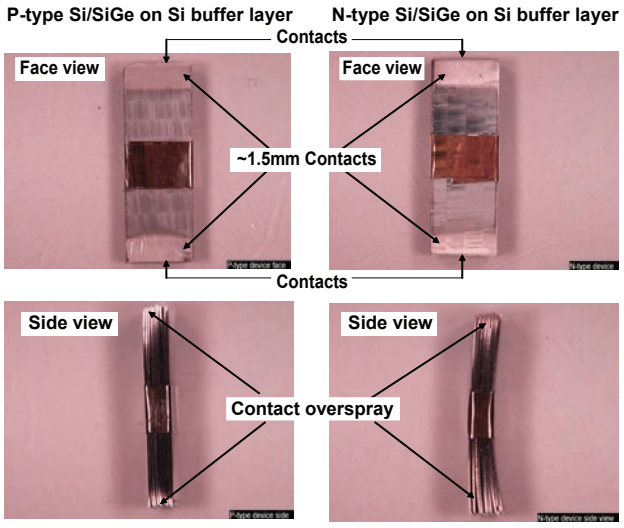


FIGURE 4. Pictures of the final, assembled P-N couple ready for conversion efficiency testing.

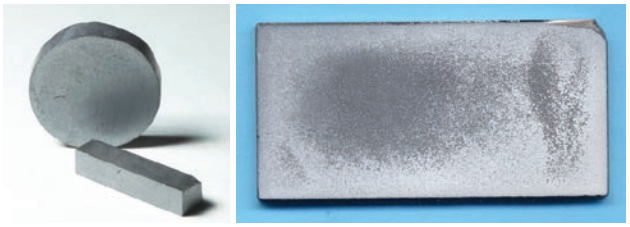


FIGURE 5. Representative bulk heterogeneous nanocomposite samples fabricated at UTRC. (A) silicon germanium, and (B) boron carbide.

Kapton®, was evaluated as a risk reduction measure. This couple also exhibited very high electrical resistivity and gave a Seebeck coefficient that was low for QW films, but consistent with bulk values. The measured conversion efficiency was also very low (<1%).

Figure 5 shows examples of the heterogenous bulk nanocomposite materials fabricated as part of this budget period. For the silicon germanium system, two methods were evaluated: (i) hot isostatic pressing of Si nanoparticles into a coarse $Si_{0.8}Ge_{0.2}$ powder mixture to form $(Si)_x/(Si_{0.8}Ge_{0.2})_{1-x}$ and (ii) arc melting of a uniformly mixed, pre-consolidated powder mixture of Si, Ge, and an insoluble additive phase, A, to form $(A)_x(Si_{0.8}Ge_{0.2})_{1x}$. The hot isostatic pressing method yielded samples that had densities ranging from 90–95% of theoretical, while arc melting yielded samples that had densities ranging from 85–100 % of theoretical. TE property measurements were acquired for the nanocomposites produced from both routes. ZT values for the $(Si)_x/(Si_{0.8}Ge_{0.2})_{1-x}$ nanocomposites formed by the hot isostatic pressing ranged from 0.17–0.21 at 175°C. These values are comparable to bulk silicon germanium. ZT values for undoped $(A)_x(Si_{0.8}Ge_{0.2})_{1-x}$ nanocomposites, formed by hot isostatic pressing, ranged from 0.01–0.04 at 175°C. These values are significantly lower than fully doped, bulk silicon germanium, but are comparable to the undoped, bulk silicon germanium sample prepared for the purpose of baseline comparison.

For the boron carbide system, one fabrication route was evaluated. Within this route, phenolic resin was demonstrated as a suitable carbon source to generate nanostructured boron carbide in-situ via reaction with amorphous boron powder. Formation of boron-rich boron carbide was demonstrated via direct reaction of B_4C with additional amorphous boron. Hot pressed boron carbide heterogeneous nanocomposites exhibited densities that ranged from 77–97% of theoretical, with retained nanocrystallinity between 45–100 nm. TE property measurements were acquired for the fabricated boron carbide nanocomposites up to 400°C. Results were comparable with bulk TE properties.

Conclusions

- Moving the TEG upstream to a hotter location in the exhaust and dedicating a cooling loop to the system design resulted in an additional 2.2% improvement in fuel economy.
- QW films on Kapton® were unable to produce high ZT needed for TEG design.
- The bulk heterogeneous nanocomposite routes evaluated, for both silicon germanium and boron carbide, produced ZT values comparable only to bulk. If performance benefits exist in these materials, they would likely be observed at higher temperatures.

References

1. Trip report, Terry Hendricks, PNNL – Review of Hi-Z Quantum Well Efficiency Test System (Rig), submitted to DOE on 09/29/06.

FY 2006 Publications/Presentations

Presentations

1. 12th Annual Diesel Engine Emission Reduction (DEER) conference, August 24th, 2006, Detroit, MI.

2. Phase II, Budget Period 2 Program Review, Oct. 10th, 2006, Washington, D.C.

IV.4 Thermoelectric Conversion of Waste Heat to Electricity in an IC Engine Powered Vehicle

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Objectives – Phase II (30 months)

- Using thermoelectric energy recovery from the exhaust system, determine material performance needed to produce a 10% improvement in brake specific fuel consumption for an over-the-road (OTR) truck operating under cruise conditions.
- Evaluate currently available thermoelectric materials to determine engineering developments required for their implementation in a thermoelectric generator (TEG) for an OTR truck, to be demonstrated within five years.
- Determine requirements for a heat exchanger needed in this application.
- Determine power electronic and control requirements for this application.
- Assemble the equipment needed to conduct the necessary material synthesis, fabrication and hardware necessary for a scaled demonstration.
- Determine if Phase II results warrant a prototype engine – TEG final design in Phase III.

Accomplishments in Phase II

- Systems for material synthesis, powder processing, hot pressing, leg preparation, material mechanical and thermoelectric property characterization, and couple fabrication have been demonstrated. In addition to the facilities at Michigan State University, this includes the use of facilities at the Jet Propulsion Laboratory (JPL) and DOE's Oak Ridge National Laboratory (ORNL). Upon completion of Phase II we expect to meet the objectives of being able to successfully fabricate the modules required for the TEG.
- Using the measured properties of known materials for the temperature range of operation we estimate that a segmented couple can provide a 12.3% conversion efficiency.
- Analytical studies were performed to obtain operating points and efficiencies of various TEG configurations using materials that have been developed. Calculations show estimated improvement of up to 6.2% in fuel economy for a Class 8 OTR truck operating at cruise conditions.

Future Directions for Phase II

- Conduct design and analysis of the power conditioning system to optimize thermoelectric system performance including fault remediation.
- Explore leg fabrication methods (e.g. wet milling/ dry milling, hot pressing) for improving mechanical properties and microstructural characteristics.
- Develop fabrication techniques for scaleable couple/ TE modules.
- Improve results of analytical studies on the full engine system by coupling current simulations to the 3-D heat transfer studies performed at Iowa State University.
- Improve the coefficient of performance (ZT) by exploring several more promising thermoelectric material compositions, with emphasis this period on PbTe systems with Eu doping.
- Extensive mechanical, thermal cycling and thermoelectric property testing of segmented hot-pressed legs including Bi_2Te_3 and LAST/(T).
- Continue development of module fabrication methods.

Introduction

At peak efficiency, current diesel engines are capable of converting 40 percent of fuel energy to useful energy. When a Class 8 diesel truck is loaded, the engine

might deliver 300 kilowatts of power to drive the wheels, while at the same time, another 300-400 kilowatts of energy goes out through the exhaust stack as wasted energy. This research project is attempting to find ways to capture that wasted energy and convert it to back into useful energy. A reasonable long term goal would be to increase the diesel power plant efficiency to greater than 50%!

This unique project requires input from a number of researcher collaborators and experts inside and outside of the College of Engineering at Michigan State University (MSU). The aim of the research is to use a direct conversion device--fabricated out of thermoelectric materials--to recover waste heat from the exhaust of internal combustion engines and turn it into useful electricity. The team is working with thermoelectric materials that have already been developed and is assessing them to see if they can be implemented in a powertrain in a cost-effective manner. The team is also developing new high efficiency thermoelectric materials that will permit a 10% improvement in fuel economy of OTR Class 8 trucks. We expect that completion of the project through Phase 4 will result in a scaled demonstration of the engine and thermoelectric energy recovery system.

Approach

This MSU-led multidisciplinary research effort is to evaluate the entire system and identify the required processes needed to bring thermoelectric technology to a cost-effective commercial product for an OTR truck. The Phase II effort is 30 months in duration involving an exploratory analysis and feasibility study which includes system design, new TE material synthesis, power electronics design, material thermoelectric and mechanical property characterization, heat exchanger design, TE material fabrication methods, module fabrication and evaluation of system performance.

Results

1. Couple and Module Design

An important part of this effort includes transport measurements of the thermoelectric materials, design, assembly, and testing of the thermoelectric modules, which includes the investigations of protective coatings and contacts to the materials. From software developed in the LabView® programming environment, the expected efficiency is calculated for various module loading conditions and module leg geometries to determine the optimal ratio of cross-sectional areas for the *n*-type and *p*-type legs. This iterative modeling procedure was used for the following boundary conditions which were provided by the engine analysis of Novak, Hartsig, and Schock as shown in Table 1. Results for the six conditions are given in Table 2.

TABLE 1. Temperature and Heat Flow Conditions from the Engine Analysis

	T2	T2'	T3	T3'	q (calc)
6-1	731	**727**	524	**342**	50493.822
6-1	781	**777**	546	**338**	57445.870
6-1	831	**826**	567	**334**	64397.918
EGR Cooler	495	**493**	408	**331**	21222.041
EGR Cooler	636	**633**	474	**331**	39516.904
EGR Cooler	834	**829**	568	**334**	64885.781

TABLE 2. Results for 4 mm and 7 mm Leg Modeling for the Given Engine Conditions

Leg length	T_c (K)	T_h (K)	η (%)	R (mΩ)	V (V)	P (W)	#/kW
4 mm	342	727	11.0	6.1	0.142	0.73	1,370
4 mm	338	777	12.3	6.75	0.165	0.90	1,112
4 mm	334	826	13.4	7.3	0.188	1.10	910
4 mm	331	493	5.48	4.76	0.067	0.21	4,762
4 mm	331	633	9.05	5.26	0.110	0.52	1,924
4 mm	334	829	13.5	7.32	0.189	1.12	893
7 mm	331	493	5.48	8.32	0.067	0.12	8,333
7 mm	331	633	9.05	9.20	0.110	0.30	3,333
7 mm	334	829	13.5	12.8	0.189	0.62	1,612

2. Design of Power Electronics and its Control

Using commercially available 5.7 W TE modules from Tellurex Corp. it has been calculated that at least 200 modules are required to generate a reference power target of 1 kW. Although an all-in-series module configuration would make the power conditioning circuit easier and more efficient and an all-in-parallel module would result in a more reliable circuit with higher power output, a combination of series and parallel (Figure 1) is preferred as it will alleviate some inherent operating and robustness problems. The smart power electronic circuit would provide load matching to maximize output power, bypass failed modules to continue operating, protect each module from thermal and electrical stresses and it would enable each TE module to be operated at different heat flux and ΔT conditions.

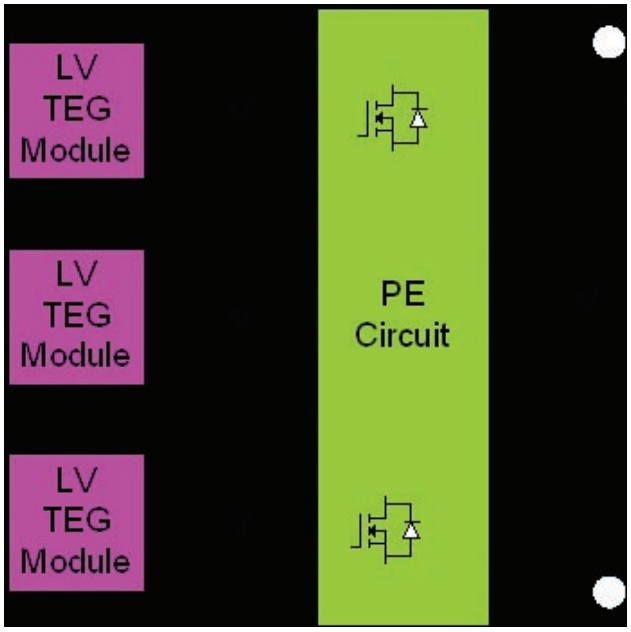


FIGURE 1. Using Power Electronic Circuits to Improve TEG reliability, Provide Load Matching, and Protection

3. Production and Property Characterization of TE Materials

Over the last 12 months a major effort related to production, powder processing and material characterization of LAST/T material has been underway. Powder processing by wet and dry milling has been explored. The particle size and distribution of these powders were analyzed using Coulter counters and scanning electron microscope micrographs. Powder was hot pressed at the University of Michigan and ORNL. Over 90 LAST/T ingots of various stoichiometries were synthesized during the past year. Material property characterization was performed on these ingots by studying hardness, elastic modulus, fracture toughness and internal strain.

4. Leg Segmentation

JPL assisted MSU in their efforts to mature LAST-based thermoelectric technology to quantify the thermoelectric and electrical properties of this material as well as helping to develop hot pressing methods for the LAST material. A puck of LAST ETN121 was metallized using JPL's *in situ* hot pressing technique (Figure 2). JPL has also been involved with designing and developing Skutterudite/PbTe/BiTe technology for the waste heat application.

5. Engine-Thermoelectric Systems Performance

The analytical study continues with the objective of a more accurate prediction of the potential benefits of TEG design alternatives for converting exhaust gas heat into electrical energy. The WAVE engine system model simulates the complete engine system. Contrary to the Phase I model, the TEG now functions as the exhaust gas recirculation (EGR) cooler and resides within the EGR bypass subsystem.

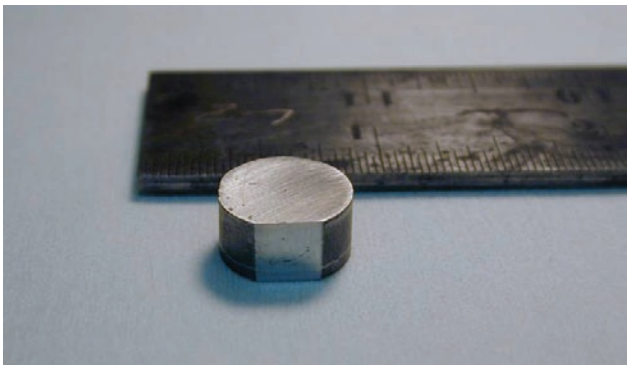


FIGURE 2. A 0.5" LAST ETN 121 Puck Metallized with Ni on One End and Fe on the other

One of the primary objectives of this analysis is to better understand and quantify the balance of exhaust gas mass flows between the TEG (EGR cooler) and the exhaust turbine. The temperature variation along the length of the TEG at this instant in the engine cycle spans over 300 K. Calculated improvements in fuel economy are shown in Table 3.

TABLE 3. Improvement in BSFC for Different TEG Configurations

TEG configuration	% Improvement in BSFC
1 Cylinder into 1 TEG (6 TEGs)	6.2%
3 Cylinders into 1 TEG (2 TEGs)	4.0%
6 Cylinders into 1 TEG (1 TEG)	2.8%
TEG used as EGR Cooler (1 TEG)	1.5%

6. Heat Transfer Enhancement

As part of the proposed efforts on heat transfer enhancement, literature on gas-turbine thermal management was reviewed to identify heat transfer enhancements techniques for the hot-gas side. Some examples of heat-transfer enhancement techniques are shown in Figure 3, which involve ribs in various arrangements. This survey indicates that the maximum heat transfer enhancement is approximately three to four on the average at best. However, it was noted that locally the heat transfer enhancement can be higher.

7. ZT Amplification

By the end of Phase 2 our goal is to achieve not only a doubling of our current ZT of 1.4-1.7 but also close matching of the temperature profiles of the ZT to the temperature profile available from the diesel engine

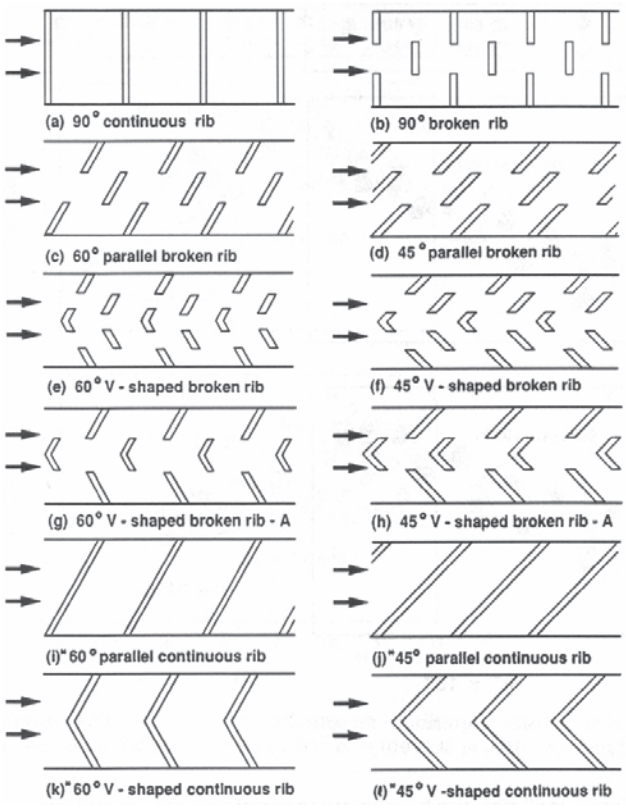


FIGURE 3. Examples of Heat-Transfer Enhancement Methods Involving Ribs

selected for the project. Emphasis will be on long-term material stability and cost.

We are focusing on the $AgPb_{18}SbTe_{20}$ class of materials but also on KPb_mSbTe_{2+m} and PbTe derivatives which show good promise for high efficiency. We expect materials with lower Pb content such as $KPb_{16}SbTe_{20}$ and $KPb_{14}SbTe_{20}$ to have lower thermal conductivity which should help reach higher ZTs. We have investigated the PbTe systems containing Eu nanoparticles. Preliminary data for these samples have been obtained and they are promising. Details of this work can be found in our Septembr 30, 2006 quarterly report to DOE.

Conclusions

Completion of the Phase II effort will provide the following results:

- Preliminary TEG design will be completed using material properties that have been measured.
- Demonstrate the viability of a module which can produce between 20 and 40 watts of power with a temperature difference of less than 800 K on the hot side and 300 K on the cold side.
- Accurately quantify the bulk mechanical properties for the LAST/T material for use in the FEA studies of the thermoelectric generator.
- Complete selection of appropriate metallization for segmented couples, voltage insulators and required sublimation suppression.
- Couple detailed heat transfer models of Iowa State University to WAVE and FEA models of thermoelectric generator. Perform comparison of system efficiency for various options.
- Estimate of possible performance gains using demonstrated materials with known mechanical and thermoelectric properties will be provided.

FY 2006 Publications and Presentations

Published archival journal papers

1. F. Ren and E. D. Case, E. J. Timm, M. D. Jacobs and H. J. Schock, "Weibull analysis of the biaxial fracture strength of a cast p-type LAST-T thermoelectric material," 2006, Philosophical Magazine Letters, 86[10]: 673 – 682.

Submitted journal papers

1. F. Ren, E. D. Case, E. J. Timm and H. J. Schock, "Hardness as a function of composition for n-type LAST thermoelectric material," submitted, Journal of Alloys and Compounds.

2. A. L. Pilchak, F. Ren, E. D. Case, E. J. Timm and H. J. Schock, "The effect of milling time and grinding media upon the particle size distribution for LAST (Lead-Antimony-Silver-Tellurium) powders," to be submitted, Materials Science and Engineering.

3. T. Hogan, A. Downey, J. Short, J. D'Angelo, C.-I. Wu, E. Quarez, J. Androulakis, P. F. P. Poudeu, J. Sootsman, D.-Y. Chung, M. G. Kanatzidis, S. D. Mahanti, E. Timm, H. Schock, F. Ren, J. Johnson, E. Case, "Nanostructured Thermoelectric Materials and High Efficiency Power Generation Modules," submitted to *Journal of Electronic Materials*.

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IV.5 Exhaust Energy Recovery

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NETL Project Manager: Ralph Nine

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

- Identified the prime path working fluid for the Rankine cycle system. Honeywell Genetron R245fa has been identified as the most appropriate working fluid for use as it is available, has good environmental and thermal performance properties, and is expected to be a cost-effective choice.
- Performed thermodynamic cycle analysis to predict performance across engine duty cycle. Basic thermodynamic analysis has been conducted to determine the amount of power recoverable from the Rankine cycle system. Analysis has identified the optimum arrangement of heat exchangers and system components within planned engine system architectures to provide the maximum amount of power recovery with a minimum of system complexity and expense.
- Identified supporting technologies to enhance the recovery of waste heat energy using common electric power engineering components. Recovered waste heat energy will be converted to electricity. This electricity is most efficiently handled at higher voltages (approximately 340 VDC, common with hybrid electric vehicle technology). The presence of a high-voltage bus and its associated components creates a power system which can accommodate high-voltage power producing and consuming devices. More efficient electrically driven parasitics (such as coolant pumps, fans, etc.) will be explored to most effectively utilize the recovered electric power.

Future Directions

Continuing effort is planned in the pursuit of an effective and efficient Rankine cycle waste heat recovery system. The past activities have identified key components and have defined their performance for a successful, integrated system. Based on this analysis we expect to:

- Create specifications for prototype hardware and control software. Suppliers were identified during FY 2006 and we will be working with them to design, fabricate, and test their prototype devices prior to their delivery for laboratory, engine-system level testing.
- Perform subcomponent testing of prototypes and verify model predictions for their performance.
- Perform model-based simulation of integrated systems for vehicle-level performance prediction across operating duty cycles.
- Define expected hardware performance in-vehicle.
- Start laboratory-based, integrated system testing.

Also, we will continue pursuit of an electric-assist turbocharger which will use the high-voltage power electronics introduced in support of the energy recovery system. This development also supports potential significant emissions improvement and engine performance (responsiveness for improved driveability). Towards this goal we expect to:

- Create an appropriate turbocharger model for the target engine application (Cummins' ISX, 15-liter, 6-cylinder engine)
- Perform modeling exercises to determine the potential performance improvement this technology may offer to exhaust gas recirculation (EGR) engines.
- Pursue hardware for testing should modeling results indicate significant benefit.

Introduction

With the advent of low-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.

The Rankine cycle 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 work. This work is used to turn a generator which then provides additional power above what the diesel engine produces for the same amount of fuel burned. Using the Rankine cycle to extract energy (or to thereby provide cooling) from waste heat streams serves to reduce the amount of heat which must be rejected while simultaneously providing extra power. 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 improving fuel economy.

The Exhaust Energy Recovery program at Cummins Inc. was initiated by experiments conducted under the Heavy Duty Truck Engine program. During this testing, a Rankine cycle was employed in support of that Program's high engine efficiency demonstration. In the current work, Rankine cycle heat recovery is being focused on the heavy-duty diesel engine's EGR and fresh, compressed charge air streams as these sources of waste heat drive the most significant performance increase to the vehicle's cooling package. Also, in combination to this recovery work, electric-assist turbocharging will be pursued to add to and use power provided by the Rankine cycle energy recovery system.

Approach

Cummins' approach to the Program 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 additional EGR and fresh charge air to thereby achieve low intake manifold temperatures (in pursuit of clean combustion) drives an increase in vehicle cooling system performance.

A Rankine cycle extracting heat energy from the engine's EGR and fresh, compressed charge air streams reduces the heat load on the cooling package and simultaneously provides extra power from 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 coolant pumps, fans, etc.

To efficiently accommodate power from the Rankine cycle generator and to minimize its size, higher voltage than what is traditionally used on heavy-duty vehicles (12 VDC) is required. The recommended 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. The electric-assist turbocharger is one example of this. Efficient coolant pumps, fans, etc. are others.

Results

Research has been focused on identifying the most effective techniques and tools for Rankine cycle application to a heavy-duty diesel engine installed in a Class 8 tractor.

Simulation Analysis

A simple Recuperated Rankine Cycle is schematically presented in Figure 1. Saturated liquid working fluid (blue) comes from the system condenser and first passes through a Recuperator which transfers energy left over after turbine energy extraction. The fluid then passes to the engine heat exchangers (charge

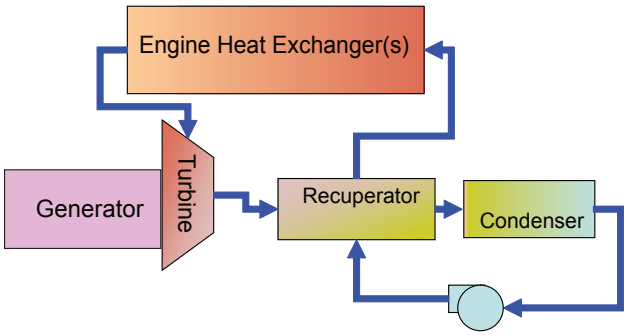


FIGURE 1. Simple Recuperated Rankine Cycle

air cooler, CAC, and EGR cooler) where it reaches a superheated state. The superheated vapor is then passed through the turbine to generate electricity. The fluid then passes through the recuperator and then the condenser.

A performance analysis using R245fa in a recuperated Rankine cycle extracting energy only from EGR and charge air resulted in a maximum brake thermal efficiency (BTE) improvement of 10.6% over the base engine alone at the B100 operating condition. Heat rejection out of the engine system from the EGR and compressed, fresh charge air was reduced by 16.3% (or by the Rankine cycle efficiency). The table below summarizes results from this study.

TABLE 1. R245FA Recuperated Rankine Cycle Analysis using only CAC and EGR Heat

Condition	Engine Power (kW)	Total Heat Rejection (kW)	Net WHR (kWe)	%BTE Improvement
C100 – Max Power	338	234.9	35.68	10.55
B100 – High speed, high torque	336	235.4	35.8	10.64
B50 – cruise	170	96.7	14.7	8.62
A100 – low speed, high torque	283	151.8	23.1	8.2

The optimum configuration for energy recovery from the ISX engine has continued beyond this analysis and has considered a Rankine cycle architecture which best fits within the expected engine architecture for future diesel engines. The recovery of heat energy from only EGR flow offers a simpler packaging challenge with acceptable performance results.

Hardware Design

An initial design study (see Figure 2) of a turbine generator for this application has been made. The turbine for this application will be either a variable nozzle turbine (VNT) or variable admission turbine (VAT) to increase Rankine cycle efficiency over the base engine operating map as much as possible. Also, this design includes a reaction-type turbine wheel (similar to existing turbocharger compressor wheels) and hydrodynamic bearings for good performance in-vehicle against shock and vibration (again, similar to turbocharger technology).

Generator output voltage for this system is expected to be 340 VDC in order to be compatible with currently available heavy hybrid transmission and driveline equipment. This higher voltage also minimizes the physical size of the generator.

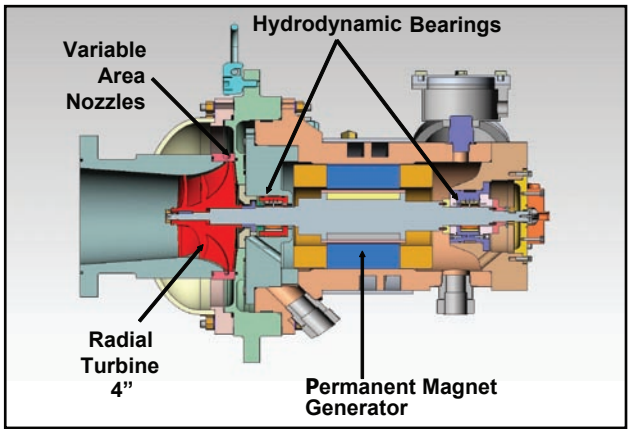


FIGURE 2. Proposed Turbine/Generator Design

Heat exchangers for the system are being pursued through outside suppliers who are providing design, fabrication, modeling, analysis, and performance testing of their components prior to integrated system testing at Cummins. The work is similar to the effort made for typical EGR coolers and CACs. Of critical concern is the maintenance of a temperate operating environment for the working fluid as over-temperature conditions will lead to fluid breakdown.

The system’s driveline motor and high voltage power electronics are being designed and developed by Cummins Power Generation and Generating Technologies groups. Typical efficiencies for the major components in the power electronics architecture are expected to be approximately 96%, resulting in very little loss due to power conditioning.

Conclusions

Modeling and analysis performed to date, supported by the previous experiments with Rankine cycle systems on the Heavy Duty Truck Engine Program leads us to expect significant efficiency improvement from the heavy-duty diesel engine through the incorporation of this concept. 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 is technically feasible and appropriate components (working fluid, turbine/generator, flywheel motor-generator) for the Rankine cycle concept are being developed.
- Significant cooling system benefit is possible from this concept and will therefore provide benefits beyond base engine fuel efficiency to the vehicle original equipment manufacturer customer.

- Provision of appropriately conditioned charge air for clean combustion is promoted through the incorporation of this system.
- Additional benefits through the utilization of optimized parasitics are possible.
- Utilization of other high-speed rotating electric machinery (electric-assist turbocharging) is enabled through this concept.

FY 2006 Publications/Presentations

1. 2006 DEER Conference Presentation – "Exhaust Energy Recovery", presented by Christopher R. Nelson, 24th August, 2006.

IV.6 Very High Fuel Economy, Heavy Duty, Constant Speed, Truck Engine Optimized via Unique Energy Recovery Turbines and Facilitated by a High Efficiency Continuously Variable Drivetrain

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Subcontractors:
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- Volvo Technology, Gothenburg, Sweden

Objectives

- Increase engine efficiency by 10% while meeting U.S. 2010 emissions standards.
- Achieve efficiency increase by implementing energy recovery devices in the form of turbocompounding and narrowing the engine operating speed range. Couple the engine to a continuously variable transmission (CVT) to enable the engine to operate in a narrow or constant speed (1,000-1,300 RPM).
- Test the engine-CVT combination over road cycles in a test cell to demonstrate system efficiency increase.

Accomplishments

- Through simulation, demonstrated an engine efficiency increase of 8.2% when operating over a road cycle and 10.5% during steady-state operation over the ESC/OICA at U.S. 2010 NOx levels (0.2 g/bhp-hr).
- Met the milestone that the added investment for the CVT and energy recovery devices will be returned in less than 1.5 years assuming fuel prices of $2.50 per gallon.
- Net fuel efficiency when coupled to a CVT was estimated to be a 5% increase.

Future Directions

- Design a compressor and two turbines (turbocharger and compound), tailored for the highly weighted operating points. Design of complete turbocharger and turbo compound units.
- Test these compressor and turbines in special rigs in order to verify the theoretical performance.
- Build prototype high efficiency turbo and turbo compound units for testing.
- Begin baseline engine development that will include high efficiency turbo and turbo compound units.
- Demonstrate the engine and CVT system in a test cell environment to determine system efficiency.

Introduction

Fuel prices have remained high for the last several years hovering at times around the $3.50 per gallon mark. The heavy-duty trucking industry is very sensitive to fuel pricing and at times passes the increased cost on to the consumer. With new and more stringent emissions standards taking effect in 2007 and than again in 2010, fuel economy will suffer as more energy is needed to drive the emissions control devices. Even as little as a 1% improvement in fuel consumption can mean huge savings for a fleet of say 100 trucks operating 100,000 miles per year.

One way to increase the engine's efficiency is to recover some of the energy that is lost through the exhaust. A mechanical turbo compound device has the ability to direct some of that energy back to the engine gear train by coupling directly to the compound turbine thus reducing a portion of the energy lost through the exhaust as can be seen in Figure 1. It is worth mentioning that a turbo compound engine reacts more positively to improved turbo efficiency than a conventional turbocharged engine. This project has taken an energy recovery approach along with operating the engine in a different speed range than today's engine. Narrowing the engine operating speed range allows the designer to select the optimum speed where engine efficiency is highest. Conventional standard transmissions operate with gear steps too wide to run the engine in a constant or narrow range but with the development of a CVT, narrow range operation is possible which will allow the engine to operate at peak efficiency over its entire operating range.

Besides the more narrow operating range, the average engine speed is also lower. This makes it possible to optimize valve timings, combustion specification etc. High efficiency turbo compressors are also important to realize increased overall efficiency.

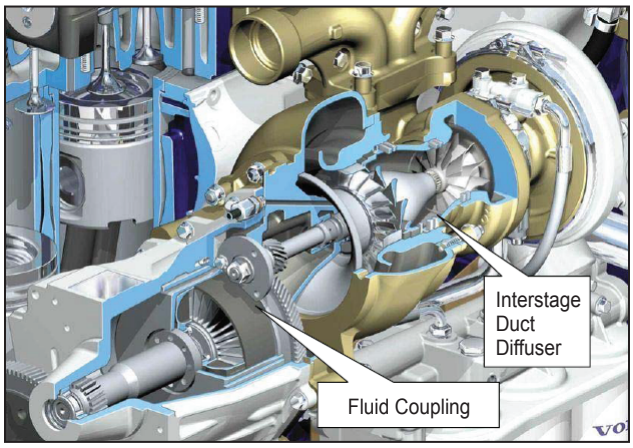


FIGURE 1. Close-up Showing the Turbocharger, Interstage Duct Diffuser and Turbocompound

The more narrow speed range allows the use of a compressor with a vaned diffuser which has higher efficiency compared to a vaneless diffuser. In order to achieve the efficiency goal, four techniques were combined: mechanical turbo compound, high efficiency turbochargers, narrow range operation and optimized combustion and valve timings.

Approach

To determine the efficiency improvement potential detailed engine simulations were done considering the Volvo MD13 (485 hp/2,600 Nm) engine to determine the benefit of reducing engine speed and impact on efficiency. The simulations guided the development of the narrow range approach and allowed the study of different operating ranges so the best one could be chosen. Simulations were also done to determine the best turbocharger and turbo compound combination that would return the highest efficiency improvement without adding significant cost to the engine. The turbo compound unit is based on a production unit for the Volvo D12 500 hp engine in Europe. Cost analyses were performed on the engine system including the CVT to determine the added cost and return on investment.

Based on the engine simulations, prototype turbocharger and turbo compound hardware will be designed and manufactured. The prototype hardware will be installed onto a 13L Volvo engine for testing to compare simulation results with actual.

The final plan is to assemble the engine with the high efficiency turbocharger and turbo compound units and CVT and place in a test cell capable of running the same road cycles that was done during the simulation phase. The results of the testing will be compared to that determined through vehicle simulations.

Results

The simulation result showed the fuel consumption reduction compared to the U.S. 2007 reference engine is 8.2% when using the U.S. 2007 weight factors (flat 70%, rolling hills 25% and hilly 5%) and 10.5% when using the European Steady State Cycle (ESC). These improvements are achieved by a number of measures compared to a conventional turbocharged engine. The main contributor is the mechanical turbo compound system which converts exhaust energy into mechanical work. This unit has a high efficiency axial turbine with a stator. The duct between the turbocharger and the compound turbine is annular with low pressure loss and high pressure recovery. The turbocharger has both a high efficiency compressor and turbine. The turbo compound system also has the advantage of positive driving pressure for the high-pressure exhaust gas recirculation (EGR) system. If a conventional turbocharged engine has too high turbine efficiency, the exhaust pressure will be too low compared to the inlet manifold pressure and the driving pressure for EGR will be negative. The other source of the improvement is the narrow range operation which allows optimized camshaft timings and combustion.

Two different engine speed control strategies were studied, constant speed and narrow range. The narrow range strategy means that the engine speed is not fixed but optimized over a certain cycle ranging from 1,000-1,300 rpm at part load. The result of this study showed that the narrow speed engine is more efficient than the constant one when the engine is not working in full power range. It can be seen from Figure 2 that, it is more economical to reduce the speed at part loads.

The engine cost estimate has been divided into four different sub-groups including turbocharger, turbocompound unit, interstage duct diffuser and modification necessary to the engine to accommodate the turbocompound unit which results in additional cost in producing the engine. This additional cost can

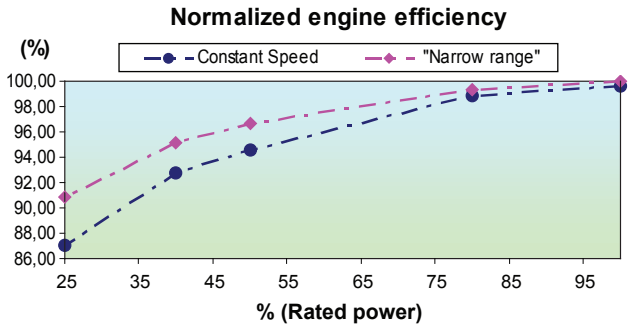


FIGURE 2. Engine Efficiency Comparison in "Constant" and "Narrow range" Speeds

be paid back by decreased fuel consumption over a period of time which depends on the fuel price and the recovered efficiency. To calculate the payback time the following premises have been used:

Truck mileage per day	600 miles (966 km)
Working days per year	240 days
Average fuel consumption	6.5 MPG (reference) (36.2 lit/100 km)
Increased fuel economy	5 – 7 – 10 % improvement
Fuel price	2.5 - 3.0 - 3.5 - 4.0 - 4.5 - 5.0 $/gallon

The added cost for the system will be returned in less than 15 months assuming fuel prices of $2.50 per gallon and the lowest recovered efficiency. Figure 3 shows the payback time for the higher fuel prices and efficiencies.

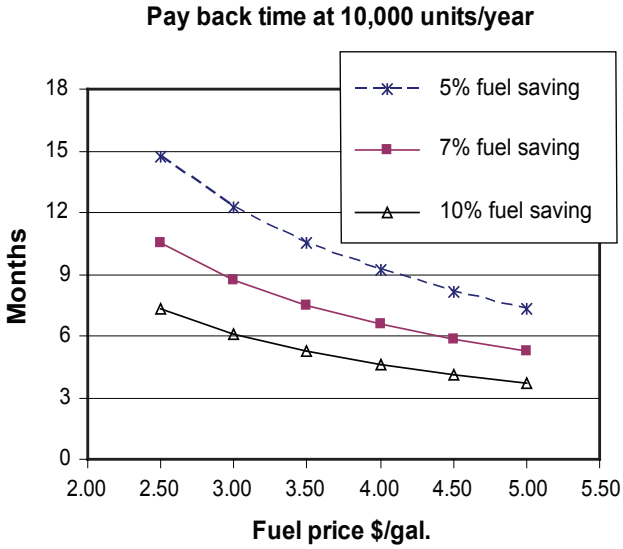


FIGURE 3. Pay Back Time in Months at Various Fuel Prices and Increased Fuel Efficiencies for 10,000 Unit Production Volume per Year

Conclusions

The target for engine efficiency increase was 10% – 13% which was met by achieving 10.5% efficiency improvement when the engine was operating over a steady-state cycle. However, the achievement in the road cycle was 8.2% increase in efficiency. When the engine was coupled to a CVT the efficiency increase was only 5%.

A comprehensive study showed that with a 5% increased efficiency and the fuel price of $2.50/gal, it takes a little less than 1.5 years to compensate the initial charges added to the engine due to the efficiency recovery units. This study has been done for a 10,000-unit production volume per year. With increase in annual production numbers and considering a learning factor of 0.87 the pay back time will reduce significantly.

At the moment, detailed design work is on going to understand the turbo flow characteristics and stress levels with the compressor, turbocharger turbine and compound turbine. This design will satisfy the highly weighted operating conditions.

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FY 2006 Publications/Presentations

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V. OFF-HIGHWAY ENGINE EFFICIENCY R&D

V.1 Exhaust Aftertreatment and Low-Pressure Loop EGR Applied to an Off-Highway Engine

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Objectives

The 2006 objective of this project was to use the MTU 1-D diesel oxidation catalyst (DOC) model and the MTU 1-D 2-layer catalyzed particulate filter (CPF) model to predict the engine exhaust back-pressure, and the filtration and oxidation characteristics of the aftertreatment components as a function of engine loads, configurations and loading time. The loading experimental data was then used to characterize the performance of the DOC and CPF.

Accomplishments

- The MTU 1-D and 2-layer models have been enhanced and calibrated.
- The models predict the pressure drop across the DOC and CPF.
- The models estimate the amount of particulate matter (PM) entering the CPF, the amount oxidized and the amount exiting.

Future Direction

- The project is complete but the next step would be to apply the models to transient operation.

Introduction

An experimental and modeling study was conducted using emissions data measured from the exhaust of a John Deere 6.8 liter, turbocharged and after-cooled engine with a low-pressure loop exhaust gas recirculation (EGR) system which includes a DOC-CPF in the exhaust system. A series of experiments were conducted to evaluate the performance of the DOC, CPF and DOC+CPF configurations at various engine speeds and loads. Pressure drop across the devices, mass of PM deposited in the CPF at the end of loading, upstream and downstream gaseous and particulate emissions, and particle size distributions were measured at different times during the experiments to characterize the pressure drop and filtration efficiency of the DOC-CPF system at each engine load case as functions of loading time.

The project was divided into two tasks. Results from Task I focused on meeting the off-highway Tier 3 emission standards and were reported in 2004; results from Task II focused on meeting the Tier 4 emission standards with improved fuel economy and were reported in 2005. Finally in 2006 the results from the aftertreatment modeling studies are reported in this study.

Approach

The MTU 1-D DOC model was developed as part of this research [1] and is based on similar models available in references 2, 3, 4 and 5. This model uses a one-dimensional single channel representation of the DOC, as shown in Figure 1. The exhaust gas mixture flows through the DOC in a 2-phase flow (gas-phase and solid-phase), and all gaseous species reactions are considered to be occurring in the solid-phase, and at the local substrate wall temperature. The kinetics scheme considered in the model uses equations of the Langmuir-Hinshelwood form [4] for expressing the rates of chemical reactions. There are eight global one-step reactions available in the DOC model.

The detailed description of the MTU 1-D 2-layer CPF model developed as part of previous research at MTU is given in references 6 and 7, and is based on the

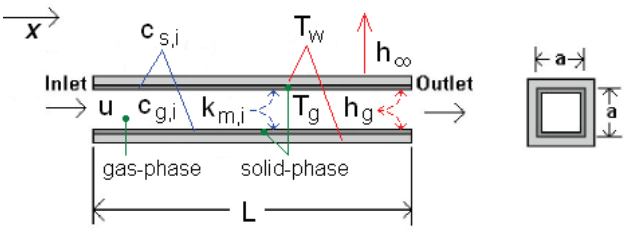


FIGURE 1. Schematic Representation of the Single Channel DOC

regeneration framework presented in reference 8, and the filtration process is based on the model presented in references 9 and 10. Figure 2 shows the representation of the CPF, which uses a single inlet channel, a substrate wall and a single outlet channel, with cross-sectional average values of velocity and exhaust temperature as input to represent all the CPF channels. The oxidation of PM deposited in the CPF takes place through two mechanisms – NO_2/temperature-assisted and thermal. The NO_2/temperature-assisted mechanism for PM oxidation occurs due to the inlet NO_2 as well as NO_2 produced as the exhaust gas mixture passes through the substrate wall. A description of the oxidation sub-model used in the CPF model is given in references 1, 6 and 7.

Results

Figure 3 shows a comparison of experimentally measured and model-predicted pressure drops obtained from the calibrated CPF model in the CPF configuration at the four engine load cases (25, 50, 75 and 100%) at 2,200 rpm, and Figure 4 shows a similar comparison for the four engine load cases in the DOC+CPF configuration at 2,200 rpm. A point-to-point comparison of pressure drop between experimental and model-predicted values showed a maximum variation of 0.85 kPa (in the 50% engine load case) in the CPF configuration and 0.80 kPa in the DOC+CPF configuration for the model-predicted values of ΔP. In the DOC+CPF configuration at 100% engine load case, a maximum variation of 1.22 kPa of the model-predicted ΔP from the experimental ΔP was observed, which is due to the CPF pressure drop model not being able to predict the highly transient variation in PM oxidation rates in the wall. Overall, good agreement of model-predicted CPF pressure drops was obtained in all cases, especially in the cake filtration regime.

Figure 5 and 6 show the mass balance curves from the calibrated CPF model outputs for the four

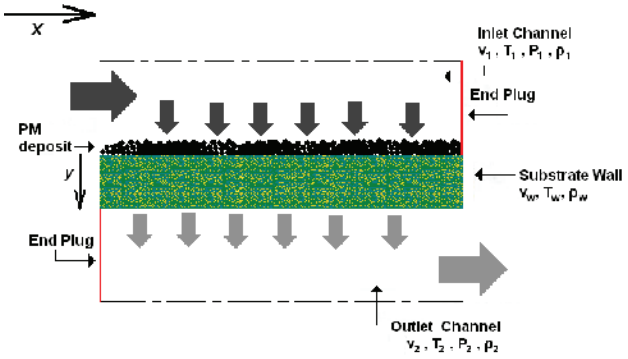


FIGURE 2. Schematic of Single Channel Representation used in CPF Model

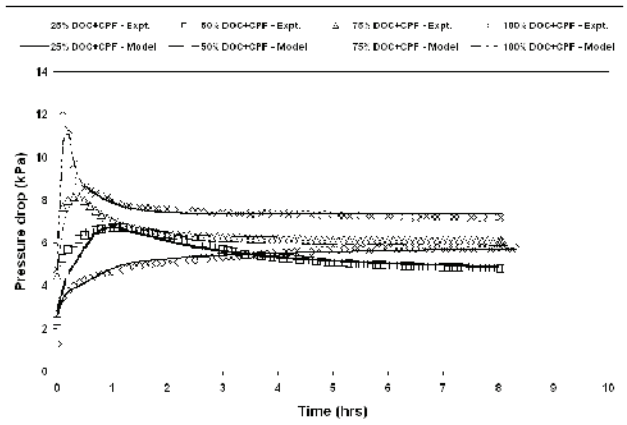


FIGURE 4. Comparison of experimental and model-predicted CPF pressure drop at various engine load cases in the DOC+CPF configuration at 2,200 rpm.

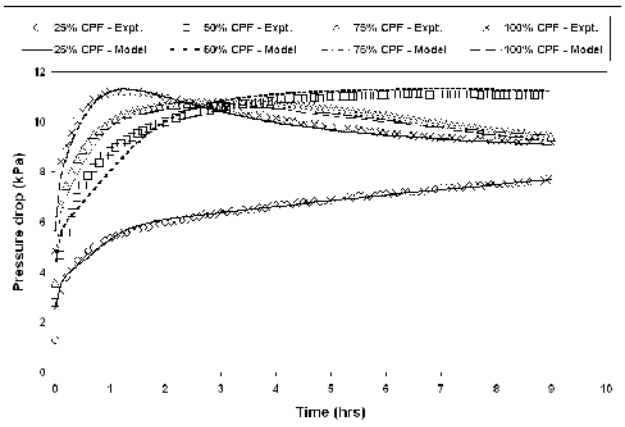


FIGURE 3. Comparison of experimental and model-predicted CPF pressure drop at various engine load cases in the CPF configuration at 2,200 rpm.

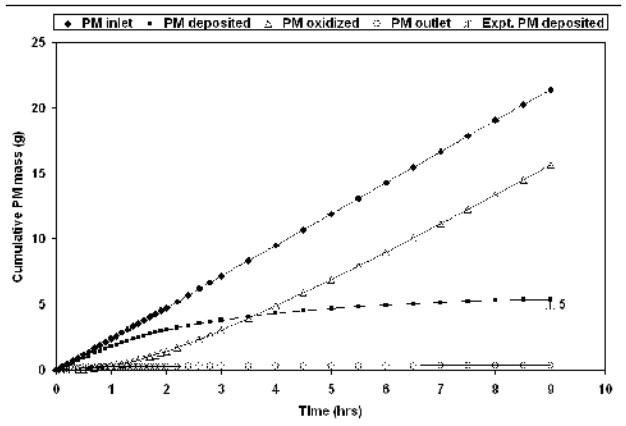


FIGURE 5. Particulate mass balance curves obtained from the calibrated CPF model at 100% engine load case in the CPF configuration at 2,200 rpm.

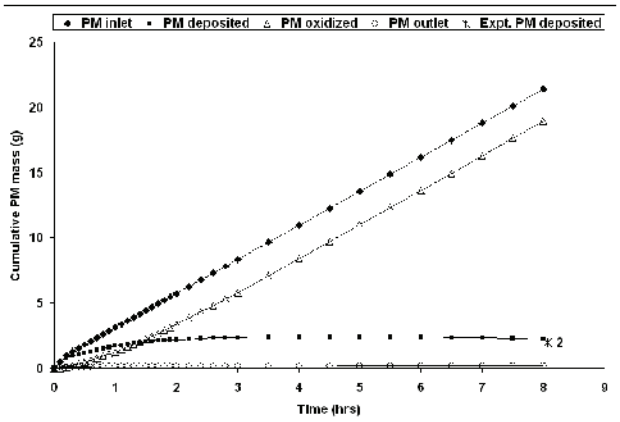


FIGURE 6. Particulate mass balance curves obtained from the calibrated CPF model at 100% engine load case in the DOC+CPF configuration at 2,200 rpm.

engine load cases studied. The experimental PM mass deposited in the CPF at the end of loading are also shown, labeled by their numeric values in *grams*. 'PM inlet' curves for each engine load case were linear since the CPF inlet PM concentrations and volumetric flow rates for the CPF model were considered to be the load-average values. 'PM deposited' for each engine load case shows the cumulative values, and was the sum of PM deposited in the PM cake layer as well as the substrate wall, although the majority of PM mass deposited was in the PM cake layer. Similarly, 'PM oxidized' curves also were the sums of PM mass oxidized in the PM cake layer and substrate wall. 'PM outlet' curves show the cumulative PM mass that had exited the CPF till the particular loading time since start of loading simulation. For both Figures 5 and 6 the PM deposited agreed well with the total PM mass measured in the CPF. Note that the DOC+CPF configuration had significantly higher PM oxidized due to the higher concentration of NO_2 in the exhaust.

Conclusions

- The MTU models accurately predicted the pressure drop across both the DOC and the DOC+CPF aftertreatment for various engine speeds and loads under steady-state operation.
- The MTU models also accurately predicted the amount of mass deposited and oxidized in the CPF as a function of time.
- The next step would be to apply transient operation to the MTU models to determine if they can be used to predict when an active regeneration would be required.

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V.2 Electrically Coupled Exhaust Energy Recovery System Using a Series Power Turbine Approach

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NETL Project Manager: Ralph Nine

Subcontractors:
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- International Truck, Fort Wayne, IN

Objectives

The overall objective of this project is to demonstrate the technical benefits of electrically coupled turbo compounding. Specific objectives for 2006 included:

- Develop hardware and software suitable for vehicle demonstrations.
- Confirm compatibility of the technology with Tier 3 emissions regulations.
- Demonstrate performance characteristics on the dyno and in vehicles.

Accomplishments

- Through component optimization and turbo system matching, performance goals of 20% power growth and a 10% increase in fuel economy have been demonstrated at Tier 3 emissions levels.
- A compact 50 kW flywheel mounted motor/generator system was developed and tested. System efficiencies of over 95% in the key operating areas for off-highway equipment were demonstrated.
- A Deere 8530 tractor has been built and tested with a complete turbo compounding system. Power recirculation and system compatibility has been successfully demonstrated. The tractor is ready for fuel economy and productivity testing on the test track and field.
- A Deere 9L engine has been installed in an International 8600 truck and tested at the National Renewable Energy Laboratory (NREL). Results showed mileage equivalent to the base M11 truck engine. Turbo compounding hardware including a high power hybrid transmission and battery pack have been designed, built and tested. This equipment is now being installed into the truck and will be retested at NREL in early 2007.
- A variable geometry power turbine was developed and tested. The ability to increase part load system output by 50% was demonstrated. Fuel economy improvements were limited to less than 2%.
- Based on successful demonstration of concept demonstrator hardware, a second generation system has been designed. A more automotive-style turbo generator has been designed that uses higher rotor speeds with a revised speed control algorithm to improve system efficiency.

Future Directions

- Test vehicles under realistic operating cycles to document real world benefits in both fuel economy and vehicle productivity. This includes both tractor and truck evaluations.
- Develop second generation hardware with improved performance and greater commercialization potential. Updated turbo machinery will be critical here, particularly development of a turbocharger system that will provide high efficiency and adequate surge margin.
- Define optimal system architecture and power splits for Tier 4 emissions compatibility. Emphasis will be on aftertreatment and exhaust gas recirculation (EGR) plumbing.
- Increase scope of application of turbo compounding by evaluating performance enhancements in both larger and smaller engine platforms. Start with modeling to define potential and adapt existing hardware to demonstrate if advantages justify.

Introduction

The objective of this project is to characterize fuel economy and power growth benefits of electrically coupled turbo compounding, a waste exhaust heat recovery technology. This technology is becoming viable due to the commercialization of cost-effective high efficiency electrical components and controls, and

because of increased emphasis on fuel economy. Bare engine and in-vehicle testing are being employed to develop valid performance assessments of the concept. Integrating the technology with emissions-driven engine changes to synergistically optimize system performance is a key requirement for successful implementation.

Approach

High power steady-state duty cycles glean maximum benefit from turbo compounding due to the greater time averaged energy availability compared to lighter duty cycles. Agricultural tractors fit this definition as do many on-highway trucks. A Deere 9.0L Tier 3 engine was selected as a demonstration platform since this engine is in a power class that fits both large agricultural tractors and on-highway Class 8 trucks. Special turbo compounding hardware including a high performance single stage high pressure ratio turbocharger, a high efficiency turbo generator, and a compact and efficient flywheel motor generator were designed, analyzed, built, and tested. Engine performance characteristics using this experimental hardware were compared to baseline engine performance. Performance development work completed in FY 2006 was focused on comparisons at Tier 3 emissions levels, while efforts are continuing to define optimal architecture for Tier 4.

Although bare engine performance provides an acceptable measure of the potential benefit offered by turbo compounding, it is ultimately necessary to apply the hardware to vehicles that can be evaluated under typical duty cycles to assure the benefits translate to real world fuel savings. This is due to different levels of benefit over the operating envelope, as well as potential transient effects. Vehicle testing is also useful in defining challenges that must be addressed in order to allow successful commercialization. Two vehicles were built to evaluate fuel economy benefits. A large 8530 Deere row crop tractor was upgraded to provide an additional 50 kW of power to the ground. The additional power was provided by the turbo compounding system. A 50 kW motor generator system was also integrated into the tractor drive train to couple the turbo generator output back into the tractor drive train. The base tractor was upgraded in order to be able to deliver the added power to the ground. This was done by stretching the wheelbase and applying significantly larger experimental tires.

In order to explore broader application of the technology, a Deere 9L engine was installed into an 8600 International truck. Baseline testing of the truck was required since this engine has not been applied to truck applications before. Testing was completed at NREL, showing the same fuel economy as the original truck engine. Hardware to add the complete turbo compounding system including an electric hybrid transmission and electrical energy storage system were also designed and built. Vehicle testing with the turbo compounding system is scheduled to be completed in early FY 2007.

Results

Output characteristics of a 50 kW electrically coupled turbo compounding system applied to a Deere 275 kW 9L diesel engine are shown in Figure 1. The engine meets Tier 3 off-highway standards. Results show output power from the turbo compounding system being reasonably linear with load and speed with maximum contribution at rated speed. The fuel economy plot in Figure 2 shows the benefits compared to a baseline non-turbo compounded engine over the speed range.

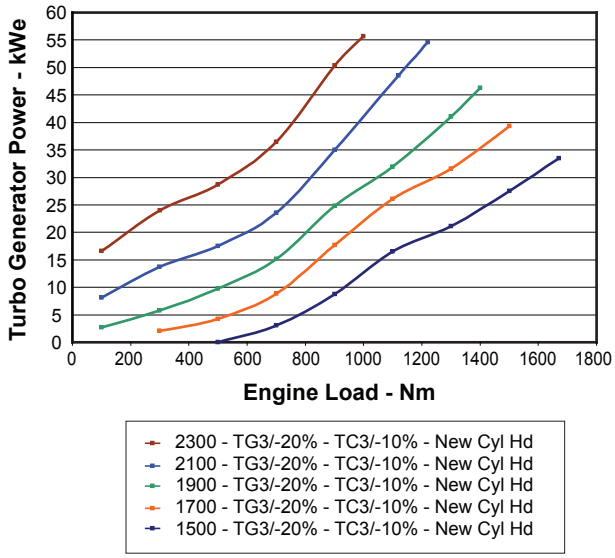


FIGURE 1. Typical System Output Characteristics

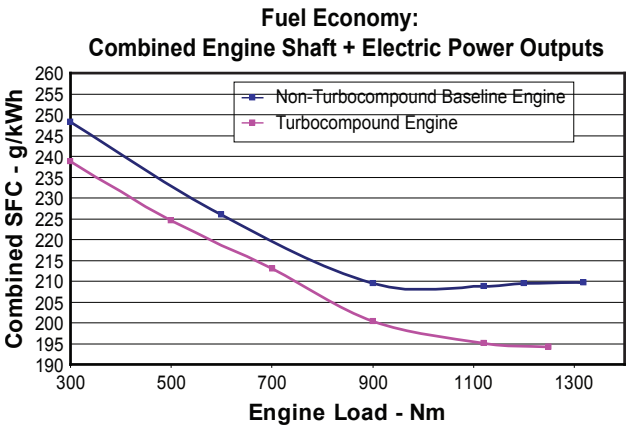


FIGURE 2. Specific Fuel Consumption (SFC) Characteristics at 2,100 RPM

Figure 3 shows a photo of the hardware as it was tested in the dyno. A variable geometry power turbine was developed and tested in an effort to extract more power at light loads common in many applications. An increase in output of 60% was demonstrated at the design point with modest improvements is overall fuel economy. Figure 4 shows the brake specific fuel consumption at 1,900 RPM.

Vehicle testing is needed to accurately characterize fuel economy benefits. A complete turbo compounding system was applied to a John Deere 8530 tractor. The machine is shown operating at high load on the power take-off dyno in Figure 5. The tractor is now ready for test track evaluation. Figure 6 shows the Deere 9L engine in the 8600 International truck. The truck was tested at NREL to define baseline fuel economy. Test results matched the baseline engine in the truck at 5.44 MPG on the West Virginia test cycle. Figure 7 shows the truck on the chassis dyno. The truck is now being rebuilt with turbo compounding hardware and is planned to undergo testing some time after March 2007.

Tier 4 emissions significantly impact the benefit of turbo compounding. Higher EGR rates rob the power turbine of flow with high-pressure loop EGR architectures. Flow restrictions due to diesel particulate filters are multiplied by the turbine pressure ratios, and

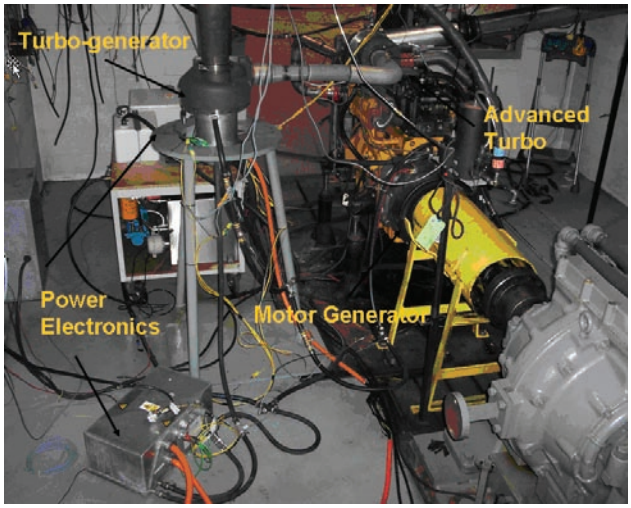


FIGURE 3. Electric Turbo Compounding System Hardware – Dyno Installation

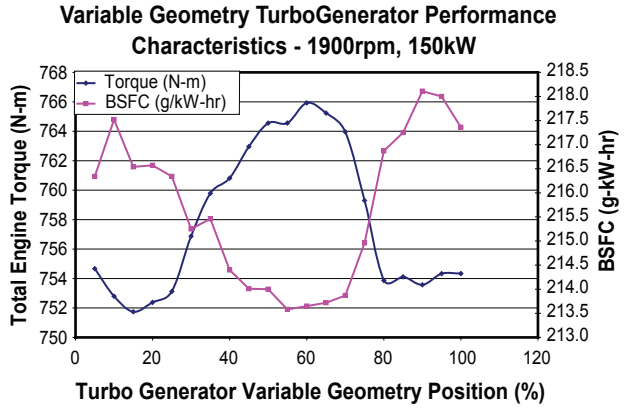


FIGURE 4. Performance of Variable Geometry Power Turbine



FIGURE 5. Turbo Compounded 8530 Tractor on Dyno



FIGURE 6. View of Truck Showing Deere 9L Engine in 8600 International Truck



FIGURE 7. Truck Running on NREL Chassis Dyno

this can significantly reduce the allowable pressure ratio and system output. Fuel economy with low-pressure loop EGR has been shown to be 3% better than with high-pressure loop and heat rejection is also significantly lower. Power growth with low-pressure loop EGR is also substantially greater. Turbo compounding eliminates the need for a variable geometry turbocharger, significantly reducing system complexity and cost.

Conclusions

Electric turbo compounding can deliver fuel economy benefits of 10% and provide power growth capability of 20% or more at Tier 3 emissions levels.

Turbo compounding is compatible with Tier 4 emissions regulations, but additional work is required to define optimal system architecture and performance. This is the subject of FY 2007 work that will address not only emissions, but also development of truly automotive hardware. Low-pressure loop EGR provides significant benefit, but also presents technical challenges.

System integration and performance has been demonstrated. Hardware has been shown to be reliable, and controls have proven manageable.

VI. HEALTH IMPACTS

VI.1 Health Effects from Heavy-Duty Diesel Emissions at the Watt Road Environmental Laboratory

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DOE Technology Development Manager:
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Objectives

- Improve understanding of "real-world" mobile source evolution as a function of meteorology, geography, and traffic at unique site near Knoxville, TN with high volume of heavy-duty truck traffic (>20,000 trucks per day on Interstates 40&75).
- Understand potential impact of developing fuel, combustion, and aftertreatment technologies on air quality and, thereby, human health.

Accomplishments

- Three remote sensing techniques were deployed in two field campaigns at the I-40/75 weigh station. Ultraviolet (UV), light detection and ranging (LIDAR) and acoustic techniques measured NOx, PM, and engine parameters, respectively, to obtain emission distributions as a function of truck weight, speed, and other parameters.
- In cooperation with the Federal Highway Administration (FHWA), a project concentrating on ambient air quality near the Watt Road-I-40/75 interchange was completed. The project showed that idling trucks typically dominate the air quality near the roadway despite the large number of trucks traveling on I-40/75 per day.
- Presented results to and interacted with stakeholders at four conferences.

Future Directions

- Characterization of mobile source air toxics (MSATs) from advanced engine and aftertreatment systems.
- Measurement of MSATs at higher time resolution measurements in order to understand mobile source impacts.
- Continued deployment of the remote sensing instrumentation for evaluation of end use emissions.

Introduction

The Watt Road Environmental Laboratory (WREL) is an active real-world laboratory devoted to (1) the study of actual in-use emissions of heavy trucks and (2) defining their impact on local air quality and thereby on human health. This unique laboratory is located near Oak Ridge National Laboratory where approximately 20,000 heavy-duty trucks per day pass by an interstate interchange that also contains multiple travel center facilities. The mid-south location means that the atmospheric conditions, in particular relative humidity, more accurately reflect the climate in which 75% of the U.S. population lives than the desert southwest, where most air quality studies are performed. This real-world laboratory serves as a national resource for studies of the impact of mobile emissions on local and regional air quality and the health effects from those emissions. Because of interest in the Watt Rd. site from multiple stakeholders, there have been a variety of sponsors including the Knox Co. Municipal Planning Organization (MPO), the Federal Highway Administration (FHWA) as well as DOE.

This project, under the direction of Dr. James Eberhardt, has focused on the health effects of in-use diesel truck emissions. By combining field measurements of emissions sources with air quality, meteorological and geographical data, air quality models are developed and validated so that contributions of mobile sources to local and regional air quality can be defined. The link between mobile sources and air quality must be understood to determine the health impacts on the human population by mobile sources.

Approach

The emphasis of the Watt Road Environmental Laboratory project has been on real-world measurement of emissions and air quality. In general, the approaches involved can be categorized into three areas: (1) mobile source characterization, (2) ambient air quality characterization, and (3) simulation and understanding of source contributions to air quality. Remote sensing has enabled the mobile source characterization, and various analyzers have been employed for ambient

air quality studies. The tasks for simulation and understanding of source contributions to air quality have involved multiple techniques, but in general, efforts have centered on analyzing the data obtained from remote sensing and ambient air quality studies to compare the data with models. The comparison of data and model outputs allows further interpretation of the environmental chemistry of mobile source impacts on ambient air quality; in addition, the data allows validation and databases for models. A particular focus of the analysis and modeling has been fine-scale modeling. This report will present FY 2006 results from remote sensing campaigns to characterize mobile source emissions from heavy-duty trucks.

Results

Two remote sensing field campaigns were conducted in FY 2006 to measure the emissions from heavy-duty trucks. Both campaigns were conducted at the eastbound weigh station on I-40/75 just west of Knoxville, TN. The campaign was conducted in cooperation with the Tennessee Department of Safety which operates the weigh station, and we are grateful for their support of the project. Emissions from heavy-duty trucks accelerating away from the weigh scales were measured with several remote sensing techniques. Truck weights and other general truck information were recorded as well.

The remote sensing techniques employed were ultraviolet (UV) differential adsorption spectroscopy, acoustic analysis, and LIDAR. The UV technique was deployed to measure NO emissions. The acoustic technique allowed measurement of several engine and truck operational parameters such as vehicle speed, engine speed, and turbo speed. LIDAR was employed to measure particulate matter (PM) emissions.

The UV spectroscopic technique measured NO concentration over a light beam path by measuring the absorbance of NO in the 226 nm spectral region. Essentially, the remote sensing was performed by passing a UV light beam through the air across the roadway above the height of the trucks. The UV light was actually passed across the truck lane then returned along the same path with a retroreflector mirror. The returning light was collected and analyzed with a UV spectrometer. A picture of the setup is shown in Figure 1. With this arrangement, the emissions from one truck at a time were measured. The height of the beam path above the exhaust pipe of the truck was varied in position between one and five feet above the regulation height for 18-wheeler trucks.

An example of the NO emissions as a function of time during the campaign is shown in Figure 2; here the presence of a truck pulling away from the weigh scales is noted by a yellow circle. Spikes in NO concentration occur in conjunction with the trucks accelerating away from the weigh scales, but the amount of NO and general profile vs. time varies for the trucks due to differences in truck weight, engine type, engine operation, and acceleration speed, etc. The NO emission peaks for each truck were analyzed and combined with other data obtained in the campaign for analysis.

An acoustic-based technique allowed characterization of truck engine operating parameters from data obtained by placing microphones near the truck lane. The detection equipment for the acoustic technique is simple and low cost; the strength of the technique lies in the analysis of the spectrogram which contains a wealth of information. Detailed analysis of the spectrogram for each truck allowed measurement of the engine speed and acceleration, the turbo speed and acceleration, and the vehicle speed and acceleration (via audible indicators on the road). An example spectrogram is shown in Figure 3; here the higher frequency curves represent turbo speed and the lower frequency streaks of data represent engine speed. Based



FIGURE 1. Picture of the UV remote sensing technique being deployed during a field campaign at the I-40/75 weigh station.

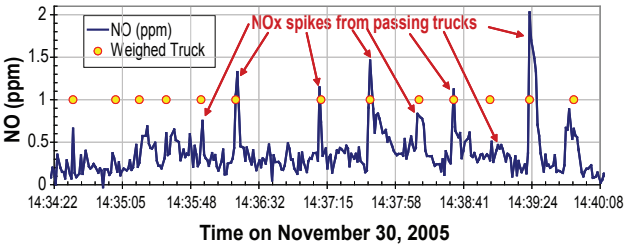


FIGURE 2. Example UV remote sensing data from a weigh station field campaign showing NOx emissions as a function of time. Yellow circles note occurrences of passing trucks.

on assumptions for engine displacement and number of cylinders, a mass flow of exhaust from the truck was computed; this mass flow was combined with the NO concentration data to determine NO mass emissions.

The combined UV NO measurements and acoustic truck operational parameter measurements allowed a database of truck emissions as a function of several parameters to be generated. An example of some of the data is shown in Figure 4; peak NOx emissions in g/minute are shown as a function of truck weight. The distribution of truck emissions obtained provides a database for models; in particular, emissions data from trucks with weights above 60,000 pounds is in relatively short supply since heavy-duty truck dynamometer emission measurements become difficult at higher truck weights.

The LIDAR technique measures PM concentration and physical location based on the backscattered light intensity. A laser diode of similar power to a common laser pointer was the light source for the LIDAR system. The laser diode was modulated at frequencies of 10-200 MHz and launched into the air above the truck exhaust port at the same height as the UV technique beam path. The backscatter laser light was detected by a collection telescope and measured with a photomultiplier tube (PMT) detector. Lock-in amplification of the modulated light and a narrow bandpass filter on the PMT allowed sensitive detection of the backscattered light in the presence of bright daylight. Analysis of the signal magnitude and phase shift for a set of different modulation frequencies results in a plot of PM concentration vs. position. The details of the analysis technique and the relationship between the detector signal-to-noise and PM concentration are given by M. L. Simpson *et al* [1]. To validate the technique, LIDAR measurements of PM from a light-duty diesel vehicle were made during a chassis dynamometer test and compared with results from a scanning mobility particle sizer (SMPS). A schematic of the LIDAR setup is shown in Figure 5. ORNL worked closely with Galt Technologies, a small company specializing in optics and spectroscopic applications, to develop the LIDAR system.

The field campaigns at the weigh station in FY 2006 represented the first deployment for the novel LIDAR technique in this application; thus, the results gave valuable insight into the feasibility of LIDAR for PM remote sensing. Example data from the campaign is shown in Figure 6. The PM concentration signal peaked above noise levels for only a small percentage of the trucks that were remotely sensed. The large signals observed with the LIDAR technique were due to trucks with soot plumes visible to the naked eye. Moderate size peaks are indicative of PM emissions below the visibility

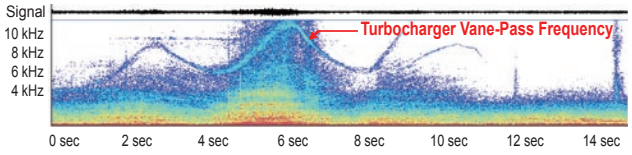


FIGURE 3. Acoustic spectrogram of a heavy-duty truck accelerating away from the weigh scales.

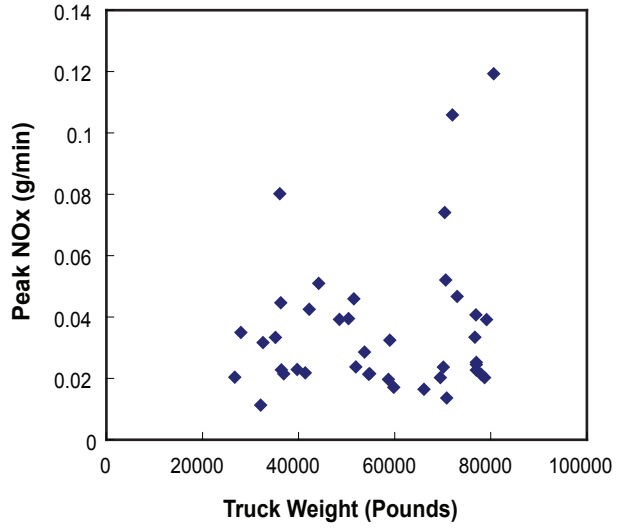


FIGURE 4. Distribution of NOx emissions as a function of truck weight.

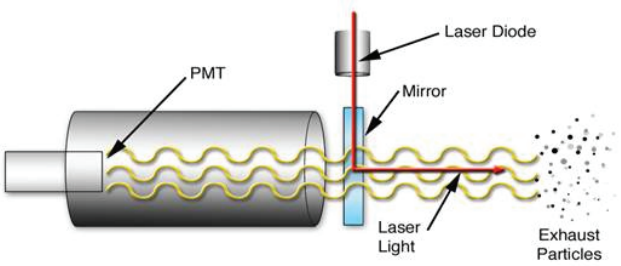


FIGURE 5. Schematic of the LIDAR technique for PM remote sensing.

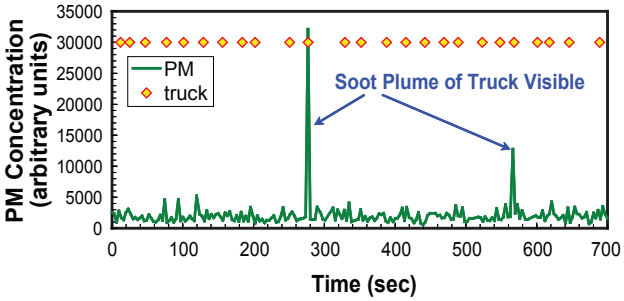


FIGURE 6. Example PM remote sensing data obtained with the LIDAR technique during a weigh station field campaign. Yellow diamonds note occurrences of passing trucks.

threshold. During these initial studies, measurements of PM emissions from heavy-duty trucks with a LIDAR technique were demonstrated for the first time. The results indicate that the technique is feasible, but improvements must be made in the dynamic range of the instrument to be capable of measuring of low PM emission trucks.

Conclusions

Remote sensing techniques have been deployed in the field to measure emissions from heavy-duty trucks at a weigh station on Interstate 40/75. UV spectroscopic measurements of NO emissions were coupled with truck operational data characterized with an acoustic analysis technique to determine mass-based emissions in a non-intrusive manner. The distribution of truck emissions obtained provides a database for models; in particular, the emissions as a function of truck weight at >60,000 pounds are of value. The first deployment of a LIDAR technique for PM measurement from heavy-duty trucks led to a demonstration of the feasibility of the technique and a definition of needed improvements in the technique (specifically dynamic range).

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VI.2 Weekend Ozone Effect Studies

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James J. Eberhardt

Subcontractors:
- Envair, Berkeley, CA
- ENVIRON, Novato, CA

Objectives

- Ambient ozone (O_3) levels in southern California are about 50% higher on Sundays than on mid-week days. The objective of this study is to identify whether this phenomenon exists in other parts of the U.S. that experience violations of the national ambient air quality standard for ozone.
- This project characterized day-of-week differences in:
  - ambient concentrations of primary pollutants, including nitric oxide (NO), oxides of nitrogen (NOx), speciated volatile organic compounds (VOCs), carbon monoxide (CO), and black carbon (BC);
  - ambient concentrations of ozone and particulate matter (PM) nitrate;
  - responses of ozone and PM nitrate concentrations to changes in the ambient concentrations of primary pollutants.

The principal focus is on the gas-phase species NO, NOx, CO, VOCs, ozone, and PM nitrate.

Accomplishments

- Completed analysis of 1998-2002 or 2003 ambient ozone precursor and ozone data from many U.S. monitoring locations.
- Wrote and sent draft report to air quality staff in the regions/states studied for technical comments and peer review. The report was sent to the states of Arizona, Texas, and Colorado; Northeast States for Coordinated Air Use Management; Mid-Atlantic Regional Air Management Association; and the Lake Michigan Air Directors Consortium.
- Submitted paper summarizing study results to the *Journal of the Air & Waste Management Association* for peer review and subsequent publication.

Future Directions

Began proximate ozone modeling study in southeast Michigan region in November 2005, in collaboration with state and local government groups and industry representatives in that area. This project will be completed in FY 2007.

Introduction

The occurrence of generally comparable – or even higher – ambient concentrations of ozone on Saturdays and Sundays than on other days of the week is commonly known as the "weekend effect for ozone," or, simply, the "weekend effect." Because emissions of ozone precursors, including volatile organic compounds (VOC), oxides of nitrogen (NOx), and carbon monoxide (CO), are lower on weekends than on weekdays, the weekend ozone effect is counterintuitive. To provide a better understanding of the implications of the weekend effect, a thorough analysis of weekday and weekend precursor concentrations and composition is needed. Observed in air quality data from the mid-1960s and early 1970s, the weekend effect in California recently has been studied at length. Fujita *et al.* [1] and Lawson [2] conclude that weekend reductions of NO emissions are the most important factor leading to higher weekend ozone, allowing ozone to accumulate earlier in the day and to reach higher concentrations compared with weekdays, and that proposed alternative hypotheses are not supported by ambient data and do not explain the weekend effect in southern California. In contrast, Croes *et al*. [3] considered the available air quality data and photochemical models inadequate to conclusively determine the causes of the weekend ozone effect in southern California.

This study provides further analysis of the weekend ozone effect in areas of the United States outside California. The weekend ozone effect provides air quality managers and scientists the opportunity to make empirical observations of the kind that are so important in testing hypotheses by asking "What if" questions regarding emission reductions that are needed to reduce ambient O_3 levels. Seldom are such opportunities available using ambient data regarding how the atmosphere actually responds to changes in emissions

because most air quality regulations provide small incremental benefits and take effect over long periods of time.

Approach

The analyses were carried out at ambient air quality monitoring sites in ozone problem areas in 23 states: the Northeast corridor (including the New York-Northern New Jersey-Long Island, Philadelphia-Wilmington-Trenton, and Baltimore-Washington metropolitan areas); the Gulf of Mexico coast (including the Houston-Galveston-Brazoria and Beaumont-Port Arthur and Baton Rouge metropolitan areas); Dallas-Fort Worth; Phoenix; and the Colorado Front Range area (including Denver, Colorado Springs, Boulder, and Fort Collins). Previous work carried out for the Atlanta area and for six Midwestern states (Ohio, Michigan, Indiana, Illinois, Missouri, and Wisconsin) was also incorporated in this study. The time period analyzed was 1998 through 2002 (or 2003 where data were available).

Results

Ambient air quality monitoring data were analyzed to evaluate the differences between mean day-of-week ambient concentrations of ozone precursors (NO, NOx, CO, and VOC) using 1998-2003 ambient air-pollutant data from monitoring sites in 23 states in New England, the Midwest, the mid-Atlantic, and isolated urban areas in the western and southern U.S. During the months of March through October, median decreases of NO, NOx, and CO at 6 a.m. Sundays compared with 6 a.m. Wednesdays were 71, 58, and 42 percent, respectively, as shown in Figure 1. The median declines of NO, NOx, and CO at 12 noon Sundays compared with 12 noon Wednesdays were 46, 40, and 12 percent, respectively. The Wednesday/Sunday PM nitrate median decline at 69 sites was 2.6%, with the difference statistically significant at only one location.

The large reductions in ambient concentrations of ozone precursors on weekends did not produce meaningful reductions of ambient ozone levels. To the contrary, median 1-hour and 8-hour ozone daily maxima on Sundays increased by 1 and 3 percent, respectively, from their mean peak levels on Wednesdays. When restricted to high-ozone days, the median 8-hour ozone daily maxima were unchanged on Sundays compared with Wednesdays, while the median 1-hour peak ozone levels decreased by 2 percent from Wednesdays to Sundays.

The changes observed in weekend ozone levels relative to weekday concentrations were the net result of weekday/weekend differences in a number of processes affecting ozone formation, including emissions, ozone transport, and local ozone formation:

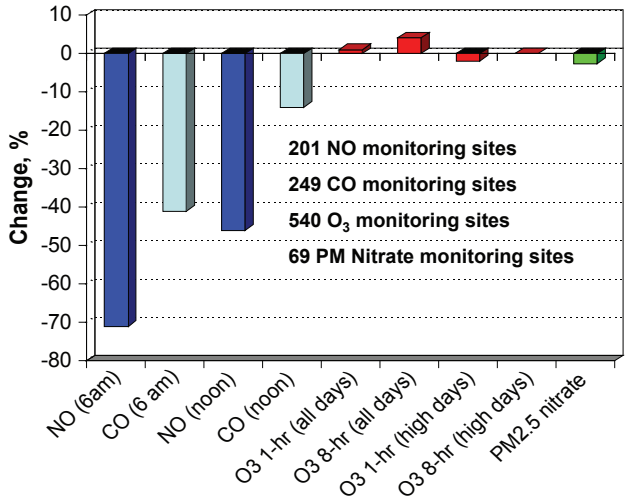


FIGURE 1. Median ambient pollutant concentration changes from Wednesdays to Sundays. Results are shown for morning and noon concentrations of NO, NOx, and CO (March – October), and for 1-hour and 8-hour peak ozone concentrations on all ozone-season days (March – October) and on high-ozone days (top three peak days per day of week per year). PM nitrate levels are obtained from 24-hour sampling periods. Negative values represent higher Wednesday concentrations than on Sundays; positive values indicate that concentrations were higher on Sundays than on Wednesdays. The time period analyzed was 1998 through 2003.

- Ozone accumulation began about one hour earlier on Sundays than on Wednesdays. Ozone can accumulate only after NO concentrations fall to low levels.
- Regional ozone levels contributed the majority of the peak ozone concentrations measured downwind of four urban areas where ozone transport was studied in detail (Atlanta, Chicago, Dallas-Fort Worth, and Phoenix).
- Statistically significant day-of-week differences in ozone levels did not occur at either upwind or downwind locations. Ozone concentrations averaged about 5 to 10 ppbv lower on Sundays than on Wednesdays upwind of Atlanta, Chicago, and Phoenix; none of these differences were statistically significant, and no day-of-week transport differences were observed for Dallas-Fort Worth. Data from the northeastern U.S. are depicted in Figure 2.

Conclusions

The weekend ozone effect provides a natural experiment for understanding how urban ozone and PM nitrate respond to large reductions in ozone precursor emissions. The data suggest that, for ozone problem areas in and downwind of urban U.S. locations, VOC emission reductions reduce ozone, while NOx emission reductions increase ambient ozone levels. Despite large weekend reductions of NO emissions, there is little

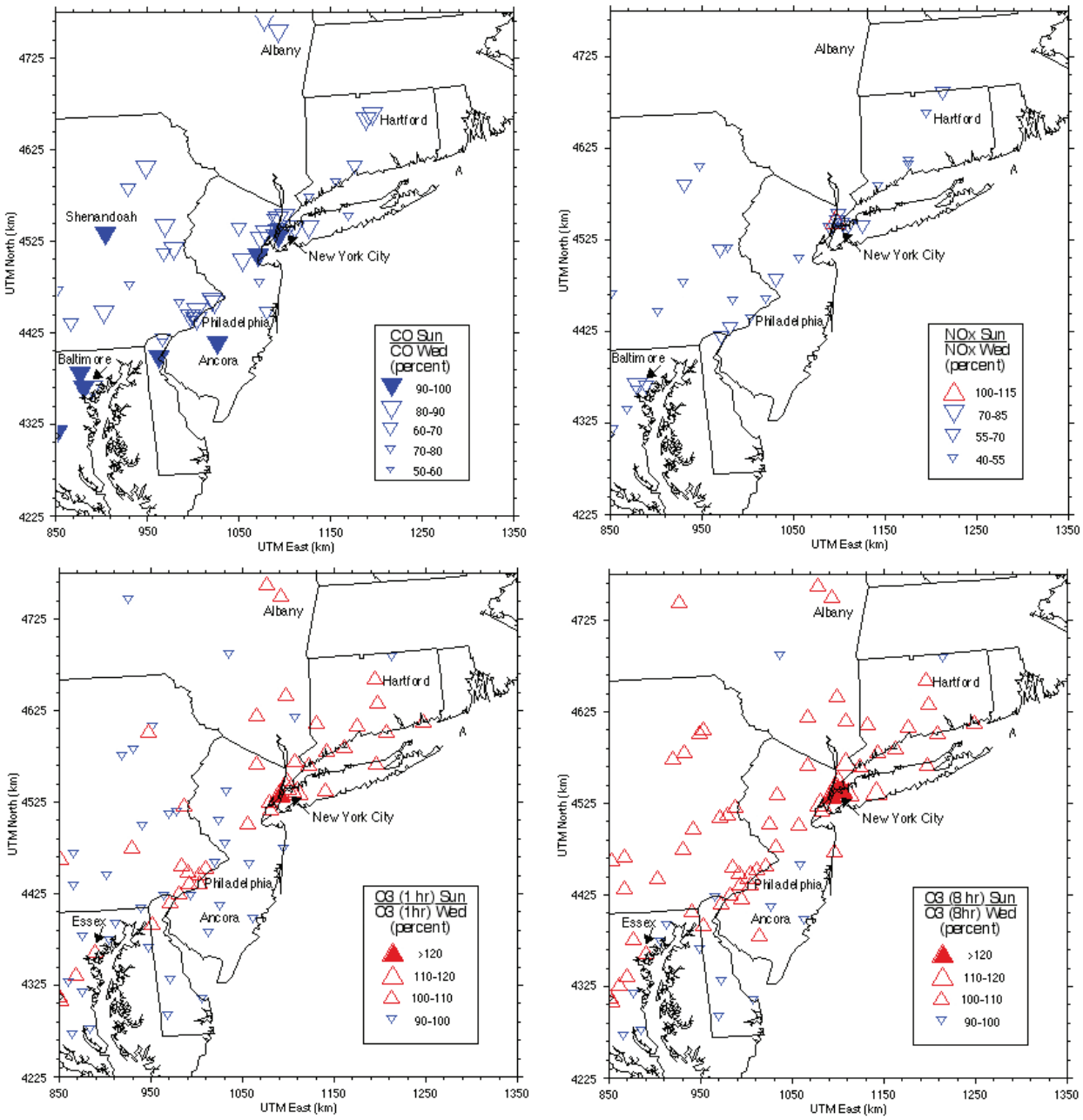


FIGURE 2. Geographical comparisons of mean Sunday to mean Wednesday daytime (6 a.m. through 3 p.m.) concentrations of CO and NOx and mean peak daily one-hour and eight-hour ozone in the Northeast. The differences were determined from all days, March-October 1998-2003.

change in PM nitrate concentrations on weekends. The findings from this study may require a rethinking of present control strategies to reduce urban ozone and PM nitrate exposure and ozone transported downwind of urban locations in the U.S.

We interpret the observed absence of differences between weekday and weekend ozone levels, in combination with significantly lower ambient levels of NOx, as an indication that ozone formation in our study areas is VOC-limited. Our analyses of weekday/weekend differences in ozone precursor emissions show that different emission reductions of ozone precursors than normally take place on weekends will be required before significant reductions in ambient ozone can be achieved. Yet, in relative magnitudes, the emission changes that are projected to occur between now and 2010 more closely resemble the weekend reductions that we report here than the historical emissions trends, in which VOC emission reductions have exceeded reductions of NOx emissions on a relative basis. Our

results call into question the rates of future progress in reducing peak ozone levels in major metropolitan areas in the United States.

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VI.3 Health Impacts: Respiratory Response

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Objectives

- Define relative health hazards of competing existing power technologies
- Determine contributions of different fractions of emissions to health hazards
- Evaluate health benefits of emission reduction technologies
- Evaluate emerging technologies for unanticipated health hazards

Accomplishments

- Developed technology to generate nanoparticle aerosols from engine crankcase oil
- Discovered that used diesel crankcase oil nanoparticles have low lung toxicity, but may suppress systemic immune responses
- Completed a comprehensive study of the effects of repeated inhalation exposure to laboratory-generated gasoline emissions
- Discovered that non-particulate emissions from gasoline engines can cause vascular changes in a mouse model of atherosclerosis

Future Directions

- Complete work to clarify health importance of nanoparticle (< 50 nm) components of diesel emissions, and relative importance of black carbon- vs non-solid condensate-based particles
- Complete study testing the hypothesis that artifactual formation of nitro-aromatic compounds on filter samples is responsible for much of the mutagenicity of diesel particle extracts
- Complete analysis and publication of results from study of gasoline emissions, and comparison to effects of diesel emissions

Introduction

This project is the biological evaluation component of the Health Impacts Program, and supports meeting DOE technical targets by: 1) placing in proper context the health hazards of engine emissions relative to other air quality hazards, and the relative hazards of emissions from different fuel, engine, and emission reduction technologies; 2) determining the key toxic components among the hundreds of components of vehicle emissions; and 3) evaluating emissions from emerging technologies to avoid unintended health consequences prior to commercialization and demonstrate that reductions in emissions are paralleled by reductions in health hazards. This project addresses potentially technology-limiting issues that are not addressed in other DOE or non-DOE programs. This project complements other Health Impacts projects that are characterizing emissions, determining the impact of emissions on air quality, and conducting long-term health studies of 2007-2010-compliant diesel systems.

Approach

This project employs a four-tactic strategy to placing the health hazards of vehicle emissions in proper context, identifying the key toxic components, and evaluating new technologies. The first tactic involves laboratory evaluations of emission samples collected from vehicles and environments elsewhere. The second tactic involves animal studies of inhaled whole emissions, separated fractions of emissions, and specialized aerosols generated in the laboratory. Tissue oxidative stress, lung inflammation, cardiovascular effects, and immune responses are evaluated. The third tactic employs multivariate and univariate statistical analyses of data on composition vs. biological response to identify components that cause adverse effects. The fourth tactic involves working with DOE program managers and industry partners to identify advanced technologies having the greatest near-term commercialization potential, and using the above approaches to evaluate those technologies for unintended health consequences.

Work during the past year focused primarily on two issues pertaining to current technologies in order to clarify issues that must be addressed for emerging technologies: 1) the health importance of organic condensate nanoparticles; and 2) the health effects of particulate and non-particulate components of gasoline engine emissions. There has been considerable speculation about the health effects of so-called “nanoparticles” (under 50 nm diameter)

from combustion and other sources, and the non-solid condensate species are hypothesized by some to be of concern for future emissions. Such particles have always existed in engine emissions, but no technology has been successful for separating condensate particles from other emissions for health studies. Because crankcase oil is the primary source of this material, this project undertook to develop a method for generating nano-sized aerosols from crankcase oil in the laboratory. Developmental work led to the successful generation of aerosols by a vaporization-condensation method followed by carefully controlled cooling and dilution to produce suitably small particles.

Despite the overwhelming attention to the potential health hazards of diesel emissions, there has been little evaluation of gasoline emissions. Because gasoline emissions contain a greater proportion of mass in the vapor phase, parsing the effects of particulate vs. non-particulate effects can provide important insights into the physical-chemical species responsible for effects of whole emissions. This project collaborated with other federal and non-federal partners (including several major large engine and fuel providers) to conduct a detailed study of the respiratory and cardiovascular effects of inhaled emissions from "fleet average" light-duty gasoline engines. Of special interest in view of recent epidemiological results linking traffic emissions to cardiac mortality and morbidity was the inclusion of an animal model of atherosclerosis and other vascular effects.

Much of the concern for carcinogenicity of diesel emissions stems from the bacterial agenicity of solvent extracts of material collected on filters. There is evidence that the passage of nitrogen oxides through filters during collection increases the formation of nitroaromatic compounds that drive much of the mutagenicity. To determine the extent to which the mutagenicity of diesel particles might result from this artifact, this project began testing the mutagenicity of material collected with and without removal of oxidizing gases by denuders.

Results

The many detailed results of this project are communicated in numerous technical presentations and peer-reviewed scientific publications (FY 2006 products listed below, full listing available on request). Only example key results are summarized here.

After developing and validating the technology to generate nanoparticles, a study of the health implications of oil condensate began this year with an inhalation exposure of mice to an aerosol generated from used crankcase oil from a 2000 model Cummins ISB 5.9 liter 6-cylinder turbocharged engine operated on the EPA heavy-duty certification cycle. The oil was Shell Rotella-T® 15W-40, a diesel lube oil with a high market share. Control mice were exposed to clean air. This was the first of a planned series of exposures to aerosols from new and used oil from diesel and gasoline engines. Mice were exposed six hours/day for seven days to an aerosol of 17 nm particles at a mass concentration of 300 $\mu g/m^3$ and a particle number count of 1 million/cc. Health evaluations included lung inflammation, lung tissue oxidative stress, and the responses of systemic immune cells (spleen lymphocytes).

The exposure did not cause evidence of lung inflammation, either by histopathology or cell and biochemical markers in airway fluid. The only effect observed in the lung was an increase in heme oxygenase-1 in lung tissue, a marker of oxidative stress that is increased by many inhaled pollutants. The exposure caused two indications of a mild disturbance of the systemic (outside the lung) immune system. In a systemic immune response, different types of lymphocytes in the spleen and other lymphoid tissues must divide to produce more cells, and also produce antibody to foreign materials. Two types of lymphocytes, T and B cells, were removed from the spleen and treated with materials that stimulate cell division. In condensate-exposed animals, the cell division responses of both cell types were modestly, but significantly reduced (Figure 1). The T lymphocytes were also challenged with a foreign protein to test for the ability to form antibody, which was also significantly reduced by the exposure (Figure 2).

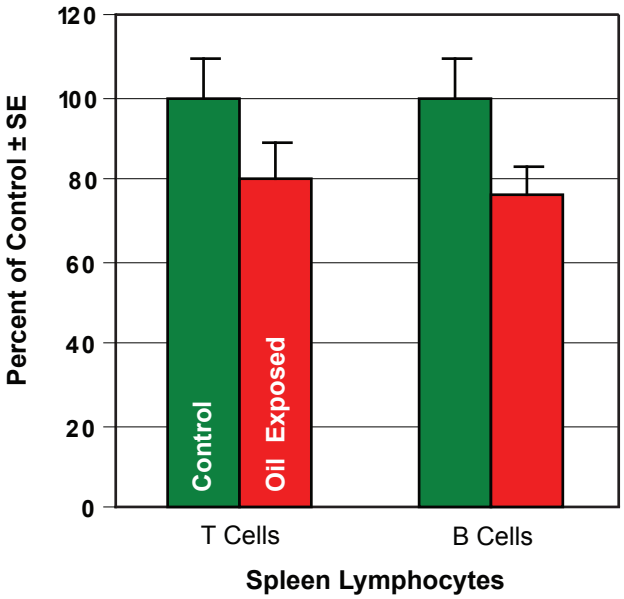


FIGURE 1. Oil nanoparticle exposure-related reduction in response of T and B lymphocytes from the spleen to a proliferative stimulus.

The study of oil condensate nanoparticle aerosols is still underway. The initial finding described above is being compared of the effects of unused diesel lube oil from the same lot, and both new and used gasoline lube oil. We will also explore lower exposures to determine if realistic environmental exposures present a hazard. Parallel studies at Lovelace funded from other sources are providing additional comparisons by evaluating carbon fullerene and nanotube particles.

During the past year, a jointly-funded comprehensive laboratory study of the health hazards of repeated inhalation exposure to "fleet average" gasoline emissions was completed. Animals were exposed daily for up to six months to emissions from 1996 model General Motors 4.3 liter V-6 engines burning national average regular unleaded gasoline and operated on the California Unified Driving Cycle. Animals were exposed to clean air as controls, to whole emissions diluted to particle mass concentrations of 7, 30, or 60 µg/m^3, or to the highest concentration with the particles removed by filtration (particle mass at background level of 2 µg/m^3). Many different respiratory and cardiovascular health indicators were measured, in accordance with a standardized protocol used in companion studies of diesel emissions and wood smoke (www.nercenter.org).

Of special interest concerning both current and future emissions, this study demonstrated for the first time that some health effects were driven primarily by particles, some by the non-particle gases and vapors, and some by both. A concentration-related reduction in the resistance to lung infection with bacteria, for example, was shown to be caused by both fractions, because the effect was reduced approximately by half with particles removed. The new finding most relevant to recent epidemiological results was that non-particle emissions were primarily responsible for changes observed in blood vessels associated with the heart. These changes were of a type that would promote the development of atherosclerosis – the root cause of most myocardial infarctions. A genetic strain of mouse used by cardiologists to study atherosclerosis was exposed for seven weeks, followed by measurement of several indicators of stress and damage in the aorta adjacent to the heart. The results for endothelin-1, a marker of vascular stress, are shown in Figure 3; similar results were shown by other indicators of vascular stress and damage. Endothelin-1 was increased slightly at the lower exposure levels, and markedly at the highest level. The finding of no significant difference between responses to filtered and unfiltered emissions at the high level indicated that the non-particle gas and vapor phases were responsible for the effect. Work is underway to determine the specific gases or organic vapors responsible for the effects, which will point toward emissions to target in evaluating emerging technologies.

Conclusions

Emissions from all technologies evaluated to date are attended by potential adverse health impacts of some nature and degree that need to be understood and mitigated as new technologies develop. Evidence to date indicates that attention to crankcase oil emissions is warranted, and that emissions of non-solid organic condensate nanoparticles should be minimized.

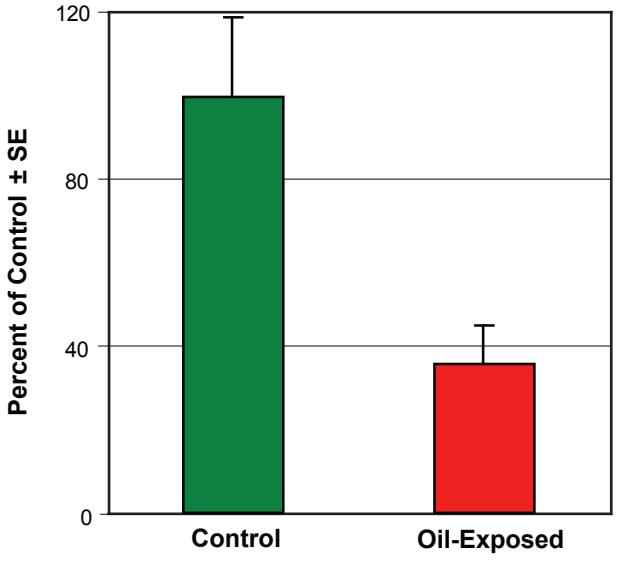


FIGURE 2. Oil nanoparticle exposure-related reduction in ability of spleen T lymphocytes to produce antibody to a foreign protein.

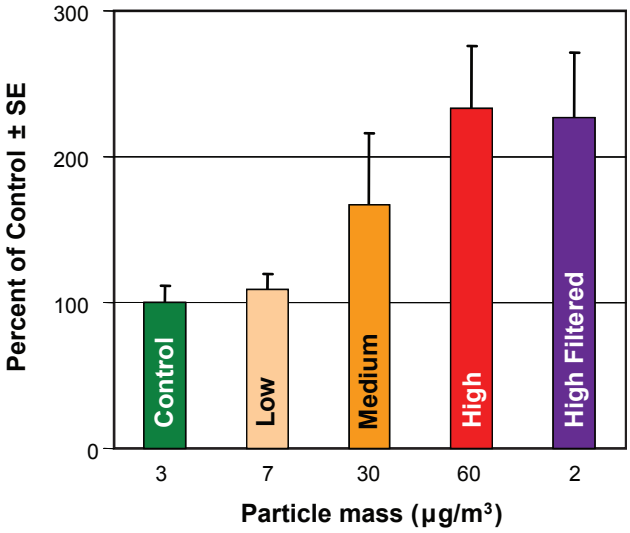


FIGURE 3. Exposure-related increase in endothelin-1in aorta of mice exposed for seven weeks to clean air (control), one of three concentrations of whole gasoline emissions, or to the highest concentration with particles removed by filtration.

Evidence also suggests that the non-particle components of emissions require continued attention. Fortunately, the fuel-trap-catalyst technologies required to meet 2010 on-road diesel emission standards will markedly reduce emissions of the organic vapors that condense to form nanoparticles, and constitute the vapor phase of emissions. After completion of the work described above, the project will shift completely to the evaluation of emissions from emerging fuel, engine, lubrication, and after-treatment technologies, with priorities based on the likelihood of commercialization.

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VI.4 The Advanced Collaborative Emissions Study (ACES)

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Objectives

- **Phase 1:** Extensive emissions characterization (at an existing emissions characterization facility) 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 in a specially-designed emissions generation and animal exposure facility (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 and shorter term biological screening assays in rats and mice similar to the standard National Toxicology Program (NTP) bioassay (Phase 3B) as well as emission 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 shorter-term biological screening activities at the beginning and during Phase 3 are components of the DOE ACES contract.)

Accomplishments

- Conducted site visits to potential facilities in Albuquerque, NM, Oak Ridge, TN, and Richland, WA (November 2005).
- Issued a Request for Proposals for Phase 1 (and 2) emissions characterization (CRC February 2006, see *www.crcao.com*) [1].
- Issued a Competitive Solicitation for Phase 3 emissions and health effects assessment, including RFP 06-1 for the emissions characterization and chronic bioassay and RFA 06-2 for shorter term biological screening studies. (HEI May 2006, see *www.healtheffects.org/funding.htm)*[2].
- Reviewed six proposals for Phase 1 and requested revised proposals from the top two contenders (May/June 2006).
- Reviewed two revised proposals for Phase 1 (July 2006).
- Selected Southwest Research Institute (SwRI) to conduct emissions characterization in Phase 1 (August 2006).
- Reviewed one proposal for Phase 3A and B, the core emissions characterization and chronic bioassay, from the Lovelace Respiratory Research Institute (LRRI) and determined that it was responsive to the RFP (August/September 2006).
- Finalized protocols and methods for emissions characterization to be performed in Phase 1 and initiated contract negotiations with SwRI (September/October 2006).
- Discussed details of facility development, emissions characterization, and health effects assessment for Phase 3 with the LRRI principal investigator and the ACES HEI Oversight Committee, specifically regarding cost savings options (September 2006).
- Finalized dates for delivery of test engines to SwRI and degreening procedures to be performed by the engine manufacturers (September 2006).
- Discussed composition of fuel and lubricants and delivery to SwRI for January 2007 (September 2006).
- Planned meetings with the ACES Oversight, Advisory and Steering Committees regarding finalization of emissions generation and characterization, health effects assessment, and cost savings options for Phase 3, and to finalize financial commitments (September 2006).
- Received initial letters of intent for shorter term biological screening studies during Phase 3B (September/October 2006).

Future Directions

Phase 1

- Finalize the contract with SwRI and start preparation of the engine testing facility for Phase 1 (Fall 2006).
- Select fuel and lubricant suppliers and arrange for delivery to both SwRI and LRRI (Fall 2006).
- Start emissions characterization work in Phase 1 (Winter 2007).

Phase 3

- Review cost and project options for emissions characterization and health effects assessment in Phase 3 through meetings with the ACES Oversight, Advisory and Steering Committees; finalize financial commitments (Fall 2006).
- Assuming adequate cost reductions, begin contract negotiations with LRRI (Fall 2006).
- Initiate Phase 3 (Spring 2007).
- Solicit and select shorter term biological screening study contractors for Phase 3B (Spring 2007).

Introduction

The Advanced Collaborative Emissions Study (ACES) is a cooperative, multi-party effort to characterize the emissions and assess the safety of advanced heavy-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 the Health Effects Institute (HEI; contractor) and the Coordinating Research Council (CRC; subcontractor). 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 Health Assessment Document for Diesel Engine Exhaust [3] 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 (NTP) bioassay utilizing two rodent species. Other specific shorter-term biological screening studies also will be undertaken, informed by the emission 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 health effects 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 database to inform future assessments of these advanced engine and control systems.

Approach

Experimental work under ACES will be performed in three phases, as outlined in the Objectives. Detailed emissions characterization (Phases 1 and 2) will be performed by an existing engine laboratory that meets the U.S. Environmental Protection Agency specifications for 2007 and 2010 engine testing. In Phase 1, emissions from four 2007-compliant engine/control systems will be characterized. One engine will be selected for health testing in Phase 3. In Phase 2, emissions from four 2010-compliant engine/control systems will be characterized. In Phase 3, one selected 2007-compliant engine/control system will be installed in a specially designed emission generation facility connected to a health testing facility 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 will be overseen by the subcontractor (CRC) and its technological panels. The health effects assessment will be overseen by HEI and its ACES Oversight Committee. Set-up of the emission generation facility at the health effects testing facility (for Phase 3) and establishment of periodic emission characterization throughout Phase 3 will be done with input from the team of investigators selected to conduct emissions characterization in Phase 1 and CRC.

Results

At this time, the engine facility to perform emissions characterization in Phase 1 (and 2) has been selected. Contract negotiations are currently underway. The emissions characterization and health testing facility for conduct of Phase 3 has also been identified. Negotiations are underway to finalize the feasibility set-up, emissions characterization, and health assessment plans to keep them within the available funds by considering various cost saving options.

Conclusions

By identifying the teams for emissions characterization and core chronic bioassay we have made substantial progress towards the implementation of the project. Furthermore, the emissions characterization work for Phase 1 is being finalized in order to be ready to start the work upon delivery of the engines to SwRI early in 2007. Final negotiations for emissions characterization and health effects assessment in Phase 3 are underway.

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2. Platform Presentation at the HEI Annual Conference in San Francisco CA, April 2006, in the session "Hot Topics, Breaking News"

VII. UNIVERSITY RESEARCH

VII.1 University Consortium On Low-Temperature Combustion For High-Efficiency, Ultra-Low Emission Engines

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Objectives

- Investigate the fundamental processes that determine the practical boundaries of low-temperature combustion (LTC) engines.
- Develop methods to extend those boundaries to improve the fuel economy of these engines, while operating with ultra-low emissions.
- Investigate after-treatment, alternate fuels, and ignition options for partially premixed compression ignition (PPCI) engines.

Accomplishments

- Single-cylinder experimental results and a modeling study have shown that pilot injection of fuel during negative valve overlap (NVO) can be used to extend the lower load limit of homogeneous charge compression ignition (HCCI) operation.
- A coupled computational fluid dynamics (CFD)/chemistry model has been used to show and quantify the burn rates and combustion efficiency in an HCCI engine configuration. Modes of combustion failure have been identified at the operation boundaries and the influence of operation and design variables on those limits is being investigated.
- A multi-cylinder engine simulation based on GT-Power® and enhanced with user derived HCCI combustion and heat transfer models has been used to demonstrate the effects of transient wall temperature excursions on ignition timing and combustion rates. The simulation shows that an open-loop controller can improve the combustion phasing and overall fuel economy of a vehicle in normal driving cycle.
- Spark assist has been shown in optical engine experiments to have an effect in stabilizing combustion under limiting conditions. The high speed images show that although a small flame is present at the spark plug, the main combustion event begins at other locations in the chamber.

Future Directions

- Carry out single-cylinder investigations of upper load combustion limits with super/turbo charging and fast thermal management of intake temperature.
- Develop a "model-based" correlation of burn rates and combustion efficiency from the CFD/kinetic model results. Incorporate the correlation into the GT-Power® system model.
- Simulate the full range of operation of a dual-mode (spark ignition homogeneous charge compression ignition, SI-HCCI) engine and evaluate the fuel economy implications of various control strategies.

Introduction

Low temperature combustion (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 25%, and in the case of diesel engines, providing the means of satisfying the new, more stringent emissions regulations.

Because LTC implies operation at temperatures below or at the limit of flame propagation, combustion must be initiated by auto-ignition which requires successful management of the thermal history of the engine and the gas charge. In principle this can be

achieved with adequate thermal management and control and various methods have been suggested for accomplishing this. However, as shown in Figure 1, full use of LTC has been limited at both high and low load and 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 focus of this consortium is to investigate the limit phenomena and to propose methods of extending the limits.

Approach

Our new research project, now in its first year, combines experiments and modeling at four university research centers in order to acquire the knowledge and technology to develop the knowledge and methods to extend the load range of LTC engines. This project builds on skills and facilities developed in our previous consortium on HCCI combustion and focuses more closely on understanding and removing the limits to LTC combustion. 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 possible roles of alternate 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 LTC environment both for HCCI and for PPCI systems.

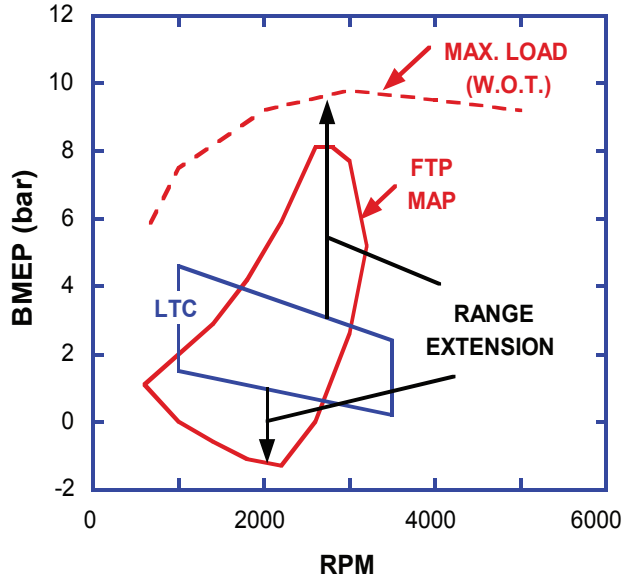


FIGURE 1. Performance map showing limited current achievable LTC range relative to a typical automotive range for maximum load and over the FTP driving cycle.

An array of modeling tools, developed in the earlier project, are being refined and brought to bear on the specific limit problems of importance. These models cover a range of detail from system models for both engines and after-treatment devices, through detailed and reduced chemical mechanisms, to fully coupled CFD/kinetic models. Our intent is to take advantage of the broad range of capabilities of the university partners and the existing collaborative relationships among them.

Results

Engine Experiments on LTC Limit Extension

Experiments at Stanford University on a variable valve actuation (VVA) single-cylinder engine have shown the potential of fuel injection during the negative valve overlap (NVO) period of the engine cycle to extend the lower load limit. Figure 2 shows the extension from 3 bar to near 1 bar of load (net mean effective pressure, NMEP) using this technique. Normally the NVO is used to trap hot exhaust gases to provide heat to successfully ignite the next cycle. When fuel is injected during this overlap period the ignition is advanced so that lower loads can be obtained. The

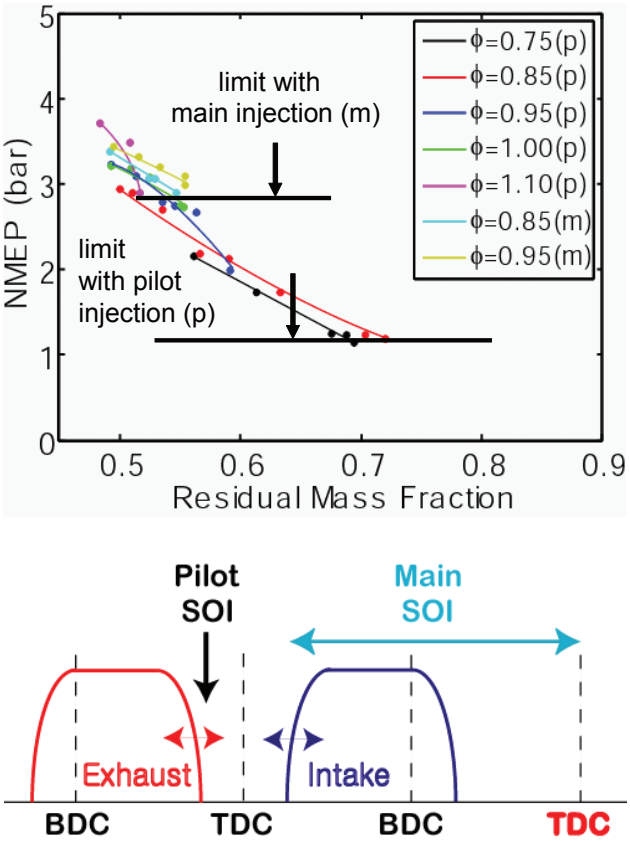


FIGURE 2. Lower load limit extension by pilot injection during negative valve overlap (NVO).

possible mechanisms responsible for this enhancement are thought to be fuel reforming, exothermicity, and charge cooling. A cycle model with detailed kinetics is being used to investigate the effect further.

Meanwhile work is underway at M.I.T. and University of California Berkeley (UCB) to evaluate the effect of turbo/supercharging on the upper limit of LTC operation in a single- and multi-cylinder engines respectively. Turbo/supercharging raises the load limit by increasing the operating pressure (and air loading), thereby permitting higher fuel loading while keeping the mixture lean and cool enough to avoid rapid combustion. The M.I.T. approach will use a computer-controlled turbocharger emulator to simulate a multi-cylinder application. The UCB approach will use an actual turbocharger and a fast thermal management heat exchanger/flow management system for further control. Both test setups are currently wrapping up hardware and software installation.

Modeling and Simulation Tools

This year we have exercised the fully-coupled CFD/kinetic model developed earlier to investigate the behavior of combustion rate and combustion efficiency near the combustion limits with particular attention paid to the role of heat transfer and internal temperature distribution. A parametric study was carried out of an initially uniform mixture compressed from intake valve closing, through ignition and the combustion process. Extensive data was gathered from over 400 simulations for variables such as engine speed, equivalence ratio, turbulence level, wall temperature and piston shape. Analysis of the results is underway. Figure 3 shows pressure traces and corresponding combustion efficiencies for a typical timing sweep made by varying inlet temperature, at 1,200 RPM, $\Phi = 0.26$, 5% residual gas fraction (RGF), and compression ratio (CR) = 12.5. The numbers identify three cases with high, medium and low combustion efficiency.

A plot of the maximum temperature distribution in the cylinder provides insight into how the combustion begins to fail under marginal conditions. Figure 3c shows the maximum temperature envelopes for the three cases. For the healthiest combustion case (1) the temperature distribution has a smooth shape and suggests a well developed boundary layer. For the other two cases (2, 3) there is a decided kink in the curves which appears to occur at or near the point of local ignition (1,000-1,100K). This point is also close to a value of cumulative mass distribution equal to the amount unburned, i.e. (1-Combustion Efficiency/100). In this case it appears that locally, combustion is limited by ignition failure. Analysis of the data set is continuing with the ultimate goal of developing a fast, realistic correlation of burn and efficiency behavior for use in engine system models.

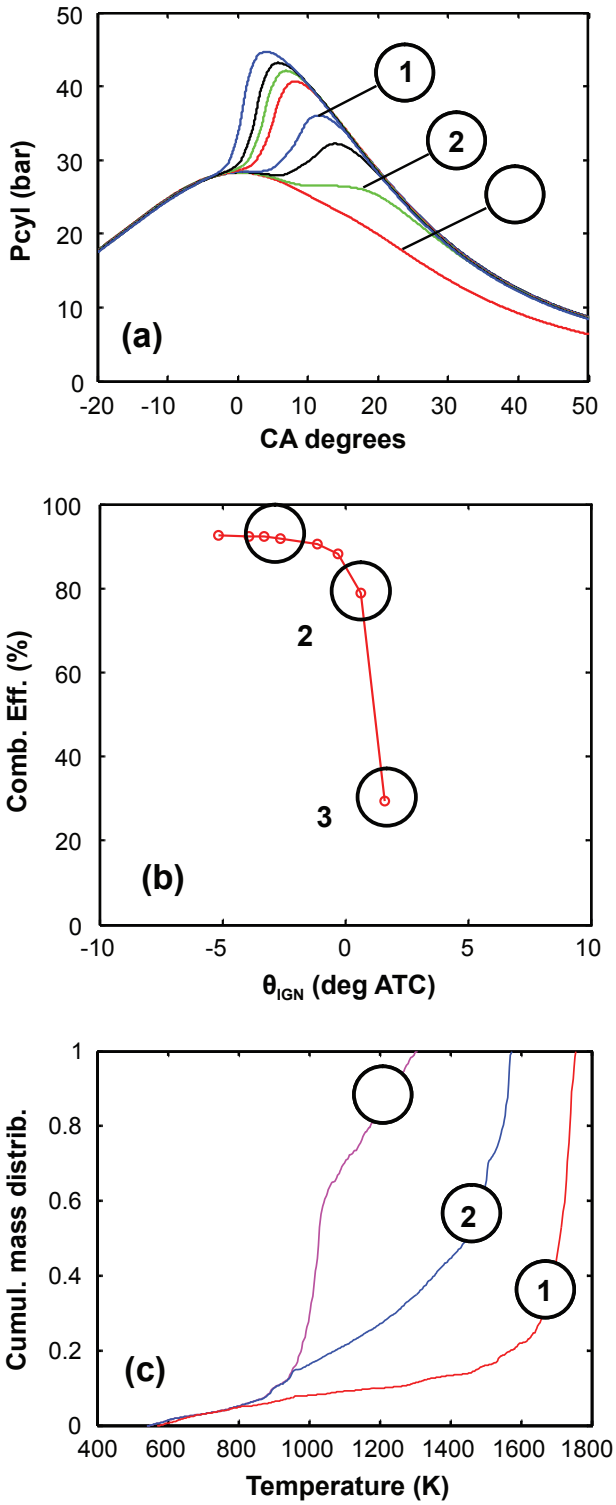


FIGURE 3. Coupled CFD/kinetic results for an HCCI timing sweep; a) pressure traces; b) corresponding combustion efficiencies; c) corresponding maximum in-cylinder temperature distributions. Numbers identify three cycles with high, medium and low efficiency.

In order to reduce computational time in CFD calculations an artificial neural network (ANN) based combustion model has been developed and integrated

into a fluid mechanics code (KIVA3V) to produce a new analysis tool (titled KIVA3V-ANN) that can yield accurate HCCI predictions at very low computational cost. The neural network predicts ignition delay as a function of operating parameters (temperature, pressure, equivalence ratio and residual gas fraction). KIVA3V-ANN keeps track of the time history of the ignition delay during the engine cycle to evaluate the ignition integral and predict ignition for each computational cell. After a cell ignites, chemistry becomes active, and a two-step chemical kinetic mechanism predicts composition and heat generation in the ignited cells.

KIVA3V-ANN has been validated by comparison with isooctane HCCI experiments in two different engines. The neural network provides reasonable predictions for HCCI combustion and emissions that, although typically not as good as obtained with the more physically representative multi-zone model, are obtained at a much reduced computational cost. KIVA3V-ANN can perform reasonably accurate HCCI calculations while requiring only 10% more computational effort than a motored KIVA3V run. It is therefore considered a valuable tool for evaluation of engine maps or other performance analysis tasks requiring multiple individual runs.

Beyond the fundamental work with CFD codes there is a need for systems modeling of the HCCI engine-in-vehicle, for investigating transient effects and demands on the engine system. In this regard it is known that wall temperatures have a great effect on HCCI combustion timing and burn rates especially during transient operations. In this system modeling study, control of the wall temperature effect on combustion is simulated by modulating the RGF to compensate for the wall temperature.

A multi-cylinder engine simulation with detailed geometry is carried out using a 1-D GT-Power® system model that is linked with Simulink. The model includes a finite element wall temperature solver and is enhanced with user specified HCCI combustion and heat transfer models. Initially, the required residual gas fraction for optimal brake specific fuel consumption is determined for steady-state operation. The model is then used to derive a map of the sensitivity of optimal residual gas fraction to wall temperature excursions. The map is then used to determine the necessary changes in the control strategy to compensate for the thermal inertia effects during transients. Figure 4 is a schematic of the control algorithm used.

The results show that, when the non-equilibrium transient wall temperature difference from the steady-state value is moderate, load and speed transitions in the HCCI operating regime can be managed by using controllers based on steady-state RGF maps. However, with large wall temperature excursions from the steady-state, the results indicate the need for wall temperature dependent calibration of combustion parameters for best fuel economy and knock-free performance. Compensating for the wall temperature effects results in improved fuel economy while satisfying knock and misfire constraints.

After-Treatment System for LTC Engines

The goal of this task is to develop successful models of after-treatment devices and systems for the low-temperature applications in HCCI and PPCI. As seen in Figure 5, after-treatment is made more difficult by the increasing CO and HC emissions that accompany lower exhaust temperatures. The strategy of this project is to take advantage of the existing work on diesel oxidation catalysts (DOCs) and develop specific kinetic models where needed and to build on the existing UM

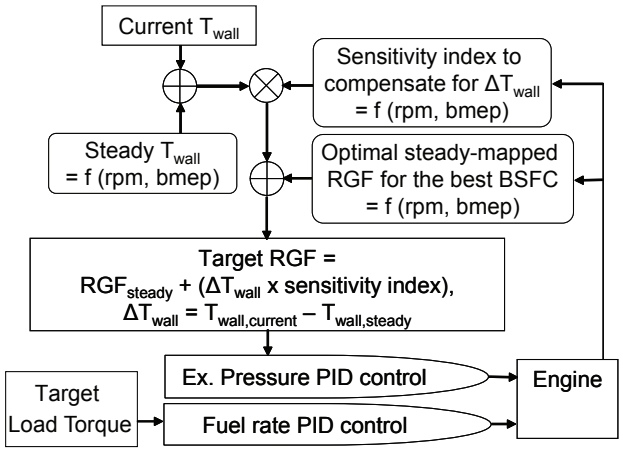


FIGURE 4. Schematic of simulated control strategy to compensate for wall temperature effects.

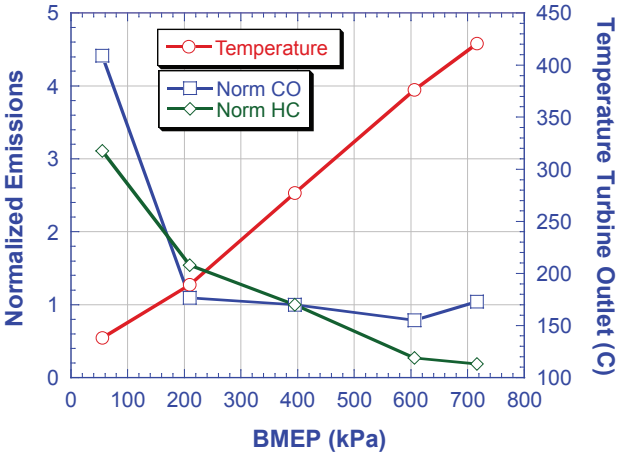


FIGURE 5. Typical rapid increase in CO and HC emissions with decreasing turbine exhaust temperature in a diesel LTC application.

after-treatment system models, supplemented with experimental data from the UM diesel/PPCI test facility.

To date a fundamental kinetic model of a DOC has been developed from reactor data provided by GM as part of the GM collaborative Research Laboratory work at UM. This model uses a single component (C_3H_6) to represent the unburned hydrocarbons and has demonstrated good agreement with experimental light-off curves. The model is currently being incorporated into the UM system model for validation against low-temperature diesel and PPCI data from the test cell. Improvements to the model will be made as needed depending on the validation work.

Spark-Assisted HCCI and Alternate Fuels

In a combined experimental and modeling approach, this task is investigating the possible use of a spark plug to enhance combustion at the combustion limits. Recent optical engine experiments have demonstrated the beneficial effects of a spark in extending the stability limit. Figure 6 shows a series of pressure traces with decreasing equivalence ratio (and load) from left to right. As the load is progressively reduced the peak pressure decreases and becomes more retarded until at the next to last equivalence ratio of 0.42, the combustion is on the verge of misfire. When the spark is turned on for the last pressure curve, the combustion is advanced and the load can be reduced to equivalence ratio of 0.40 while the combustion remains stable.

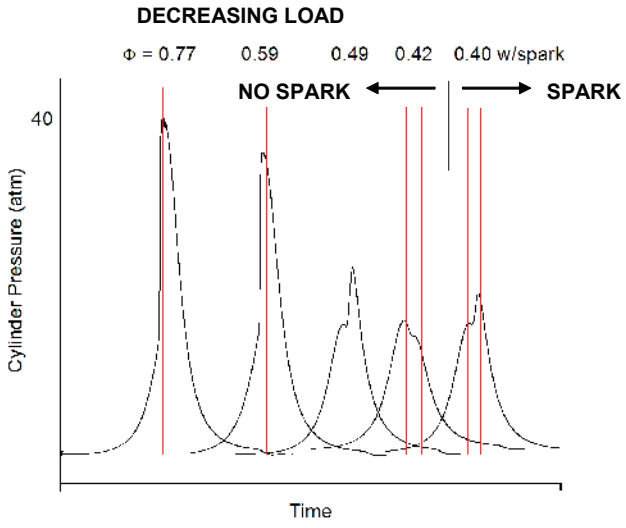


FIGURE 6. Sequence of LTC pressure curves in order of decreasing load (Φ) showing effect of spark at leanest Φ in advancing combustion and increasing stability.

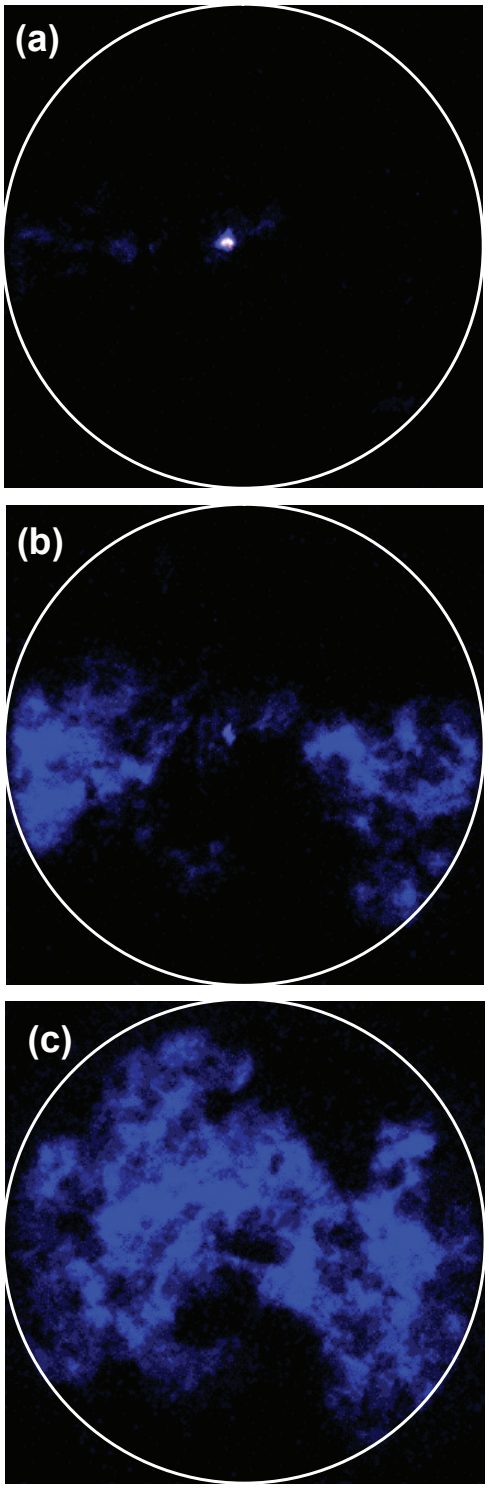


FIGURE 7. Sequence of images from the UM optical engine showing spark assisted HCCI at $\phi = 0.4$ and 700 rpm with Indolene fuel. (a) t =0: shows spark and localized reaction zone, (b) t = 0.67 ms: shows initial ignition occurring at edges of chamber, (c) t = 1.33 ms: main combustion event.

Figure 7 shows three high speed images of the spark assist process taken for the leanest condition. The sequence reveals the presence of a faint flame-like areas originating from the centrally located spark plug; however the main combustion event consistently starts near the edges of the chamber. The mechanism for this is under investigation, but it is attributed to favorable temperature gradients at the edges of the chamber.

A second approach to spark assist is directed at exploring the possibility of using a prechamber based ignition source as shown in Figure 8. The idea is to enhance dispersion of the heat or partially burned combustion products throughout the chamber by the jet action of the prechamber. Modeling work is underway to identify the processes involved in this type of ignition process. To date the results show that early sensible heat release of a part of the charge can advance ignition in a mixture that is near the point of ignition by the compression process. Next steps will use CFD and chemical kinetics to investigate flow and chemistry aspects.

Studies of normal LTC ignition of alternate fuels are underway in the optical engine and in the rapid compression facility (RCF) at UM. Optical engine studies of indolene (a reference grade gasoline), pump gasoline and isooctane have been conducted which focus on understanding the effects of real fuels compared to reference fuels and chemical surrogates. The data indicate neat isooctane behaves markedly differently from the gasoline fuels at the lean operating limits, where isooctane was capable of extremely prolonged combustion events. During stable HCCI operation, the three fuels exhibited similar ignition and combustion characteristics. From the imaging data, we found the fuels each ignited in the same location within the cylinder volume, indicating these areas were zones of preferential thermal gradients.

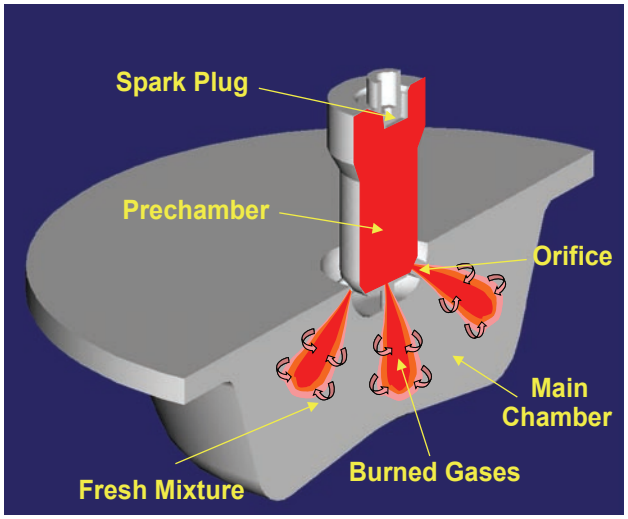


FIGURE 8. Prechamber Concept for Spark Assisted LTC Combustion Control

The ignition of a non-petroleum based biodiesel fuel surrogate has been investigated with the UM RCF. The surrogate used is methylbutanoate, an oxygenated ester that is one of the simplest representative compounds for biodiesel. The initial data demonstrate ignition is slower than predicted based on the most recent reaction mechanisms developed by Pitz and colleagues at Lawrence Livermore National Laboratory. Work is continuing.

Conclusions

- The low load limit has been extended in a single-cylinder engine operating with NVO for exhaust gas retention. By injecting the fuel during the NVO period the low load has been extended to near 1 bar NMEP. This is thought due to in-cylinder fuel reforming, exothermicity or charge cooling prior to the combustion cycle.
- A fully coupled CFD/kinetic model has been used to investigate the combustion behavior near the combustion limits. The maximum in-cylinder temperature distribution is shown to be a dominant factor, modified by rpm, equivalence ratio and design variables.
- An engine system model based on GT-Power® and user supplied combustion and heat transfer models has demonstrated a potential HCCI engine control strategy for compensating for non-steady state wall temperatures with improved fuel economy of the in-vehicle application.
- Based on reactor and engine experiments, a system model for LTC after-treatment is being developed to explore emissions issues in transient vehicle operation.
- Spark assist of HCCI has been observed in an optical engine under near limit conditions. Although the stabilizing effect is clear, no significant flame activity is observed at the spark; rather the combustion begins elsewhere in the chamber but earlier than without the spark. The investigation is continuing.
- The ignition and combustion of alternate and biodiesel fuels are being studied under HCCI conditions in an engine and in a RCF. In this study isooctane was shown to have much longer combustion than a typical gasoline fuel.

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VII.2 Optimization of Low-Temperature Diesel Combustion

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Objectives

- Develop methods to optimize and control low temperature combustion diesel technologies (LTC-D) that offers the potential of nearly eliminating engine 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, NOx, unburned hydrocarbon (HC) and 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).

Accomplishments

- Combustion models and reaction mechanisms have been formulated and applied to analyze low emissions operation. A low emissions window of operation has been identified as a benchmark for further testing.
- In-cylinder optical diagnostics have been implemented for H_2O species, temperature and turbulence dissipation measurements for chemistry and turbulence model validation.
- A prototype valve actuation system for intake valve timing control has been installed and tested and demonstrated to achieve 2010 emissions levels with LTC-D operation.
- A new single-cylinder high-speed direct-injection (HSDI) diesel homogeneous charge compression ignition (HCCI)/low temperature combustion (LTC) laboratory has been commissioned and exploration of high exhaust gas recirculation (EGR) rate (>55%) conditions has been successful.
- Advanced large eddy simulation (LES) turbulence models have been developed and shown to reveal more detailed flow information than standard Reynolds Averaged Navier Stokes (RANS) models.
- Analysis tools have been developed for development of engine control algorithms, and strategies for thermal and load changes and mode transitions have been explored

Introduction

This project was initiated in response to a Department of Energy (DOE) solicitation for research and development on homogeneous charge compression ignition (HCCI) diesel-fueled engines under the "FreedomCAR and Vehicle Technologies Program Solicitation for University Research and Graduate Automotive Technology Education (GATE) 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 particulate and nitrogen oxides (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 after-treatment 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 low temperature combustion diesel technologies (LTC-D) that offer the potential of nearly eliminating engine NOx and particulate emissions 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.

Outcomes from the research include providing guidelines to the engine and energy industries for achieving optimal low temperature combustion operation and low emissions engine design concepts will be proposed and evaluated.

Approach

- Use fully-instrumented engines with prototype fuel injection systems and combustion sensors to map and define 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.

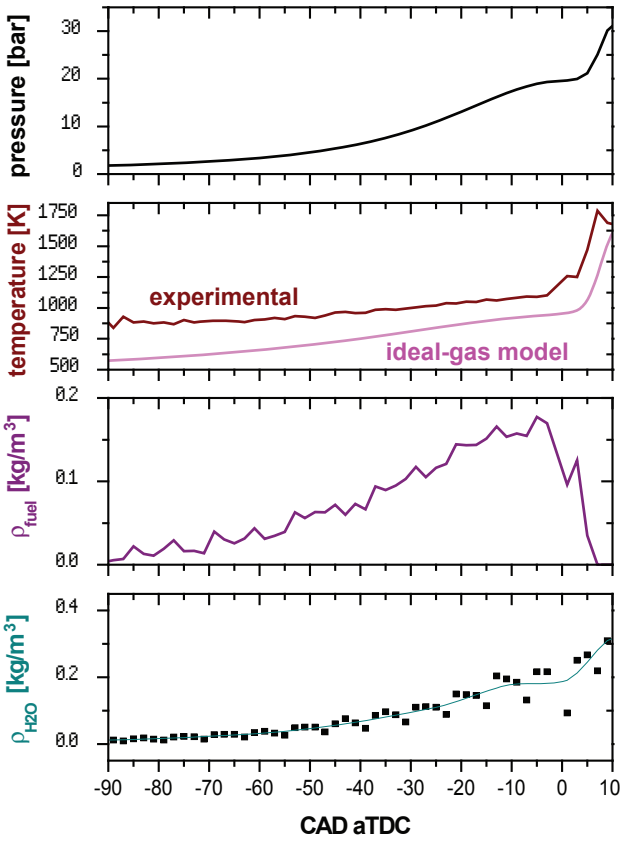


FIGURE 1. Measurements of pressure (by piezoelectric transducer), temperature, fuel, and H_2O vapor (all by absorption spectroscopy of 1600-1850 nm @ 0.75 nm resolution) in a metal engine operating in HCCI mode.

Results

Task 1 - Fundamental Understanding of LTC-D and Advanced Model Development

Kinetic mechanisms for diesel combustion are being tested. 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. Validation of the mechanism predictions will be done by comparing measured and simulated in-cylinder gas compositions, under LTC-D conditions. Significant progress has been made in H_2O vapor sensing (recent H_2O vapor measurements is available at www.erc.wisc.edu - click on “optical diagnostics”, then mouse over and click on “absorption”), while initiating measurements of other species (H_2O_2, CH_2O, OH, CO_2, and fuel). Initial simultaneous optical measurements of fuel and H_2O are shown in Figure 1.

The kinetic mechanisms have been used to identify low emission operating conditions in a HSDI diesel engine. Parametric calculations have been performed using the KIVA3V-ERC code coupled with CHEMKIN for simulating chemistry. The model has been applied with operation over wide ranges of equivalence ratio, inlet temperature, intake valve closure timing, engine speed and fuel amount under the assumption of ideal homogeneous charge. The CO, HC, NO and soot emissions have been summarized on equivalence ratio-peak cycle temperature maps, and low emission regions have been found to be located in the region approximately from 1,600 K to 1,800 K peak cycle temperature, and on the lean side of stoichiometric equivalence ratio, as shown in Figure 2.

The results reveal that clean HCCI combustion is possible with reduced EGR levels by retarding the intake valve closure timing, and the low emission window moves toward higher temperatures as engine speed is increased. The idealized HCCI emission characteristics reveal a low emission window (lower than 10 g/kg-f CO, 0.5 g/kg-g NO and almost soot-less) or “sweet spot” operation with intake valve closing (IVC) = 100° after top dead center (ATDC) and $0.6<\Phi<0.95$, $50<EGR<60\%$, and $0.25<Pboost<0.3$ MPa. These results are useful to serve as guidelines for future engine tests.

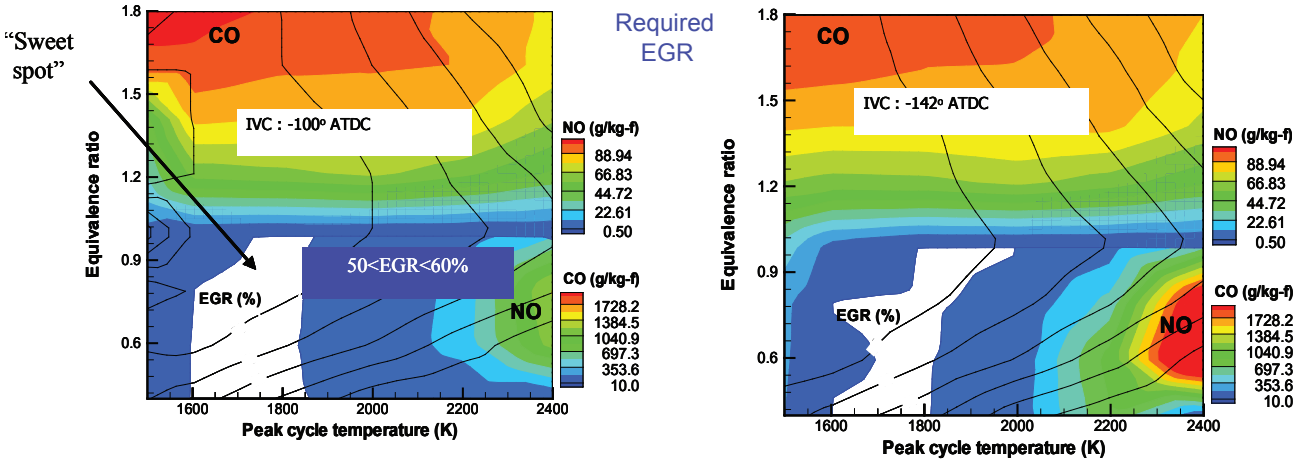


FIGURE 2. Effect of intake valve closure (IVC) timing on CO and NO emissions as a function of EGR. (White region indicates low emission window.)

Task 2 – Experimental Investigation of LTC-D Combustion Control Concepts

A prototype intake valve actuation system has been installed and tested on the Caterpillar 3401 SCOTE heavy-duty diesel engine. Parametric tests using various EGR levels, boost intake pressures, fueling rates, intake valve closings, injection pressures, and start-of-injection timings were used to explore the limitations and potential of an intake valve actuation system. At high-speed, intermediate load (56%) operation, constant airflow and no EGR, the use of late intake valve closing enabled a 70% NOx reduction while maintaining particulate matter (PM) levels. At low load operation, late IVC, and reduced intake pressure, 2010 not-to-exceed NOx and PM emissions were achieved with 40% EGR, as shown in Figure 3. At medium load, constant air flow, and early start of injection (SOI), it was found that the NOx, HC and BSFC levels at a late IVC with 30% EGR were comparable to those with the stock camshaft IVC timing of 143° before top dead center (BTDC) with 40% EGR. In comparison, the CO and PM levels decreased by nearly 70% with the use of late IVC timing and less EGR. Through these parametric studies, it was concluded that the use of late IVC actuation is successful in controlling combustion phasing and emissions.

In addition, the potential of achieving LTC-D operation with wide spray angle direct injection in a HSDI automotive diesel engine is being explored. In addition to studying spray and mixing parameters, the work will explore whether the LTC operating range can be expanded with modifications to fuel volatility and cetane number. The work is a collaborative effort between the Energy Research Center, General Motors Research and Development Laboratory and BP. After

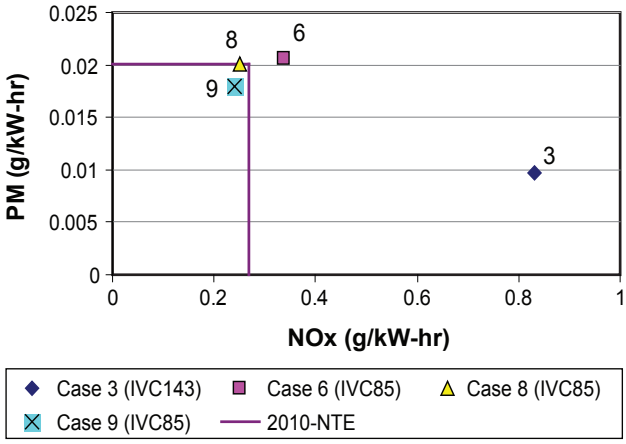


FIGURE 3. NOx vs. PM at SOI 55° BTDC, 40% EGR, with standard IVC timing (143° BTDC) and IVC 85° BTDC. Intake boost pressure is 184, 184, 179, 172 kPa for cases 3, 6, 8, and 9, respectively.

establishing operating regimes for direct injection LTC-D with a European diesel (cetane number = 53.7, sulfur = 7.5 ppm, aromatic content = 22.4%) the impact of switching to an ultra-low sulfur U.S. diesel fuel was investigated (cetane number = 40, sulfur = 15 ppm, other properties are currently being evaluated). This was done for two different nozzle hole injection angles, 148 and 155 degrees included angle.

The results show that there is a start of fuel injection timing that produces minimum CO, HC and BSFC. In all cases NO and particulate emission are at or below the resolution limit the instruments. The ignition delay curves do not show very much dependence on the fuel characteristics or nozzle hole angle, yet there is significant difference in the CO emissions and sensitivity to fuel characteristics.

Task 3 – Application of Detailed Models for Optimization of LTC-D Combustion and Emissions

In the present work optimization tools are used to recommend low-emission engine combustion chamber designs, including non-axi-symmetric piston bowls that could provide better matching with spray plume geometries for enhanced mixing. By coupling GA (genetic algorithm) with KIVA-CFD codes, and also utilizing our automated grid generation technology, multi-objective optimizations with goals of low emissions and fuel economy can be achieved. Baseline configurations have been determined for a low load running condition that is similar to Mode 6 (1,757 rev/min, 20% load) of the Caterpillar heavy-duty diesel engine simulation of the federal test cycle, which is of interest in this project. A SOI sweep under this load has been run, and the results indicate that NOx emissions are one of the primary concerns under this load. Baseline configurations for high load are being run which are similar to Mode 6 at 95% load.

Research on the spray characteristics of various nozzle types such as multi-hole (holes with uniform azimuthal spacing between holes), and group-holes (clustered pairs of holes) is being performed numerically. The concept of a group-hole nozzle is that two neighbor small holes produce smaller droplets while maintaining similar spray penetration compared to the conventional nozzle. This group hole nozzle is expected to improve engine fuel consumption at high EGR conditions, which is required for LTC-D combustion because the high momentum of the spray helps the fuel-air mixing process.

The results show that the effect of nozzle design is small at lean operating conditions (i.e., low EGR and equivalence ratios). However the multi-hole and group hole nozzles show the best indicated specific fuel consumption (ISFC) under rich combustion conditions (0.5–0.8 equivalence ratio) and near stoichiometric combustion (0.8–1.0 equivalence ratio), respectively. This result also suggests that the optimization of the nozzle hole layout is required for successful low-temperature combustion.

Computations have been made using advanced turbulence models. Large eddy simulations (LES) are being used to evaluate the effects and importance of intake flow effects (swirl, turbulence, heat transfer, etc.), variable valve actuation strategies, valve overlap including residual mixing and rebreathing operation, and early injection with moderate pressure fuel injection. LES models have been used in conjunction with detailed chemistry (CHEMKIN) and KIVA to investigate in-cylinder temperature and intermediate radical distribution for varying fuel injection timings. Comparisons of RANS-CHEMKIN and LES-CHEMKIN simulations have been made with experimental images of Singh et al. (2006). Sample images for an early injection case (SOI=22° BTDC) are shown in Figure 4, which compares an experimental image (natural emissions are representative of high temperature regions) and simulated in-cylinder temperature contours. As can be seen, the flow features from LES-CHEMKIN are more similar to the experimental features than those from RANS-CHEMKIN.

Task 4 – Impact of Heat Transfer and Spray Impingement on LTC-D Combustion

Coupled computational fluid dynamics (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. Wall films are predicted for early injection cases and this leads to increased NOx emissions due to locally high fuel concentrations. This is needed to determine the origins of NOx emissions from near wall combustion sources. A radiation model based on the discrete ordinates method (DOM) is included in the study.

Effort has focused on the establishment of methods to determine the appropriate initial conditions and boundary conditions of the engine metal components which can affect in-cylinder gas behavior and emissions through the prediction of the component temperature and heat flux distributions. The model includes gas phase and soot particle radiation, and appropriate boundary condition models on the piston and cylinder head surfaces for the present engine CFD simulations.

An in-cylinder mesh of the experimental optical diesel engine of Singh et al. 2006 (with a quartz window) has been made, and combustion cycles and heat flux at the walls have been computed with the DOM radiation model implemented into KIVA3V-ERC. A finite element model has also been made of the optical engine, and the temperature distribution within the metal components has been predicted using the finite element heat conduction code modified to calculate transient cycles, for a baseline case.

Next, the model will be applied to compute the operation of the Caterpillar SCOTE engine for

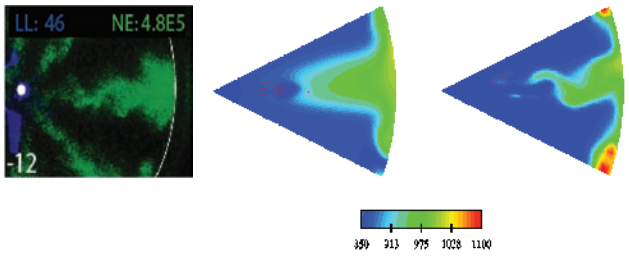


FIGURE 4. Experimental (natural emissions) and simulated temperature contours in diesel combustion using standard RANS and advanced LES turbulence models.

comparison with experimental data. A linkage system is being developed to allow investigation of the piston temperature and heat flux distribution during low-temperature diesel combustion. During this period, the optimization of the linkage assembly has been completed, and mechanical drawings have been prepared.

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 will also explore approaches to transitioning between normal and LTC operation. An engine received from GM Powertrain Europe has been installed into our transient dynamometer test cell. The engine can now be controlled during transient operation using three different techniques:

A. Changing speed/load regime by acting on the pedal of the vehicle connected to the commercial electronic control unit (ECU) and fixing load and or rpm by the dynamometer control.
B. Changing speed/load regime by emulating the pedal of the vehicle using a Labview application for accurate repeatability. This is connected to the commercial ECU and fixing load and/or engine speed by the dynamometer control.
C. Changing speed/load regime by directly interacting with an open ECU interfacing with ETAS software and hardware, for data command and retrieval, and fixing load and or rpm by the dynamometer control.

This combination of capabilities allows controlled experiments improving the repeatability and accuracy, and exercising specific parameter control, e.g., injection pressure, timing and EGR control, in conditions different to the standard calibration. Measurement of in-cylinder pressure for one cylinder, and sampling locations for fast HC and NOx in one exhaust port and after the turbocharger were also incorporated and tested.

The transient engine experiments are also being analyzed with system level analysis tools to contribute additional insights into the experimental work and to provide guidance in choosing experimental operating conditions for study. Emissions models have been used to investigate the primary sources of CO and HC emissions during steady and transient operation. Under high EGR conditions, it was observed that spikes in CO and HC or NOx emissions are formed, depending on the nature of the transient. This is attributed to the oxygen availability in the cylinder immediately after the transient. Design of fast EGR and boost controllers would help minimize the emission spikes. For example,

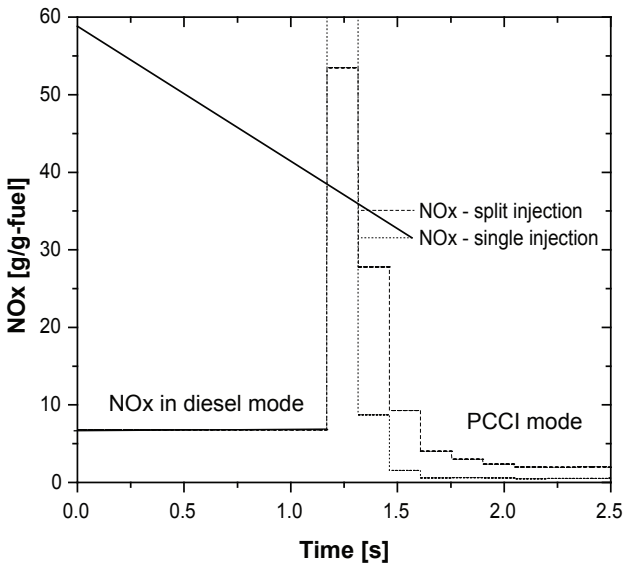


FIGURE 5. NOx emissions for diesel and PCCI combustion modes during a mode transition.

Figure 5 demonstrates a NOx peak in a diesel-to-premixed charge compression ignition (PCCI) mode transient. NOx levels decrease after the transition from diesel-to-PCCI mode due to high amounts of EGR and late IVC. In the PCCI mode, lower cylinder temperature from poor combustion results in lower NOx for the single injection case as compared to split injection strategy.

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VII.3 Low Temperature Combustion with Thermo-Chemical Recuperation to Maximize In-Use Engine Efficiency

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- Atkinson LLC, Morgantown, WV (Christopher Atkinson, Lead Investigator)

Objectives

- To substantially improve (10% fuel use reduction) the efficiency of compression ignition engines for both light-duty and heavy-duty use while meeting or exceeding the ultra-low NOx emission requirements for the 2010 engine model year.
- To utilize alternative combustion modes, coupled with thermo-chemical reforming of fuel to recover exhaust waste heat, with an optimization of the mean effective pressure versus displacement tradeoff.
- To develop technology under this project that will enable engine prototype development by 2012.

Accomplishments

- The research is in its first year. An extensive literature review was completed to define low-temperature combustion (LTC) actual operational limits with regard to load, equivalence ratio and exhaust gas recirculation (EGR) rate.
- Two models were developed as a comparative tool for diesel and LTC combustion. The LTC combustion model allows for prediction of auto-ignition onset.
- The researchers have selected a general friction model including losses from piston-ring assembly, engine bearing, valve train and engine auxiliaries.
- Steam reforming was selected as the thermo-chemical process to obtain H_2 from the fuel using the available energy of the exhaust gases, following a careful examination of reforming options. Initial modeling results show that the H_2 yield will be in the range of 5-20% (volume).
- Equipment has been selected and plans have been formulated for the reforming of fuel at GTI.

Future Direction

- The LTC combustion model will be coupled with the cooling burden model to evaluate waste energy generation.
- The LTC combustion model will be coupled with the friction model to evaluate the effect of changes in indicated mean effective pressure (IMEP) over the friction losses.
- The experimental stage at GTI will start using n-heptane as a surrogate fuel, in order to analyze the impact on H_2 and CO production due to changes in: reforming temperature, fuel flow rate, steam/fuel mole ratio and heat addition to the reformer.
- The experimental engine for the LTC project will be identified, which will complete Phase 1.
- The engine will be procured and the experimentally intensive Phase 2 LTC plan will be implemented.

Introduction

Low-temperature combustion (LTC) is a combustion process which utilizes a homogeneous air/fuel mixture, similar to spark ignited systems, but combustion is initiated by auto-ignition of the fuel due to the increase of temperature associated with the compression stroke. Although LTC combustion has emerged as an alternative to spark ignition (SI) and compression ignition (CI) combustion due to decrease in exhaust emissions and improvement in fuel economy, it is difficult to maintain LTC combustion over the entire operational engine load range. The control over ignition timing and the rate of heat release are the primary parameters affected by the nature of this kind of combustion process. The control

of LTC is the most challenging issue for commercial applications of LTC.

In general, two directions have been investigated to extend the operational range of LTC and provide the required control: modifying air/fuel mixture properties and modifying engine operation and design parameters [1]. This project is applying reforming technologies to modify the composition of a percentage of the fuel as a control tool by using heat from the exhaust gases, and a major objective is to improve overall system efficiency through the use of this heat. In parallel, an optimization of the mean effective pressure versus displacement tradeoff will be studied to address the need for broad operating range in LTC operation.

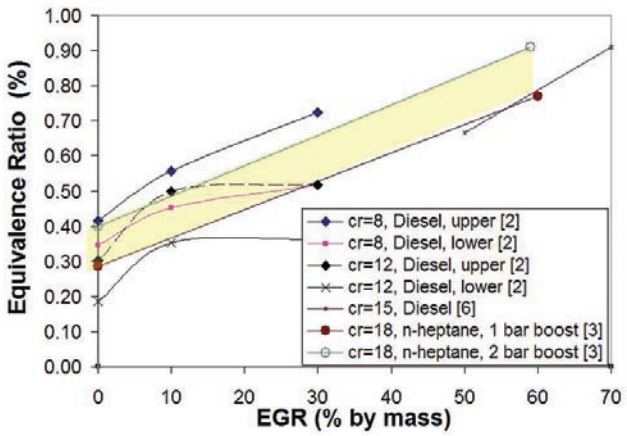


FIGURE 1. Relation between Equivalence Ratio and EGR for LTC Mode

Approach

A simplified zero dimensional model for LTC combustion has been implemented in order to understand the effect of key parameters in this combustion mode. Thermodynamic and geometric parameters have been varied and the results obtained have been compared with existing data. With the information obtained from the combustion model, the heat release data will be quantified to estimate the availability of energy for the reforming process. The models will take into account cooling load and other auxiliary loads necessary for thermo-chemical recuperation (TCR) incorporation.

The reforming process has been modeled based on exhaust temperatures and heat addition from a previous model and published experimental data. The reformer will be tested initially to verify model results, and will be coupled to an experimental engine to study the influence of parameters on a real engine running in LTC mode. The TCR stream and an untreated fuel stream will be employed as two variables to facilitate broad and rapid load control of the LTC using a well-instrumented cylinder. NOx will be monitored using both a dilution tunnel and research-grade bench and using in-cylinder sampling with a fast NOx analyzer. Optimization will take place using a neural net model based on the experimental data. Two pre-competitive (basic) engine designs and control strategies will be developed as a final product. The operating envelope will meet 2010 ultra-low NOx emissions standards.

Results

Information collected during a review has been plotted in order to define limits for this experimental research. Figure 1 shows the typical limits of equivalence ratio on LTC operation for diesel and n-heptane. There is a linear relationship between the range of operation of EGR and equivalence ratio for suitable LTC. The limits for equivalence ratio, ϕ, should be between 0.2 and 0.9.

A basic zero-dimensional model has been formulated to determine effects of variables on in-cylinder conditions. Information on in-cylinder pressure is needed to understand the effect of combustion intensity and compression ratio on irreversible losses for the engine. The present study was predicated partly on a LTC solution that would use displacement rather than power density to achieve desired power ratings. The principal objective of this model is to serve as a comparative tool to study the effect in variations of compression ratio, intake temperature and EGR content. In this model compression ratio is a variable because it is associated with the concept of increasing displacement to increase the operational range of LTC. The results obtained running the model were compared with experimental data from Shaver et al [8] and Sun et al. [9].

The inlet manifold temperature was varied between T_{min} and 430 K, and the effect on ignition onset was studied. T_{min} was the minimal intake temperature required to produce the ignition of the mix. When the intake temperature is increased, it advances the onset of ignition due to increased reaction rates (which are strongly dependant on temperature) as can be appreciated in the pressure and temperature profiles in Figures 2a and 2b. Results confirm the narrow temperature range needed to keep the ignition at the desired crank angle. The influence of compression ratio on the low temperature combustion process is shown on Figures 3a and 3b. The temperature profile tends to be bounded, while the pressure increases twofold with a 20% increment in compression ratio (Figure 3a). The results obtained from this modeling approach have shown a trend that matches the trend of previous models reported in the literature [8,9,10]. However, the numerical results are overestimated in this model.

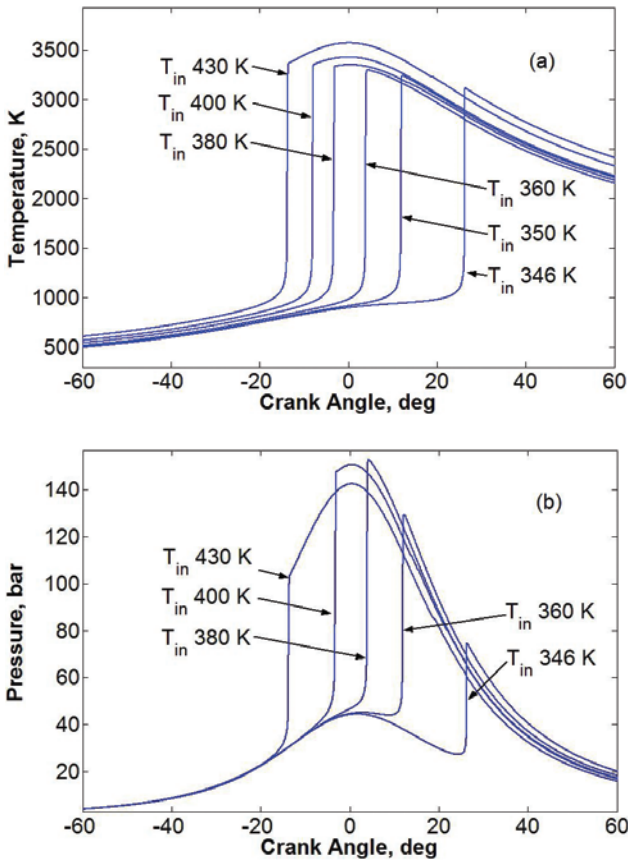


FIGURE 2. Effects of Intake Temperature in Temperature (a) and Pressure (b) Profiles for a CR=18:1

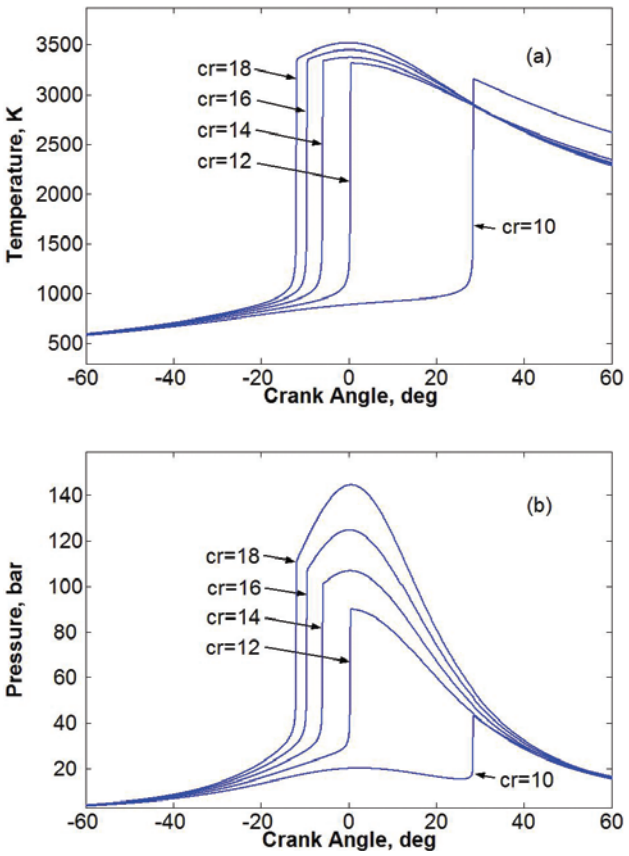


FIGURE 3. Effects of Compression Ratio on In-Cylinder Temperature (a) and Pressure (b) Profiles at T_{in}=420 K.

The constants from the Arrhenius reaction rates are the parameters that can be modified to match data. The heat release process influences the temperature history of the in-cylinder charge, and is needed to assess cooling burden. Further modeling will match results with reported experimental data from [11]. A friction model has been chosen to use in conjunction with in-cylinder pressures to predict engine efficiency trends.

The first approach proposed was to reform the fuel using exhaust gas reforming. However, modeling showed that excess oxygen reacts with fuel, leading to a loss of efficiency but a gain in reformer temperature. Stoichiometric calculations were made independently and the results showed that the penalty in fuel oxidation was harmful to the main efficiency objective of this project. GTI engineers presented a model based on a well known and successful TCR steam reforming system, and this approach has been adopted. Operational points were chosen for a six liter engine. Steam reforming was modeled with Chemkin. Engine mass flow was 0.108 kg/s; A/F ratio was 30; fuel mass flow was 0.0036 kg/s; ratio of fuel to reformer was 50% at most. The amount of fuel sent to the reformer was established in order to obtain 5-10% of H_2 on a mass basis. The fuel selected for modeling work was n-heptane. The thermo-chemical recuperation modeling permits the variation of reforming temperature, steam:carbon ratio and reactor pressure to investigate the impact on H_2 yield, reformed fuel energy content and composition. The reforming temperature is associated with the exhaust temperature of the engine, and it was set to 500°F, 750°F, 900°F and 1,200°F for modeling purposes. The steam:carbon ratio was fixed at 2:1 and the pressure at 1 atm.

Figure 4 shows the results from the Chemkin model on reformed fuel composition using n-heptane and n-butane as base fuels. The H_2 yield increases proportionally with temperature with an extra benefit from the thermo-recuperation process related with the increase on fuel energy content. GTI engineers are working on models with different alkanes to infer H_2 yield for diesel-like fuels. Some research using both n-butane and n-heptane showed that trends remained consistent as the molecular weight of these normal paraffin varied.

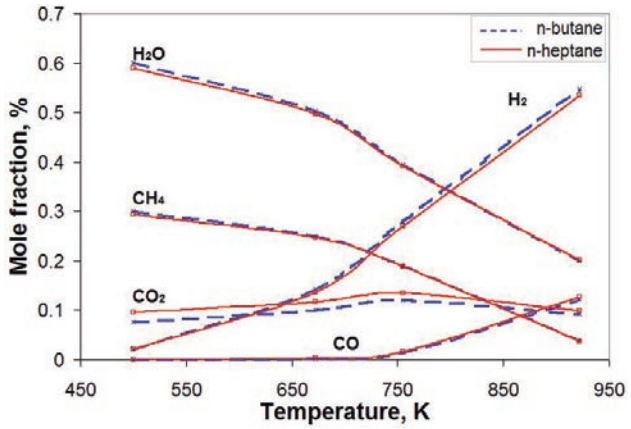


FIGURE 4. Reformed Fuel Composition for N-Heptane and N-Butane (Steam:Carbon ratio 2:1, Pressure 1 atm)

Conclusions

- The actual operational range for LTC was established based on experimental data reported in the literature. High volatility fuels are preferred because of their ability to mix with air. Diesel fuels should be premixed by pre-heating the air.
- Parametric studies have been conducted in a zero-dimensional model in order to illustrate the auto-ignition behavior on LTC mode. This model serves as a comparative tool to study the effect of variations in compression ratio, intake temperature and mixture composition (EGR).
- Predicted ignition trends were consistent with those reported in the literature as intake temperature and compression ratio were varied. The high intake temperature required to promote auto-ignition evidenced the necessity of additional boost in order to avoid volumetric efficiency losses.
- Results from chemical kinetics modeling show that H_2 yield increases proportionally with reforming temperature, and 645-700 K were found to be in the range of temperatures required to obtain 10-20% (vol) H_2 generation in the reformer.

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VII.4 Kinetic and Performance Studies of the Regeneration Phase of Model Pt/Ba/Rh NOx Traps for Design and Optimization

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Objectives

- Carry out studies of regeneration kinetics on lean-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

- Carried out bench-scale experiments of Pt/Ba monolith NOx trap. Instantaneous and time-averaged NOx conversion and product selectivities were quantified over a wide range of feed conditions and cycle timing using hydrogen as the reductant. Time averaged NOx conversions exceeding 80% were obtained with cycling protocols of 60 second storage phase and 5-10 second regeneration phase. The byproduct ammonia and nitrous oxide selectivities were determined, with ammonia selectivity as high as 50% depending on the rich pulse composition.
- Conducted transient kinetics studies of model Pt and Pt/Ba catalysts with TAP (Temporal Analysis of Products) reactor system. The TAP experiments elucidate the coupling between the precious metal (Pt) and NOx storage (Ba) components. A mechanism was proposed that is consistent with the product distribution and kinetics. A paper was published in Catalysis Today based on this work.
- Demonstrated existence of multiple periodic states during NOx trap operation using propylene as reductant. A LNT model predicts the main features of the multiplicity. A microkinetic model of the NOx storage and reduction system with hydrogen as the reductant is under development. The model is formulated as a "short monolith model" to simulate the benchscale monolith reactor experiments.

Future Directions

- Carry out comprehensive mechanistic study of the regeneration of model Pt/Rh/Ba NOx storage and reduction (NSR) catalysts with reductants H_2 and CO in the TAP reactor. We will continue with TAP experiments using model catalysts containing different loadings of Pt, Rh, and Ba. Specific TAP experiments to be conducted will include single component pulsing (NO or NO_2) and dual component pulse-probe (NO or NO_2 with H_2 or CO).
- Evaluate performance of the model NSR catalysts in a bench-scale NOx trap using synthetic lean-burn exhaust feeds. Our intent is to establish a comprehensive database of LNT performance over a wide range of experimental conditions and for different LNT catalyst compositions (containing Pt, Rh, and Ba).
- Upgrade the microkinetic model utilizing experimental data of monolith catalysts in the benchscale apparatus and of catalyst powders in the TAP reactor. The kinetic modeling will help to elucidate the mechanistic pathways and to estimate kinetic parameters. The approach we will take is systematic. The model is constructed in modules according to the different subsets of chemistries that are occurring. NO decomposition kinetic parameters will be estimated from NO pulsing over Pt catalysts while NO uptake/storage kinetics from NO pulsing over Pt/Ba catalysts, and so on.
- Apply the LNT model comprising essential transport processes and global kinetics for evaluation of alternative designs and operating strategies. Design variants to be examined will include the use of precious metal zoning.

Introduction

The objective of this project is to develop, characterize, evaluate and optimize lean-NOx trap (LNT) catalyst and reactor designs with the goal to improve the emissions performance and fuel efficiency of lean-burn and diesel vehicles. The LNT technology is an inherently transient catalytic process involving a multi-functional catalyst with multiple chemical reactions in a nonisothermal environment. Optimization of the LNT requires fundamental studies that elucidate the transient cycle to direct improvements in LNT catalyst formulations. The work plan involves four tasks: (1) carry out fundamental studies of the transient kinetics of LNT regeneration (2) evaluate and compare the effect of different reductants on LNT performance (3) incorporate the kinetics findings and develop a first-principles based predictive LNT model for design and optimization, and (4) test the LNT designs with a heavy-duty diesel dynamometer facility.

During the past year bench-scale reactor and TAP reactor studies have been conducted on model Pt/Ba catalysts. The bench-scale experiments have provided detailed performance data of monolithic NOx trap catalyst over a range of feed conditions. The experiments have provided instantaneous and time-average composition and monolith temperature data which identifies the regimes of high NOx conversion (> 80%) and NOx to N_2 selectivity (> 70%). The TAP studies provide fundamental transient kinetics under well characterized conditions, helping to elucidate the synergy between the Pt and Ba during NO pulse and NO-H_2 pump-probe experiments. A microkinetic model is under development that incorporates the underlying chemistries of hydrogen oxidation, NO decomposition, and conversion to key byproducts N_2O and NH_3.

Approach

We utilize an array of experimental and theoretical tools to advance the LNT technology. The project spans fundamental kinetic analysis, bench-scale reactor studies, microkinetic model development, LNT reactor modeling, and prototype LNT testing. Fundamental kinetics studies are carried out of model Pt/Rh/Ba NSR catalysts with reductants H_2 and CO in the TAP reactor. The TAP reactor provides the means for identifying the reaction pathways and determining the kinetics of the key steps comprising the pathways. The performances of model NSR catalysts are evaluated in a bench-scale NOx trap using synthetic exhaust, with attention placed on differences in reductant type and injection protocols. A mechanistic-based microkinetic model is developed that incorporates a detailed understanding of the chemistry and transport. We compare the NOx trap model simulations of bench-scale data obtained for the different reductants, and evaluate alternative LNT multiple zone designs. We will then test prototype LNTs on the exhaust of a diesel vehicle at the University of Houston heavy-duty diesel dynamometer facility.

Results

During the first year excellent progress has been on Task 1 (mechanistic studies in TAP reactor), Task 2 (bench-scale studies of NOx trap), and Task 3a (development of first-principles NOx trap model). Task 3b (NOx trap configurations) Task 4 (vehicle testing) will be carried out during years 2-4 and years 3-4, respectively. We carried out mechanistic studies of NO uptake and NO reduction by H_2 on Pt/Al_2O_3 and Pt/Ba/Al_2O_3 catalysts (provided by Engelhard Inc.). These studies utilized the TAP reactor system which involves rapid pulsing of reactants over a catalyst with analysis by a quadrupole mass spectrometer. The NO uptake provides information about the storage kinetics while the pump-probe experiments provide detailed information about the reaction pathways to products N_2, N_2O, and NH_3.

We carried out a systematic TAP study of NO storage and reduction over Pt/Al_2O_3 and Pt/BaO/Al_2O_3. In this study NO pulse and NO/H_2 pump-probe experiments were carried out at 350°C on pre-reduced, pre-oxidized, and pre-nitrated catalysts (Figure 1). While the findings reveal the complex interplay between storage and reduction chemistries and the importance of the Pt/Ba coupling, the data help to elucidate the catalytic processes.

NO pulsing experiments on both catalysts show that NO decomposes to major product N_2 on clean Pt but at a rate that declines as the oxygen product accumulates on the Pt. The storage on Pt/Ba/Al_2O_3 commences as soon as Pt-O species are formed. The pump-probe data provide detailed insight into the surface chemistry. The products include N_2, H_2O, NH_3 and N_2O. In most of the experiments N_2 is the major N-containing product while

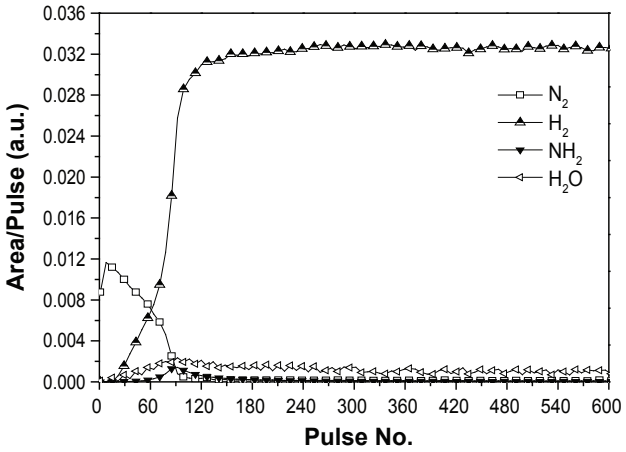


FIGURE 1. Effluent profiles during reduction of pre-nitrated Pt/BaO/Al_2O_3 at 350°C.

byproduct N_2O appears only after sufficient oxygen has accumulated. NH_3 appears only under reducing conditions. The pump-probe data show that the main role of H_2 is to react with oxygen, producing water.

Hydrogen reduction provides evidence that a fraction of NO is not stored in close proximity to Pt and is more difficult to reduce. A closely-coupled Pt/Ba interfacial process is corroborated by NO/H_2 pump-probe experiments. NO conversion to N_2 by decomposition is sustained on clean Pt using excess H_2 pump-probe feeds. With excess NO pump-probe feeds, NO is converted to N_2 and N_2O via the sequence of barium nitrate and NO decomposition. The transient evolution of the two pathways depends on the extent of pre-nitration and the NO/H_2 feed ratio. Typical results are shown in Figure 2 for an excess NO feed (NO/H_2 = 2). The first NO pulse produced N_2 which is consistent with NO decomposition. Subsequent pump-probe pairs resulted in an apparent H_2 reduction of NO stored on the barium phase (i.e. during NO pulse).

We have more recently carried out a detailed study of NO uptake and NO reduction with H_2 on Pt/Al_2O_3 catalyst over a wide range of temperatures (150 – 400°C) and pulse-probe timing protocols. These results are currently being analyzed.

Finally, recently we have made progress in the simulation of TAP experiments in order to elucidate mechanistic pathways as a first step towards estimating kinetic parameters. The TAP simulations are an essential component of the project because they enable the estimation of kinetic parameters under well defined conditions. Our initial focus has been the exposure of NO to Pt with the production of N_2 and N_2O. Together with kinetic parameter values from the literature, we have gotten good agreement in the experimental trends during NO decomposition on a pre-reduced Pt catalyst.

Bench-scale studies of NOx storage and reduction have been carried out utilizing a monolith reactor system comprising a simulated exhaust feed system, flow through reactor, and dedicated analytical system. The system enables steady-state and transient studies of all of the key overall reactions involved in NSR. These experiments provide basic data about NOx trap performance over a wide range of operating conditions (feed composition, temperature, flow rate), reductants (H_2, CO, etc.), and catalysts (Pt/Rh/Ba). Steady-state and periodic experiments identify the conditions for which the major N-containing, H-containing, and C-containing products are formed.

A comprehensive experimental study has been conducted for 2.2 wt% Pt/16 wt% Ba/γ-Al_2O_3 and 2.2 wt% Pt/γ-Al_2O_3 (Ba-free) monolithic catalysts. Steady-state data for several reaction systems were obtained over a wide range of temperatures. These data provide critical information about reaction pathways and rates that are helpful in elucidating the behavior during cycling. Some important findings are as follows:

- NO decomposition occurs to a negligible extent under steady-state conditions.
- Oxidation of H_2 is inhibited by NO, which increases the light-off temperature.
- Ammonia oxidation produces a complex mixture of N_2O, NO, and N_2. The selectivities are a sensitive function of the NH_3/O_2 feed ratio and temperature.
- The NO + H_2 reaction produces N_2O, NH_3, and N_2. The main N-containing product is dictated primarily by the NO/H_2 feed ratio.

Representative data obtained during cyclic operation with the bench-scale $Pt/Ba/\gamma$-Al_2O_3 LNT is shown in Figures 3 (effluent composition vs. time) and 4 (cycle-averaged data). The breakthrough of NO and NO_2 occurs near the end of the storage phase and

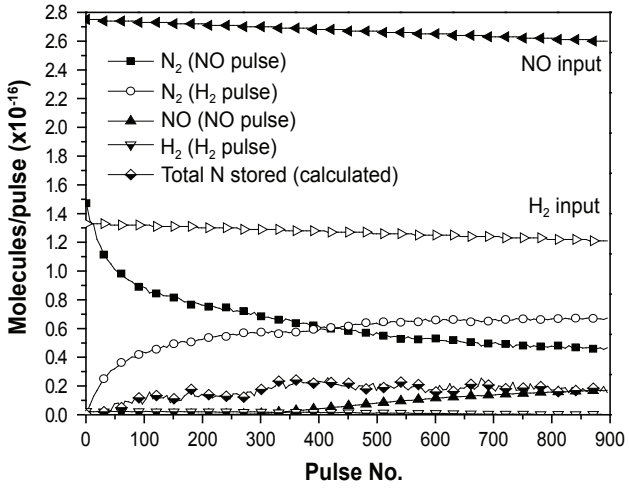


FIGURE 2. NO-H_2 pump probe over pre-reduced $Pt/BaO/Al_2O_3$ for $NO:H_2$ = 1:0.5 and 350°C.

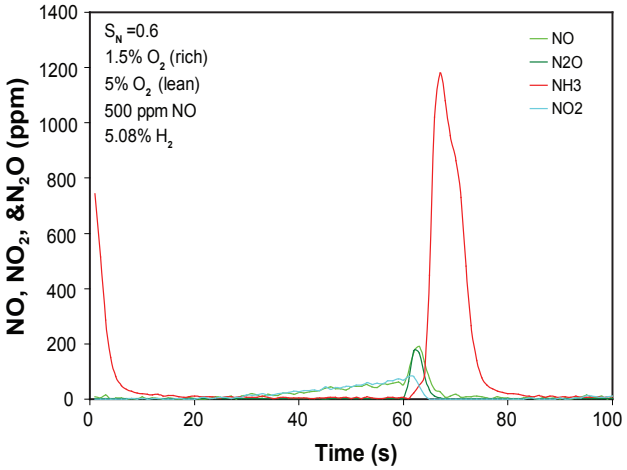


FIGURE 3. Effluent profile of N-containing species during NOx storage and reduction.

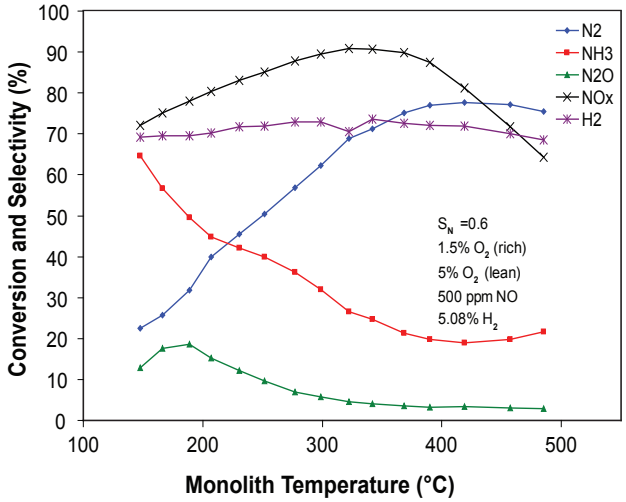


Figure 4. Cycle-averaged conversion and selectivity during NSR on Pt/Ba catalyst.

decrease to zero during the rich pulse. Product gas N_2O is followed by a much larger peak of NH_3 which appears at the end of the rich pulse. Corresponding cycle-averaged conversions and selectivities are shown in Figure 4 for a range of cycle-averaged monolith temperatures. The NOx conversion exhibits a maximum at 350°C while the N_2 (N_2O) selectivity increases (decreases) between 200 and 400°C.

This modeling component of the project complements the experimental components (Tasks 1 and 2). The objective in this part of the project is the development of a quantitative microkinetic reaction system model that can be incorporated into the NOx trap reactor model. Our near-term focus is to understand better the link between steady-state and periodic NOx reduction. The development of a predictive microkinetic model is key to success. Our approach is to build a mechanistic based model using established models of subsets of the overall chemistry. Our approach is to incorporate the continuously-upgraded microkinetic model into a "short monolith model" for direct simulation of bench-scale monolith experiments.

We are also making progress on advancing a NOx trap model developed in our group for propylene as the reductant. This model combines a detailed description of the storage of NO/O_2 mixtures on Pt/Ba catalysts with a multi-step description of propylene, including its reaction with O_2 and NO. In this study we compared model predictions with experimental measurements of steady-state and cycling on a short monolith.

Conclusions

Very good progress has been made in the objectives of this project. Detailed performance and kinetic data of model LNT Pt/Ba catalysts have been obtained in bench-scale and TAP reactors. The data provide the basis for mechanistic understanding and development of microkinetic models. During the next year we will expand the data set to include Pt/Rh/Ba catalysts and to use the microkinetics to simulate the experiments.

FY 2006 Publications/Presentations

Reports

Quarterly Report (10/1/05 – 12/31/05)
Quarterly Report (1/1/06 – 3/31/06)
Quarterly Report (4/1/06 – 6/30/06)
Quarterly Report (7/1/06 – 9/30/06)

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, **118**, Sept. 27 (2006).

2. Sharma, M., R.D. Clayton, M.P. Harold, and V. Balakotaiah, "Multiplicity in Lean NOx Traps," Chem. Engng. Sci., under review (2006).

Presentations

1. "Periodic NOx Storage and Reduction (NSR) for Lean Burn Engines," presented at AIChE Meeting, Cincinnati, 11/05 (with Manish Sharma and Vemuri Balakotaiah).

2. "TAP and Bench-Scale Reactor Studies of NOx Storage and Reduction on Model $Pt/BaO/Al_2O_3$ and Pt/Al_2O_3," presented at AIChE Meeting, Cincinnati, 11/05 (with Vinay Medhekar, Pranav Khanna, and Vemuri Balakotaiah).

3. "Experimental Analysis and Mathematical Modeling of NOx Storage and Reduction," poster presented at the Spring 2006 Symposium of the Southwest Catalysis Society, Rice University, 5/06 (with Vinay Medhekar and Vemuri Balakotaiah).

4. "Multiplicity in Lean NOx Traps," poster presented at ISCRE, Berlin, 9/06 (with Manish Sharma, Robert Clayton, and Vemuri Balakotaiah).

Special Recognitions & Awards/Patents Issued

1. First prize poster awarded at the Southwest Catalysis Society Symposium held in May, 2006.

VII.5 Investigation of Aging Mechanisms in Lean-NOx Traps

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(Todd J. Toops, Jae-Soon Choi, John M. Storey)

Partners:
- Ford Motor Co., Dearborn, MI (Bob McCabe)
- Umicore Autocat USA, Inc. (Owen Bailey)

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 spectrometer (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

- Fourteen fully formulated model catalysts were prepared (on cordierite monoliths), in which the concentrations of the four main active components, Pt, Rh, CeO_2 (or CeO_2-ZrO_2) and BaO (supported on alumina), were systematically varied.
- The optimum desulfation temperatures for the model catalysts were determined, while simultaneously examining the effect of catalyst composition on desulfation behavior. The ceria content of the catalysts was found to exert a significant influence on their desulfation characteristics: specifically, the higher the ceria content (within the range studied), the lower the required desulfation temperature.
- The effect of ceria on LNT NOx storage and regeneration behavior was examined by means of powder reactor and diffuse reflectance infrared Fourier-transform spectroscopy (DRIFTS) measurements. A number of effects associated with the presence of ceria were identified: increased NOx storage capacity (particularly at low temperatures), increased water-gas-shift activity, and improved regeneration characteristics.

Future Directions

- Evaluate NOx storage/reduction performance of fresh (de-greened) model catalysts using a bench-scale reactor.
- Perform accelerated aging of model catalysts using repeated sulfation-desulfation cycles in a synthetic gas reactor.
- Perform *in situ* DRIFTS studies in order to relate reactivity at the catalyst surface to catalyst composition (for both fresh and aged catalysts).
- Apply SpaciMS to study transient catalyst response in fresh and aged catalysts.

Introduction

Lean-NOx traps (LNTs) represent a promising technology for the abatement of NOx under lean conditions. Although LNTs have found application on lean-burn gasoline vehicles in Europe, 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_2 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 LNT 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, the evolution of catalyst microstructure upon aging can be related to NOx storage and reduction characteristics. 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

Preparation of model catalysts

Rather than using poorly characterized proprietary catalysts, or simple model catalysts of the $Pt/BaO/Al_2O_3$ type (representing the first generation of LNTs), we have elected to employ $Pt/Rh/BaO/Al_2O_3$ catalysts which also incorporate CeO_2 or CeO2-ZrO_2, representing a model system which more accurately reflects current LNT formulations. Catalysts were prepared in which the concentrations of each of the main components were systematically varied: Pt (50, 75 or 100 g/ft^3), Rh (10 or 20 g/ft^3), BaO (15, 30 or 45 g/L), and either CeO_2 (0, 50 or 100 g/L) or CeO_2-ZrO_2 (0, 50 or 100 g/L). Catalysts were obtained by washcoating onto standard cordierite substrates, the total washcoat loading being set at 280 g/L. La-stabilized alumina was used as the balance.

Desulfation studies

The catalyst aging cycle selected for the project is based on that developed by Ford Motor Co. for LNT aging. A key variable to be fixed in the cycle is the desulfation temperature: in practice the temperature used should be high enough to completely restore the activity of the catalyst (i.e., achieve complete or near-complete desulfation), but low enough to avoid unnecessary thermal damage to the catalyst. In order to determine this optimum temperature for the model LNT catalysts prepared above, sulfation-desulfation cycles were performed at Ford Research and Innovation Center, in which the desulfation temperature was systematically varied. Desulfation temperatures required to restore catalyst activity after poisoning with sulfur to a level of 6.2 g S/L were found to fall in the range 700-750°C; furthermore, the higher the ceria content (within the range studied, 0-100 g/L), the lower the required desulfation temperature. This observation is in general agreement with a study by Theis and co-workers [1], in which it was found that a trap containing no oxygen storage material required higher temperatures to recover its performance than traps containing such a material. This can be rationalized on the basis of the higher water-gas-shift activity of ceria-containing catalysts, although the ability of ceria to store sulfur, thereby potentially lessening the amount of bulk $BaSO_4$ formed, may also play a role (given that $Ce(SO_4)_2$ is less thermally stable than $BaSO_4$ and hence more readily decomposed). Future X-ray diffraction (XRD) studies will address this point.

Effect of Ceria Addition on LNT NOx Storage and Regeneration Behavior

The effect of ceria on LNT NOx storage and regeneration characteristics was also examined. Representative results obtained using Oak Ridge National Laboratory's powder reactor are shown in Figure 1, which compares NOx storage for two LNT formulations: 1 wt% $Pt/Ba/Al_2O_3$ (denoted as catalyst PBA) and (ii) 1 wt% $Pt/Ba/Al_2O_3$ (74 wt%) + 1 wt% Pt/CeO_2 (26 wt%) (denoted as PBAC), the latter comprising a physical mixture of $Pt/Ba/Al_2O_3$ and Pt/CeO_2 powders. As shown, both catalysts exhibit their highest NOx storage capacity at 300°C; for PBA the value is 0.27 mmol/g, the corresponding value for PBAC being 0.28 mmol/g. Compared to PBA, PBAC showed higher NOx storage capacity at 200°C (0.24 vs 0.19 mmol/g), clearly showing that the addition of ceria is beneficial with respect to NOx storage at low temperature. In contrast, at 400°C the storage capacity of PBA is greater than that of PBAC, indicating that ceria does not contribute substantially to NOx storage at this temperature. This has been confirmed independently by DRIFTS measurements, thermal decomposition of surface nitrate species on ceria occurring in the range 300-350°C.

Catalyst behavior was also examined under cycling conditions, using 6 min lean and 0.5 min rich times. Figure 2 shows the outlet NOx concentration profiles with time during the lean phase (T = 300°C). The superior performance of catalyst PBAC is evident from the considerably lower NOx slip as compared to PBA, resulting in higher NOx conversion (averaged over lean-rich cycles). This was also found to be the case at 200 and 400°C. Given the lower NOx storage capacity

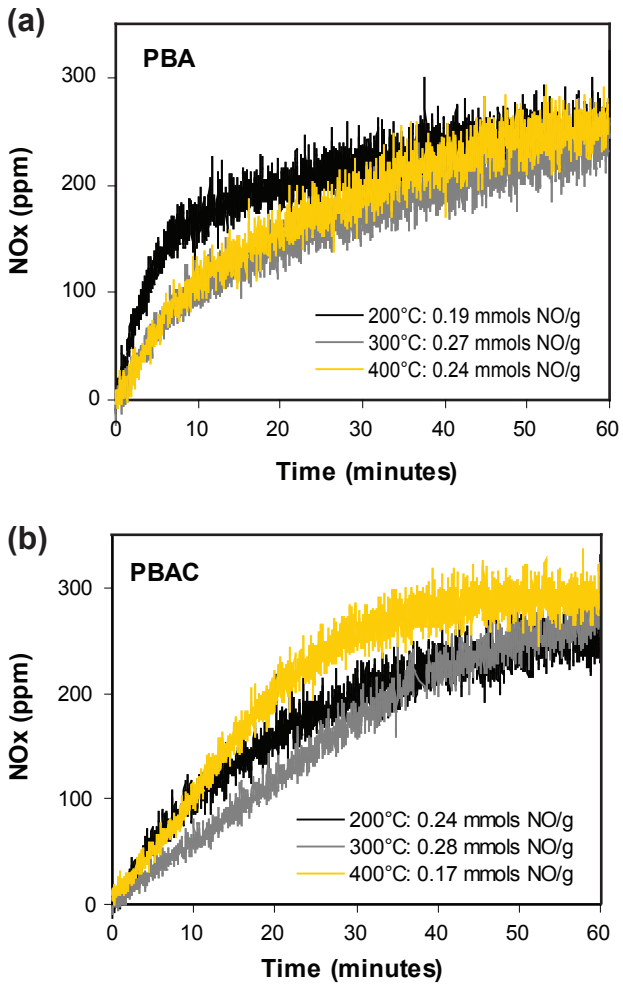


FIGURE 1. Outlet NOx Concentration as a Function of Time During Storage Capacity Measurement A: $Pt/Ba/Al_2O_3$; B: $Pt/Ba/Al_2O_3$-Pt/CeO_2 (74 wt%-26 wt%)

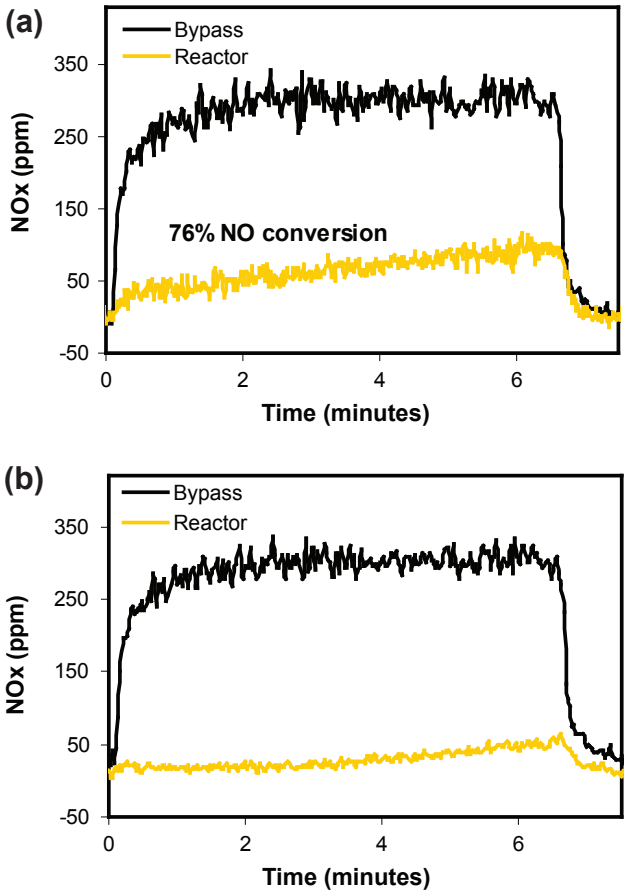


FIGURE 2. Outlet NOx Concentration as a Function of Time during Steady-State Lean-Rich Cycling

of PBAC at 400°C, its superior NOx conversion at this temperature must derive from either lower emissions of unconverted NOx during the rich phase, or a more extensive regeneration during the rich phase which results in a higher effective NOx storage capacity. The former explanation can be excluded based on an analysis of the reactor effluent, both catalysts showing near zero NOx emissions during the rich phase. Further, *in situ* DRIFTS studies provide support for the superior regeneration characteristics of catalyst PBAC. Figure 3 shows the results of experiments in which the two catalysts were loaded with NOx and then subjected to H_2-temperature programmed reduction (TPR). According to DRIFT spectra, nitrate species on PBAC are removed at a slightly lower temperature than those on PBA, as reflected in the decrease in intensity of the nitrate bands at 1415 and 1330 cm^{-1}. The origin of this effect is at present unclear, although it may be related to the ability of ceria to store NOx, thereby lessening the amount of bulk barium nitrate formed (this being the most difficult form of nitrate to reduce).

Conclusions

- Model $Pt/Rh/BaO/Al_2O_3$ catalysts have been prepared which also incorporate CeO_2 or CeO_2-ZrO_2, and in which the concentrations of Pt, Rh, BaO and CeO_2 have been systemically varied. Desulfation studies indicate that the higher the ceria content (within the range studied, 0-100 g/L), the lower the required desulfation temperature. This can be rationalized on the basis of the higher water-gas-shift activity of ceria-containing catalysts, although the ability of ceria to store sulfur, thereby potentially lessening the amount of bulk $BaSO_4$ formed, may also play a role.
- NOx storage experiments have shown that the addition of ceria is beneficial with respect to NOx storage at low temperatures (up to 300°C).

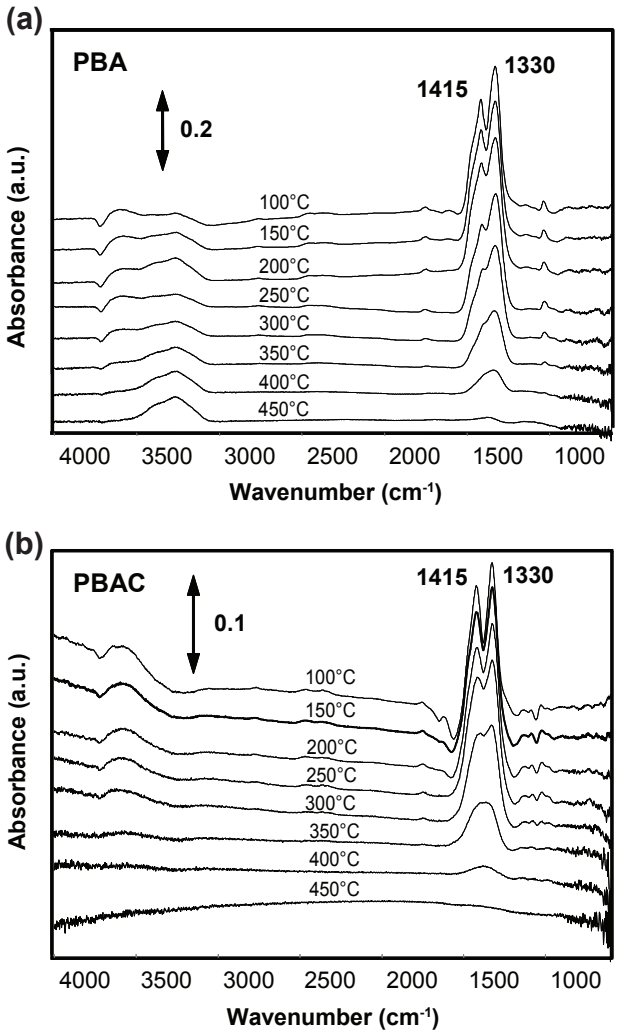


FIGURE 3. DRIFT Spectra of Catalysts PBA and PBAC Loaded with NOx during H_2-TPR

- In lean-rich cycling experiments, the presence of ceria was found to be beneficial at all temperatures in the range 200-400°C. This is attributed to the superior rich phase regeneration characteristics of the ceria-containing catalyst studied, which results in a higher effective NOx storage capacity during cycling.

References

1. J. Theis, J. Ura, C. Goralski Jr., H. Jen, E. Thanasiu, Y. Graves, A. Takami, H. Yamada, S. Miyoshi, Society of Automotive Engineers 2003-01-1160.

FY 2006 Publications/Presentations

1. Y. Ji, T.J. Toops, U.M. Graham, G. Jacobs and M. Crocker, "A kinetic and DRIFTS study of supported Pt catalysts for NO oxidation", *Catal. Lett.* **110** (2006) 29.

2. Y. Ji, T. J. Toops, U.M. Graham, G. Jacobs and M. Crocker, "A kinetic and DRIFTS study of supported Pt catalysts for NO oxidation", poster presented at the 9th CLEERS workshop, Detroit, MI, May 2–4, 2006.

3. Y. Ji, T.J. Toops and M. Crocker, "Effect of Ceria Addition on the Regeneration Behavior of a Model Lean NOx Trap Catalyst", poster presented at the 2006 Southeastern Catalysis Society Fall Symposium, Asheville, NC, September 26, 2006.

VII.6 Improved Engine Design Concepts Using the Second Law of Thermodynamics: Reducing Irreversibilities and Increasing Efficiencies

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Objectives

- Identify initial key issues to examine.
- Upgrade cycle simulation to include newer friction sub-models.
- Use the cycle simulation to examine the use of exhaust gas recirculation (EGR) for spark ignition (SI) engines.
- Use the cycle simulation to examine the use of hydrogen for SI engines.
- Complete a parametric study of the destruction of availability during the combustion process for constant pressure, constant volume and constant temperature processes.
- Complete a preliminary examination of the possible reversible combustion for a reciprocating device.

Accomplishments

- Key issues identified included the effects of EGR, and the use of hydrogen.
- The engine cycle simulation was updated to include new friction submodels which are based on engine designs of the 1990s.
- The cycle simulation was used to examine the effects of EGR for an SI engine. Both a cooled and an adiabatic EGR configuration were studied. The results included increased thermal efficiencies for increasing EGR, and a slight increase of availability destruction as EGR increased. In addition, further results were obtained as functions of engine load and speed.
- The cycle simulation was used to study the use of hydrogen in a SI engine. Because of the wide flammability character of hydrogen, engine operation with lean (~0.4) equivalence ratios is possible. By using lean equivalence ratios, the engine could be operated with less or no throttle thus increasing the thermal efficiency. Relative to isooctane, the availability destruction decreased slightly, and the nitric oxide emissions increased.
- A parametric study of the destruction of availability during the combustion process for simple systems was completed and documented. The availability destroyed during the combustion process decreased with increasing temperatures and for the same conditions varied with the selected fuel.
- A preliminary examination of hypothetical reversible combustion at high temperatures and pressures was initiated. The preliminary 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.

Future Directions

- Extend the current SI engine cycle simulation to include provisions for compression ignition (CI) engines.
- Analyze the effects of compression ratio and expansion ratio on engine performance using both the first and second laws of thermodynamics.
- Investigate the use of exhaust gas energy recovery options from both the first and second laws of thermodynamics.

Introduction

This work is aimed at using comprehensive thermodynamic evaluations to better understand the details of engine operation with the goals of defining operating conditions and design parameters which provide the highest possible efficiencies with minimal emissions. The use of the second law of thermodynamics is central to this effort. The second law of thermodynamics provides a rich and significant insight concerning the proper use of energy and its conversion to mechanical shaft power. For example, the exhaust gases may possess more energy than the cylinder heat loss, but the cylinder heat loss may be more important from the perspective of being used for "work."

The second law allows this feature to be quantified using the thermodynamic property of availability (also, known as exergy).

Throughout the world, activities are being conducted to realize higher engine efficiencies with minimal emissions. Many questions exist concerning results from these investigations. The first law has been used to provide some understanding, but the use of the second law of thermodynamics has not been widely used. The work conducted as part of this project was directed to help provide a deeper understanding of these results. This work has included a detailed study of the use of EGR by a SI engine. The thermal efficiency gains, the nitric oxide reductions, and the second law parameters are quantified as functions of EGR level, engine operating conditions and engine design parameters. Another study examined the use of hydrogen fuel by a SI engine. Different strategies are examined for the use of hydrogen which includes the use of lean operation with little or no throttle. Results include the changes in thermal efficiency, and availability destruction as functions of engine operating and design parameters.

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 new features such as the use of the second law of thermodynamics. The engine cycle simulation has been described in numerous previous publications [1, 2]. 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.

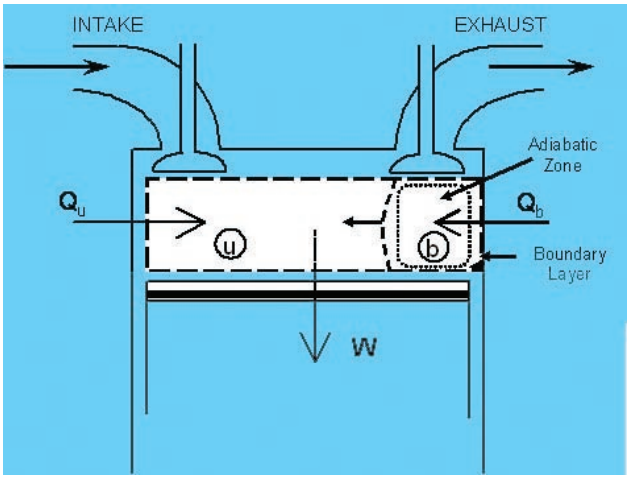


FIGURE 1. Schematic of the Engine Cylinder Depicting the Three Zones During Combustion

Results

Typical results will be reported from the EGR and hydrogen studies. Other results are available elsewhere. For both studies, a conventional, automotive V-8, SI engine is used as the framework for this work [1, 2]. Figure 2 shows the nitric oxide concentrations as functions of the percentage of EGR for the base case for the two EGR configurations. The nitric oxide concentration decreases rapidly with increasing EGR. The cooled EGR configuration results in lower nitric oxide emissions relative to the adiabatic EGR configuration since the gas temperatures are lower. Even for the adiabatic EGR configuration, however, over 90% reduction in nitric oxide is obtained with about 25% EGR.

Figure 3 shows the (net) indicated and brake thermal efficiencies as functions of the percentage of EGR for the base case for the two EGR configurations. Both the indicated and brake efficiencies increase with increasing percentage of EGR, and the results are similar for the two EGR configurations. The brake thermal efficiency increases from about 25.7% to about 29% as EGR increases from 0 to 40%. These increases of the thermal efficiencies for the use of EGR are the result of lower gas temperatures, lower heat transfer, favorable thermodynamic properties, reduced dissociation near top dead center, and lower pumping losses (a consequence of the constant load condition).

Figure 4 shows the four major availability terms as functions of the percentage of EGR for the base case for the cooled EGR configurations. The majority of the availability of the fuel is distributed between these four terms. These results can best be explained by

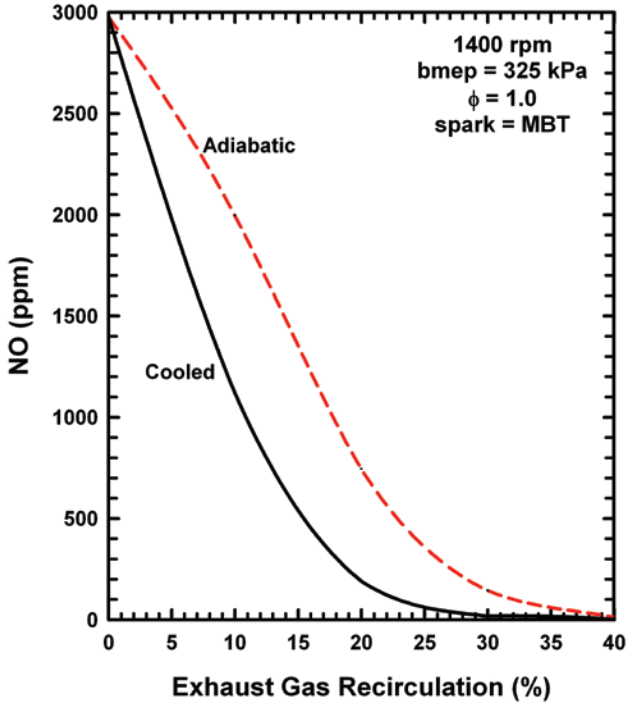


FIGURE 2. Nitric oxide concentration in the exhaust as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

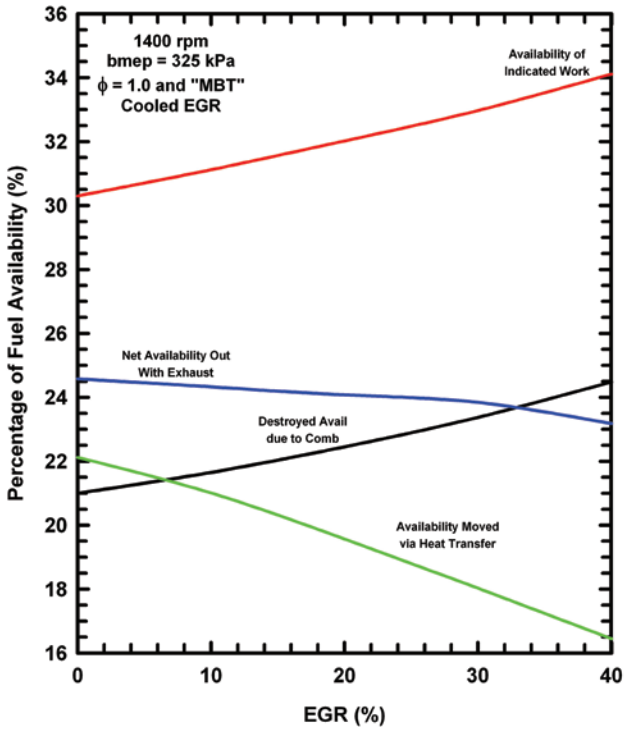


FIGURE4. Four availability terms as functions of the percentage of exhaust gas recirculation for the base case conditions for the *cooled* EGR configuration.

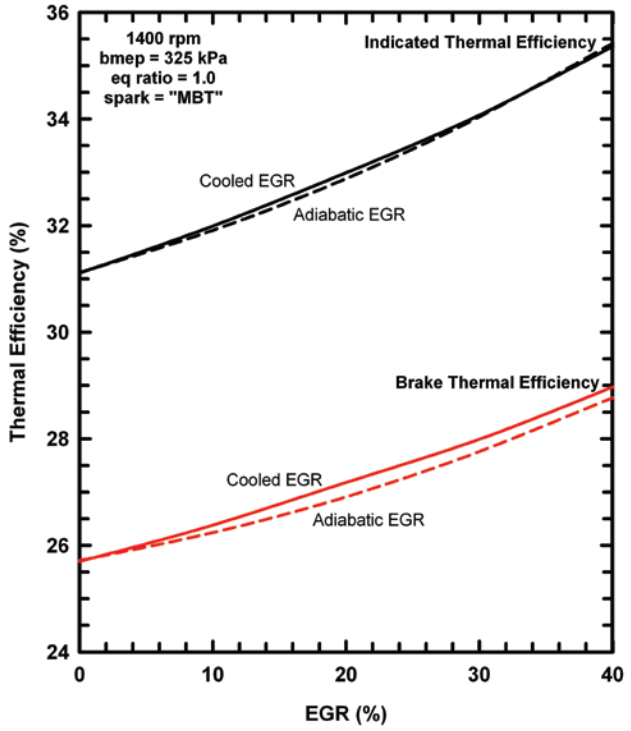


FIGURE 3. Indicated and brake thermal efficiency as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

knowing the changes in the various gas temperatures [1]. For the cooled EGR configuration, the availability associated with the indicated work increases as EGR increases. This reflects the increase of the indicated thermal efficiency (Figure 3). The net availability that leaves with the exhaust flow decreases as EGR increases, and this follows from the decrease of the exhaust temperature as EGR increases. The availability moved with the heat transfer to the cylinder walls decreases as EGR increases, and this is a result of the decreasing heat transfer as EGR increases. Finally, the availability destroyed during the combustion process increases with increases in the percentage of EGR. This is a direct consequence of the decrease in the combustion gas temperatures.

The next set of results are from the hydrogen study [2]. A number of strategies are possible for using hydrogen. For the same operating conditions, the use of hydrogen resulted in higher cylinder pressures and temperatures. Figure 5 shows the brake thermal efficiency as functions of engine load (brake mean effective pressure, bmep) for four cases: (1) isooctane with a burn duration of 60° crankangle (CA), (2) hydrogen with a burn duration of 60° CA, (3) hydrogen with a burn duration of 30° CA, and (4) hydrogen with a burn duration of 30° CA and variable equivalence

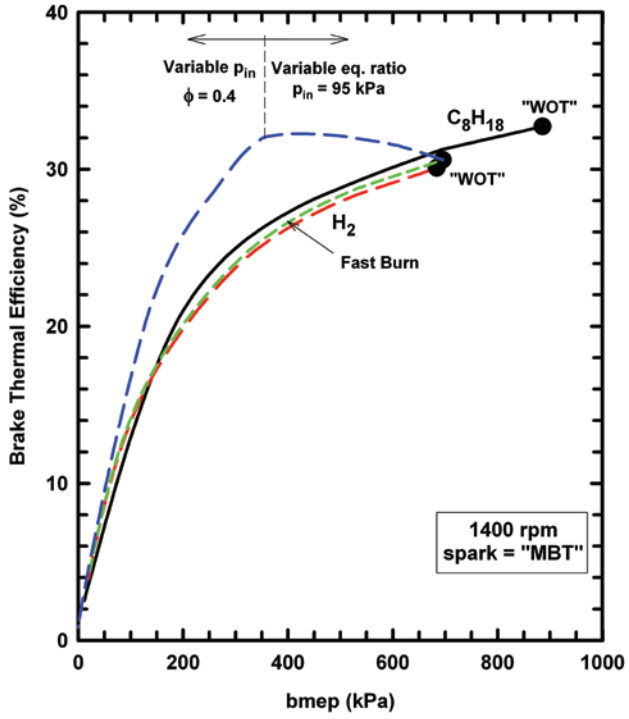


FIGURE 5. Brake thermal efficiency as functions of brake mean effective pressure for the base case using isooctane and three cases using hydrogen.

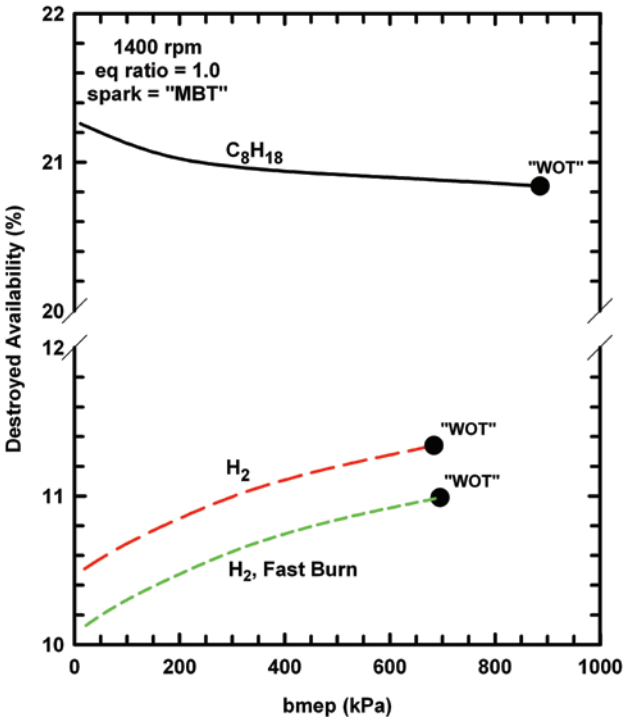


FIGURE 6. The destroyed availability due to combustion as functions of engine load (bmep) for engine operation with hydrogen with a burn duration of 60°, with hydrogen with a burn duration of 30° (fast burn), and with isooctane with a burn duration of 60°, all for an equivalence ratio of 1.0, and 1400 rpm.

ratio. The first three cases are at an equivalence ratio of 1.0, and for these cases, the brake thermal efficiency increases as engine load increases due largely to the decreasing throttle losses (pumping work) and decreasing relative heat losses. The thermal efficiency is highest for the isooctane case due primarily to the lower heat losses. The thermal efficiency for the fast-burn hydrogen case is slightly higher than for the longer burn hydrogen case.

In addition, the use of isooctane results in a higher maximum load (maximum bmep of about 886 kPa) relative to the use of hydrogen (maximum bmep of about 684 kPa). This result is due to the lower volume of fuel vapor for the isooctane stoichiometric operation compared to stoichiometric hydrogen operation.

Figure 5 also includes results for the hydrogen case which is based on a burn duration of 30° CA and variable equivalence ratio. For this case, the advantages of the lean flammability characteristics of hydrogen are used for all but the wide open throttle (WOT) condition. For these computations, the assumption was that the lean limit for hydrogen mixtures is an equivalence ratio of 0.4. For loads less than a bmep of 353 kPa, a lean mixture with an equivalence ratio of 0.4 was used.

As load increased from idle, the throttle was opened. At a bmep of 353 kPa, the throttle was wide open, and the equivalence ratio was 0.4. For higher loads (bmep >353 kPa), the equivalence ratio was increased from 0.4 to 1.0 (maximum bmep condition). The brake thermal efficiency was highest for this case as compared to the other three cases. The use of hydrogen with variable equivalence ratio results in the highest efficiencies with a maximum brake thermal efficiency of about 32.0%. The strategy of this case provides gains in brake thermal efficiency due to the favorable thermodynamics and low temperatures of lean combustion.

Figure 6 shows the destroyed availability due to combustion as functions of the engine load for the isooctane and the two hydrogen cases. The destroyed availability increases slightly with increasing load for the hydrogen cases, and decreases slightly for the isooctane case. The two hydrogen cases have between about 10–11.5% destruction, and the isooctane case has between about 20.8–21.3% destruction for the conditions examined.

Conclusions

For the EGR study:

- The level of nitric oxide emissions reductions increased for increasing EGR levels for both EGR configurations, and for the same EGR level, the cooled EGR configuration resulted in the greatest nitric oxide reductions.
- Both EGR configurations resulted in approximately the same indicated and brake thermal efficiencies. Although the heat losses were less for the cooled EGR configuration, the pumping losses were less for the adiabatic configuration (to maintain the same load), and these two effects were of approximately equal magnitude for a given EGR level.
- The availability destroyed during the combustion process increased for increasing EGR levels largely due to the decreasing gas temperatures.

For the hydrogen study:

- In general, for the cases with an equivalence of 1.0, the brake thermal efficiency was slightly lower for the hydrogen cases due to the higher temperatures and higher heat losses.
- For the variable, lean equivalence ratio cases, the thermal efficiency was higher for the hydrogen case relative to the isooctane case.
- The second law analyses indicated that the destruction of availability was lower for the base hydrogen case (11.2%) relative to the isooctane case (21.1%).
- In general, availability was preserved during the combustion process for the hydrogen cases due to the higher combustion temperatures. This availability was retained in the exhaust gases and the higher temperatures resulted in more availability moved with the heat transfer. The net effect, therefore, was a lower thermal efficiency for the hydrogen cases with an equivalence ratio of 1.0.

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2. J. A. Caton, "First and Second Law Analyses of a Spark-Ignition Engine Using Either Isooctane or Hydrogen," in the proceedings of the 2006 Fall Conference of the ASME Internal Combustion Engine Division, Sacramento, CA, 5–8 November, 2006.

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1. P. S. Chavannavar, and J. A. Caton, "The Destruction of Availability (Exergy) due to Combustion Processes: A Parametric Study," Journal of Power and Energy, Proceedings of the Institution of Mechanical Engineers, Part A, vol. 220, number 7, pp. 655–669, 2006.

2. J. A. Caton, "Utilizing a Cycle Simulation to Examine the Use of EGR for a Spark-Ignition Engine Including the Second Law of Thermodynamics," in proceedings of the 2006 Fall Conference of the ASME Internal Combustion Engine Division, Sacramento, CA, 5–8 November, 2006.

3. J. A. Caton, "First and Second Law Analyses of a Spark-Ignition Engine Using Either Isooctane or Hydrogen," in the proceedings of the 2006 Fall Conference of the ASME Internal Combustion Engine Division, Sacramento, CA, 5–8 November, 2006.

4. J. A. Caton, "The Effects of Exhaust Gas Recirculation (EGR) for a Spark-Ignition En-gine: A Second Law Analysis," in proceedings of the 2006 Spring Meeting of the Central States Section of the Combustion Institute, Cleveland, OH, 21–23 May, 2006.

5. P. S. Chavannavar and J. A. Caton, "Irreversibilities Associated with Basic Combustion Processes," in proceedings of the 2006 Spring Meeting of the Central States Section of the Combustion Institute, Cleveland, OH, 21–23 May, 2006.

Special Recognitions & Awards/Patents Issued

1. Society of Automotive Engineers 2005 Excellence in Oral Presentation Award, for presentation of "Use of a Cycle Simulation Incorporating the Second Law of Thermodynamics: Results for Spark-Ignition Engines Using Oxygen Enriched Combustion Air," at the 2005 SAE International Congress and Exposition, Society of Automotive Engineers, Cobo Hall, Detroit, MI, 13 April, 2005.

VII.7 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

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DOE Technology Development Manager:
Roland Gravel

NETL Project Manager: Sam Taylor

Subcontractor:
Visteon: James Winkelman, George Zhu
and David Hung

Goals

- Demonstrate an advanced low-pressure direct-injection engine which has a 15% improvement in fuel economy over the baseline 5.4L production engine at road load conditions.
- Demonstrate the benefits of advanced technology developed on this project including infinitely variable valve actuators (timing and lift), ionization flame detection for engine control and a cycle resolved mass air flow sensor.

Accomplishments

- A low-pressure directly injected fuel spray has been developed for this application after completing a number of experiments.
- A prototype engine controller was selected and the software developed for use in this project. A hardware in-the-loop engine simulator was developed and used to evaluate engine control software.
- During this year, we have created and validated a control oriented actuator model, developed adaptive valve lift and timing control strategies, and simulated the closed-loop lift controller with the mathematical model. This model has been implemented with the prototype closed-loop lift controller on the intake valve at engine speed ranging from 1,200 rpm to 5,000 rpm on the test bench.
- A forward-backward mass air flow sensor has been developed based on a production sensor element. We have applied for a patent on this device.

Future Directions

- Complete baseline testing of the variable cam timing (VCT) engine for performance and emissions.
- Conduct experiments with the advanced low-pressure direct injection engine which features the advanced control systems and infinitely variable valves to demonstrate an expected 15% improvement in fuel economy at road load conditions.

Introduction

The goal of this project is to demonstrate an improvement in the fuel economy of light-duty vehicles by improving the cycle efficiency of the Otto cycle based engine. Otto cycle engines have been shown to be of excellent value in cost per kilowatt, meet strict emission standards and billions of dollars have been invested in the facilities to manufacture these engines and their associated components. Thus, technologies that offer improvements in current engines provide a good value proposition for both the consumer and the manufacturer. As mentioned above, our goal is to demonstrate an advanced low-pressure direct injection engine which has a 15% improvement in road-load fuel economy over a baseline 5.4L production engine.

Approach

There are four technologies that we have been investigating to meet the goals of this project. They include a low-pressure direct injector which will increase volumetric efficiency and facilitate aggressive deceleration fuel cutoff. The second is an electronic-pneumatic valve actuator which will enable variable compression ratio control and valve deactivation. The third is a forward-backward mass air flow sensor which allows for cycle-resolved measurement of the inducted fresh air charge so that fueling can be accurately maintained. Fourth, a key aspect needed to achieve

these engine efficiency improvements is the ability to detect information associated with combustion events and in this application we have focused on the ability to use a measure of the ionization current associated with these events. The technical highlights of these developments are discussed in the next section.

Results

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 studied. Four injector spray patterns were evaluated (Figure 1). Crank angle resolved images were taken using a newly acquired high-speed imaging system. Based on extensive image analysis, an optimal spray pattern was identified. This pattern provided a good overall fuel distribution, with minimal fuel impingement on the cylinder wall. A technical paper based on these results was written and submitted for the 2007 SAE Congress.

In addition, high-speed visualization of in-cylinder flame distribution was achieved in a preliminary investigation. The color imagery allows the spray distribution, flame propagation, and fuel impingement to be studied in detail. Both in-cylinder ionization and pressure data were also obtained in synchronization with the combustion images. The entire combustion event, from the beginning of spark ignition to flame propagation and to flame quenching at the cylinder wall, can be clearly visualized. We strongly believe it is the first time that such a combination of test data has ever been collected simultaneously. We also developed a custom GUI (graphical user interface) to process the images. In Figure 2, the red line in the plot displays the image number (which can be related to crank angle) of the instantaneous combustion image with the corresponding pressure and ion voltage. The image depicts the premixed flame front (blue) propagating across the cylinder, with some small fuel-rich clusters (orange) scattered on the left side of the cylinder. Other test data can be extracted for further analysis.

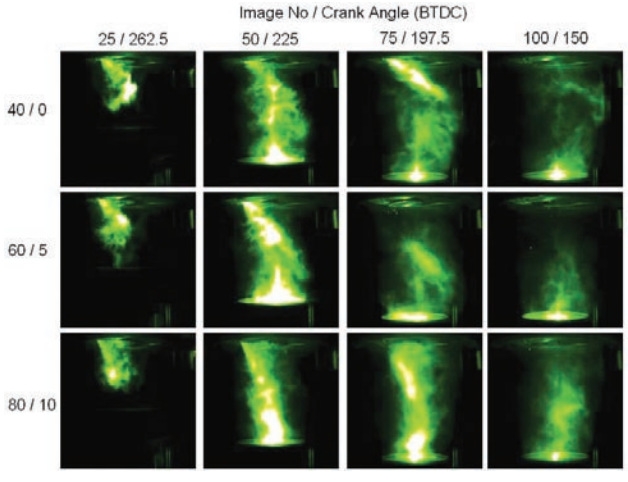


FIGURE 1. In-Cylinder Fuel Mixture Formation at 2,500 rpm/WOT/30 bar Fuel Pressure/SOI at 300° CA BTDC

Engine Control System Development

In FY 2006, we selected the Opal-RT™ real-time control system as the prototype engine controller for the project. The system was purchased in February and delivered in April. The system hardware configuration can be found in Figure 3. In a nutshell, the system consists of two CPUs, one for closed-loop control of the electro-pneumatic valve actuator (EPVA) and the other for closed-loop engine combustion control.

Real-time control software was developed based upon the Opal-RT™ real-time engine controller. The controller is capable of sampling the in-cylinder pressure, ionization, and other engine sensor signals with one crank degree resolution, calculating the engine control commands every combustion event. It updates the engine spark, fuel, valve timing (for variable compression ratio, exhaust gas recirculation rate, throttle) outputs every combustion event. A hardware-in-loop (HIL) engine simulator (see Figure 4) was developed and used to evaluate the developed engine

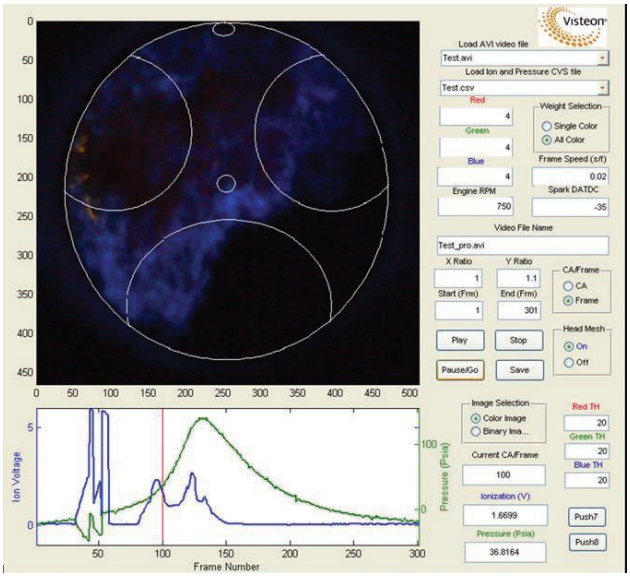


FIGURE 2. Custom-Built GUI Schematic for Flame Image Analysis (The combustion image with its corresponding pressure and ionization voltage data can be evaluated simultaneously.)

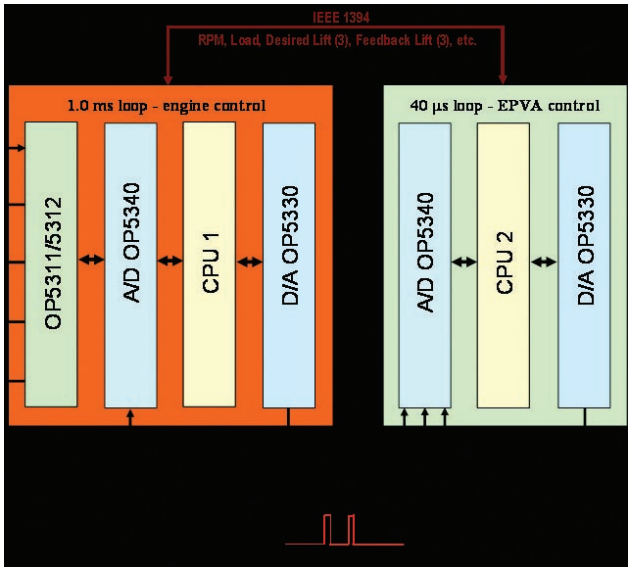


FIGURE 3. Opal-RT Hardware Architecture and System I/O



FIGURE 4. dSpace Hardware-In-Loop Simulator

control software. The real-time engine controller is going to be validated and calibrated on an engine dyno before the end of year.

Next year, we are going to focus on engine control system development in the area of closed-loop knock control, EPVA valve timing optimization, and direct injection optimization.

Development of a Forward-Backward Mass Air Flow Sensor (FBMAFS)

The goal of this component of the investigation is to develop a mass airflow sensor that is capable of measuring *unsteady*, direction-reversing, mass flow rate. Subsequently, the sensor will be integrated with the single-cylinder high-efficiency controlled combustion engine for implementation of the advanced engine control. Specifically, this sensor technology is designed to provide a net mass air flow rate entering each of the cylinders on a cycle resolved basis. Realization of this method will help provide optimum fuel-air ratio control during transients as well as in steady-state operation. As the use of variable valve timing becomes more sophisticated, speed density systems which rely on extensive calibrations become more complicated and less accurate. Proof-of-concept of the new FBMAFS has been demonstrated and we have applied for a patent on the technology. Issues related to signal noise are being addressed with appropriate filtering. Optimization of the geometrical design of the FBMAFS is underway which will provide improved signal-to-noise outputs using the sensors we have available.

Electro-Pneumatic Valve Actuator (EPVA) Control System Developments

The goal of the electro-pneumatic valve actuator control system development is to eliminate the camshaft of a traditional internal combustion engine and control the opening timing, duration, and lift of both intake and exhaust valves by these EPVAs.

Last year, a physics-based nonlinear mathematical model was built component by component and validated with experiments. In FY 2006, we have created and validated a control oriented actuator model, developed adaptive valve lift and timing control strategies, simulated the closed-loop lift controller with the mathematical model and implemented the prototype closed-loop lift controller on the intake valve at engine speed ranging from 1,200 rpm to 5,000 rpm on the test bench.

A control oriented actuator model was created to reduce computational throughput and to enable real-time implementation. This model was validated with the experimental data. The adaptive valve lift tracking, valve opening and closing timing control strategies were developed for improving actuation repeatability and response time. A model reference adaptive system identification technique was employed to obtain the nonlinear system parameters needed for generating closed-loop control signals. The convergence of the derived adaptive parameter identification algorithm was achieved within 40 cycles using the valve test bench data. Closed-loop control strategies were developed and validated in simulation. Furthermore, 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 engine speed from 1,200 rpm to 5,000 rpm. The experiment results showed satisfactory transient and steady-state lift tracking performance. For example, at 1,200 rpm, the actual valve lift reached the reference lift with less than 0.5 mm lift error in one cycle. The steady-state error was less than 0.5 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 about 45% reduction of standard deviation over the open-loop control. Please refer to the publication list for the details of all control architectures and experiment results. We are going to implement the prototype closed-loop opening and closing timing controller on the intake valve on the test bench by the end of December.

Next year, our effort will be devoted to designing the closed-loop exhaust valve controller against the random disturbance from high pressure in combustion chamber. We are going to run closed-loop EPVA lift and timing controllers on the intake and exhaust valves with the target engine head with the optimized valve lift and timing schemes.

Summary

Valve control systems are nearly complete and the final testing of valve actuators on the cylinder head is underway. The engine control system is complete in breadboard form and ready for testing on the reference 5.4L variable cam phase engine which is now complete. We believe that a solution for closed-loop feedback position control of the valves has been obtained using a recently obtained position sensor. A new emission bench is expected to be operational in December and will be available when the infinitely variable valve timing head is operational in early 2007. All systems appear to be in place to complete this project in FY 2007.

FY 2006 Publications/Presentations

1. Jia Ma and Harold Schock et. al. “Analysis and Modeling of an Electronically Controlled Pneumatic Hydraulic Valve for an Automotive Engine”, SAE 2006-01-0042, 2006.

2. Jia Ma, Guoming Zhu, Harold Schock and Jim Winkelman, “Adaptive Control of a Pneumatic Valve Actuator for an Internal Combustion Engine”, accepted by the Proceedings of American Control Conference, New York, New York, June 2007.

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VIII. ABSTRACTS OF NEWLY AWARDED PROJECTS

VIII.1 Application of Wide Spectrum Voltammetric Sensors to Exhaust NOx Measurement

Streamline Automation, LLC

Streamline Automation, LLC will perform a two-year effort to develop a NOx sensor based upon gas voltammetric technology. Liquid-phase voltammetry has been used for over fifty years for qualitative and quantitative analysis through forced oxidation or reduction at an electrode surface. In 1995, Argonne National Laboratory developed a process for gas phase voltammetry, which received an R&D 100 award for the research. The technology was licensed to Streamline Automation and is the basis for development of the NOx sensor.

The overall objective is to demonstrate that a practical automotive NOx sensor can be successfully developed based upon *voltammetric* gas sensor technology. Voltammetry is an electrochemical analysis technique that has been relied upon for many decades for *identification* and *quantification* of chemicals in *liquid* solutions and compounds. In voltammetry, an electrical current is produced by applying a high-speed, time varying potential to the cell. This forces chemical components to react (dissociate) at potentials characteristic to each species. The induced current vs. applied potential data is called a "voltammogram", or electrochemical spectrum, which is then digitally processed to extract and identify the reacting chemical species and their concentrations.

Current NOx sensors suffer from interference by exhaust gases and inability to measure ammonia, which is needed for most current NOx control strategies. The gas voltammetric method has minimal contamination and interference effects from exhaust components, can qualitatively and quantitatively measure the individual NOx species (NO_2 and NO_3), ammonia, and is capable of measuring organic exhaust species.

Several generations of gas sensors based upon voltammetry have now been produced and used as an electronic nose to detect and quantify *gaseous* chemicals in complex mixtures. While the materials that these electrochemical cells are fabricated from are similar enough to existing automotive oxygen sensors to expect similar life spans and durability - the voltammetry method of operation is significantly more capable providing far more information with which to describe the gas composition. In voltammetry *all* gases in the mixture are routinely considered "target" analytes and any issues of interferences become as simple as discarding responses outside of a defined (NOx) reaction potential. This broad-spectrum response also promotes the evolution of a voltammetric multiple gas sensor to monitor several tailpipe emissions simultaneously. The project will develop the voltammetric sensor for vehicle applications, with a form factor suitable for incorporation into standard vehicle hardware systems. This will be followed by proof-of-principle characterization and testing on operating spark-ignition and compression-ignition engines. The range of operation is expected to be from 0 to 200 ppm NOx with an accuracy of 5 ppm. The solid state device lifetime is anticipated to be 100,000 for maintenance, with a 500,000 mile lifetime.

VIII.2 Start-of-Combustion Sensor for HCCI Engines

TIAX, LLC

Homogeneous charge compression ignition (HCCI) has elevated the need for start-of-combustion (SOC) sensors. HCCI engines have been the focus of engine research recently, primarily because HCCI offers higher thermal efficiency than the conventional spark-ignition (SI) engines and significantly lower NOx and soot emissions than conventional compression ignition (CI) engines, and offer the potential for fuel neutrality.

The objective of the Phase I research is to answer two fundamental questions: can the accelerometer-based SOC sensor provide adequate SOC event capture to control an HCCI engine in a feedback loop, and will the sensor system meet cost, durability, and software efficiency (speed) targets? For successful completion of Phase I, the accelerometer-based combustion sensor must provide enough discernable signal resolution at low-load conditions (where the lowest signal-to-noise ratio exists) such that the SOC may be readily identified to the required accuracy. During Phase I, reliable algorithms for identification of SOC from the reconstructed pressure trace must be developed to meet accuracy and speed specifications. The processing code efficiency (response time of control system) must be rapid enough (meeting the specifications determined in the initial task) that control decisions may be made and implemented. The interface with the HCCI actuation/control mechanism (variable valve timing/fuel injection, etc) must be rapid and robust enough to allow the control mechanisms an opportunity to change engine conditions. The sensor(s) must be durable enough to meet all conditions of the engine operating regime and still provide accurate data for the life of the engine. The sensor and algorithm must also demonstrate “technology robustness” in application across engines of the same type (same model, different serial number) as a measure of production and commercial feasibility. The detailed specifications for each of these six criteria will be determined in the initial task of the project.

The objective of Phase II is to develop a pre-production prototype which implements the algorithms into a functional control system ready for vehicle testing. Phase II is contingent upon Phase I meeting the success criteria detailed above, in which case we assume that Continental will be heavily involved in Phase II. The team will design and optimize the SOC sensor as a system to meet commercialization targets. Phase II will address left over issues not resolved in Phase I. From Phase I, the two best algorithms will be selected, as well as the two best accelerometer sensor designs and engine mounting packages. These packages and algorithms will be down-selected and optimized. Continental will be heavily involved through this process, and from this selection process pre-production prototypes will be made.

If successful, the benefits will be significant. The emergence of a durable and effective SOC sensor will solve what is a 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.

VIII.3 On-Board Engine Exhaust Particulate Matter Sensor for HCCI and Conventional Diesel Engines

Matthew J. Hall and Ronald D. Matthews
The University of Texas at Austin

Eric Andrews and Phanindra Garimella
Cummins Engine Company

To meet the 2007/2010 particulate matter regulations, new diagnostic techniques will be useful to control the engine-out particulate emissions, control regeneration of the diesel particulate filter (DPF), and/or signal failure of the DPF. The primary goal of this 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 will be performed through a joint effort between the University of Texas at Austin and the Cummins Engine Company. The ability of this novel PM sensor concept to detect and quantify the carbonaceous fraction of particulate matter emissions in engine exhaust, with millisecond response time, has been well established.

The focus of Phase 1 will be the development of a system that will account for the velocity dependence of the sensor and will quantify the sensitivity and dynamic range of the sensor. Two concepts will be examined. First, a pitot tube will be used in the exhaust to measure the exhaust velocity. This velocity will be used in a known correlation to determine the PM concentration. The second concept is to have a separate flow circuit for the PM sensor. Instead of inserting the sensor directly into the exhaust system, a by-pass flow circuit would be attached at this point, with a small downstream blower used to create a fixed volumetric flow rate of exhaust gases past the sensor that is independent of engine operating conditions.

Phase 2 of the project will focus on applications of the PM sensor to diesel homogeneous charge compression ignition (HCCI) and on refining the design and performance of the sensor system through engine testing. The PM sensor system performance will be characterized with an EPA 2007 level-emissions diesel engine. The PM sensor will be examined for use during the mode switch from HCCI operation to conventional diesel operation at high loads and for individual cylinder control that produce PM emissions problems. Individual cylinder control of injection parameters, for example, may be an enabling technology for HCCI engines. The PM sensor system will also be evaluated as an indicator of DPF failure and as a tool to indicate when the trap needs regeneration.

VIII.4 The Development of a Robust Accelerometer-Based Start of Combustion Sensing System

Westport Power, Inc.

Westport Power, Inc. will perform a two-year project developing an accelerometer-based start-of-combustion (SOC) sensing system using standard, inexpensive automotive knock sensors (accelerometers) and advanced signal processing. An inexpensive and reliable SOC sensing system is the critical enabling technology for the introduction of high-efficiency homogeneous charge compression ignition (HCCI) engines. Other standard combustion technologies (compression and spark ignited engines) would also stand to benefit from the availability of a robust, low-cost combustion sensing system. Westport's accelerometer-based SOC sensing system will enable engine makers to improve engine efficiency (by HCCI or other means) by providing a real-time feedback signal that characterizes the combustion on every engine cycle. Westport has already demonstrated control of HCCI using the accelerometer-based SOC sensing system on two engines. As such, this technology is already beyond the proof-of-concept stage, but critical lack-of-robustness problems are preventing the commercial application of the SOC sensing technology. The work outlined in this project will resolve the key lack-of-robustness issues. Specifically, it needs a method to compensate for engine-to-engine variations, and a method to compensate for sensor-to-sensor variations. Potential solutions to these two sources of variation have been identified.

The objective of the proposed work is to resolve the main lack-of-robustness problems: the engine-to-engine and sensor-to-sensor variation issues. The work is divided into three distinct phases. In the first phase of work, methods will be developed to compensate for engine-to-engine variation. The goal of the second phase of work is to develop sensor-to-sensor compensation techniques. The goal of the third phase of work is to demonstrate the accelerometer-based SOC measurement system in a test cell.

The work outlined in this project will resolve the key lack-of-robustness issues. Upon completion of this work, SOC sensor technology will be ready for commercialization. Integration of the SOC sensor technology with any engine application which can benefit from its use will be possible. Westport's intention is that, at the end of this work, the accelerometer-based SOC sensing system could be used in a commercial HCCI-based engine. If the SOC sensing technology developed during this project enables the introduction of HCCI engines, substantial fuel economy and environmental benefits will be realized.

IX. Acronyms and Abbreviations

°C	Degrees Celsius
°F	Degrees Fahrenheit
η	Effectiveness
Φ	Fuel/air equivalence ratio
τ_{id}	Ignition delay time
Δ*P*	Pressure drop
0-D	Zero-dimensional
1-D	One-dimensional
3-D	Three-dimensional
A	Availability
a.u.	Arbitrary units
AC	Alternating current
A/C	After cooler
ACE	Advanced Combustion in Engines
ACES	Advanced Collaborative Emissions Study
Ag	Silver
AHRR	Apparent heat release rate
A/F	Air to fuel ratio
AFR	Air/fuel ratio
Al	Aluminum
Al_2O_3	Aluminum oxide
AMDC	Advanced mode diesel combustion
ANN	Artificial neural network
ANL	Argonne National Laboratory
APA	Air-power-assist
ASI	Time after the start of injection
atdc	After top dead center
ATDC	After top dead center
atm	Atmosphere
Au	Gold
B100	100% biodiesel
Ba	Barium
BC	Black carbon
BDC	Bottom dead center
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
BMEP	Brake mean effective pressure
BSDPM	Brake specific dry particulate matter
BSFC	Brake specific fuel consumption
bsNOx	Brake specific NOx emissions
btdc	Before top dead center
BTE	Brake thermal efficiency
C/N	Carbon to nitrogen ratio
CA	Crank angle
CAC	Charge air cooler
CAD	Crank angle degrees
CBM	Carbon balance method
CDPF	Catalytic diesel particulate filter
CFD	Computational fluid dynamics
Cg,i	Gas species concentration
CGIC	Clean gas induction cooler
CHEMKIN	Sandia chemical kinetics code
CI	Compression ignition
CIDI	Compression ignition direct injection
CINL	Cycle integrated natural luminosity
CLD	Chemiluminescence detector
CLEAN	Trademark for Detroit Diesel low-temperature combustion strategy
CLEERS	Cross-Cut Lean Exhaust Emissions Reduction Simulations
cm	Centimeter
cm^3	Cubic centimeters
CO	Carbon monoxide
CO_2	Carbon dioxide
COV	Coefficient of variation
CPER	Counterflow preheating with near-equilibrium reaction
CPF	Catalyzed particulate filter
Cr	Chromium
CR	Compression ratio
CRADA	Cooperative Research and Development Agreement
CRC	Coordinating Research Council
CR-DPF	Continuously regenerating diesel particle filter
CRF	Combustion Research Facility (at Sandia National Laboratories)
Cs,i	Solid species concentration

Cu	Copper
CVT	Continuously variable transmission
DC	Direct current
DEER	Diesel Engine Emissions Reduction
deg	Degrees
DEM	Delayed extended main
DGE	Diethylene glycol diethyl ether (CAS 112-36-7)
DI	Direct injection, direct injected
DIB	Di-isobutylene
DNS	Direct Numerical Simulation
DOC	Diesel oxidation catalyst
DOE	U.S. Department of Energy
DOHC	Double overhead camshaft
DOM	Discrete ordinates method
DPF	Diesel particulate filter
DRIFTS	Diffuse reflectance infrared Fourier-transform spectroscopy
DTTEG	Diesel truck thermoelectric generator
ECM	Electronic control module
ECU	Electronic control unit
EDS	Energy dispersive spectroscopy
EGR	Exhaust gas recirculation
EO	Engine-out
EOI	End of injection
EPA	U.S. Environmental Protection Agency
EPVA	Electro-pneumatic valve actuator
ESC	European Steady State Cycle
η	Effectiveness
EWHR	Exhaust waste heat recovery
FBMAFS	Forward-backward mass air flow sensor
FEA	Finite-element analysis
FHWA	Federal Highway Administration
FIE	Fuel Injection Equipment
FLRS	Full load rated speed engine condition
FSN	Filter smoke number
FSNR	Fuel specific NOx reduction
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	Gram
g	Gram
g/bhp-hr	Grams per brake horsepower-hour
gIMEP	Gross indicated mean effective pressure
g/kWh	Grams/kilowatt-hour
g/mi	Grams per mile
GA	Genetic algorithm
GATE	Graduate Automotive Technology Education
GC-MS	Gas chromatography – mass spectrometry
GDI	Gasoline direct injection
GHSV	Gas hourly space velocity
GM	General Motors
GUI	Graphical user interface
GVWR	Gross vehicle weight rating
h	Convective heat transfer coefficient
H	Enthalpy
H_2	Diatomic (molecular) hydrogen
H_2O	Water
H_2O_2	Hydrogen peroxide
H2-ICE	Hydrogen-fueled internal combustion engine
HC	Hydrocarbons
HCC	Homogeneous charge compression ignition
HC-SCR	Hydrocarbon selective catalytic reduction
HD	Heavy-duty
He	Helium
HECC	High-efficiency clean combustion
HEI	Health Effects Institute
HHV	Higher heating value
HIL	Hardware-in-loop
hp	Horsepower
HP	High pressure
HR	Heat release
hr	Hour
HRR	Heat release rate
HSDI	High-speed direct-injection
HTCD	Heavy truck clean diesel
HTML	High Temperature Materials Laboratory
HVA	Hydraulic valve actuator
HWFET	Highway Fuel Economy Test
Hz	Hertz
IC	Internal combustion
I/C	Intercooler
ICCD	Intensified charged-coupled device
ICDEM	Individual cylinder delayed extended main
ICE	Internal combustion engine
ID	Internal diameter

IMEP	Indicated mean effective pressure
I/O	Input-output
IR	Infrared
ISFC	Indicated specific fuel consumption
ITEC	International Truck and Engine Corporation
ITH	Intake throttle valve
IVA	Intake valve actuation
IVC	Intake valve closing
J	Joule
JPL	Jet Propulsion Laboratory
JWHR	Jacket water heat rejection
k	thousand
k	Mass transfer coefficient
K	Kelvin
kg	Kilogram
KIVA	Combustion analysis software developed by Los Alamos National Laboratory
KIVA-CTC	KIVA characteristic time combustion
KIVA-RIF	KIVA representative interactive flamelet
kJ	Kilojoules
kJ/L	Kilojoules per liter
kJ/m^3	Kilojoules per cubic meter
kPa	Kilopascal
kW	Kilowatt
L	Liter
L/D	Length-to-diameter ratio
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
lbs	Pounds
LD	Light-duty
LDT	Light-duty truck
LES	Large eddy simulation
LEVII	Low Emission Vehicle II
LHV	Lower heating value
LIDAR	Light detection and ranging
LIDELS	Laser-induced desorption with elastic light scattering
LIF	Laser-induced fluorescence
LII	Laser-induced incandescence of soot
LLNL	Lawrence Livermore National Laboratory
LNT	Lean NOx trap
LP	Low pressure
LPEGR	Low pressure exhaust gas recirculation
LRRI	Lovelace Respiratory Research Institute
LTC	Low-temperature combustion
m^2	Square meters
MAS	Magic-angle spinning
MB	Mercedes Benz
MCH	Methylcyclohexane
MECA	Manufacturers of Emission Controls Association
mg/mi	Milligram per mile
mi	Mile
min	Minute
MIT	Massachusetts Institute of Technology
MK	Modulated Kinetics
ML	Monolayer
mm	Micrometer
mm	Millimeter
Mn	Manganese
mol	Mole
mol/s	Moles per second
MET	More Electric Truck
MPa	Megapascals
mph	Miles per hour
ms	Millisecond
MSATs	Mobile source air toxics
MSU	Michigan State University
MTU	Michigan Technological University
N_2	Diatomic nitrogen
N_2O	Nitrous oxide
N_2O_3	Nitrogen trioxide
Na	Sodium
NCO	Isocyanate
NEDC	New European Drive Cycle
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 NO2)
NRE	NOx reduction efficiency
NRT	NOx reduction technology
NSLS	National Synchrotron Light Source
NSR	NOx storage and reduction

NTE	Not-to-exceed
NTP	National Toxicology Program
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
OEM	Original Equipment Manufacturer
OFCVT	Office of FreedomCAR and Vehicle Technologies
OH	Hydroxyl
OH*	Hydroxyl radical that emits ultraviolet photons
OH PLIF	Planar laser-induced fluorescence of OH
ORC	Organic Rankine Cycle
ORNL	Oak Ridge National Laboratory
P	Pressure
PCM	Power control module, powertrain control module
PCP	Peak cylinder pressure
PCCI	Premixed charge compression ignition
PCS	Power control subsystem
PDF	Probability density function
PFI	Port fuel injection, port fuel injected
Phi	Equivalence ratio
PHx	Primary heat exchanger
PID	Proportional, integral, and derivative
PIV	Particle image velocimetry
PLII	Planar laser-induced incandescence
PLIF	Planar laser induced fluorescence
PLRS	Planar laser Rayleigh scattering
PM	Particulate matter
PMT	Photomultiplier tube
PNGV	Partnership for a New Generation of Vehicles
PNNL	Pacific Northwest National Laboratory
Post80	Late cycle injection after the main fuel pulse at 80° after top dead center
PPCI	Partially premixed compression ignition
ppm	Parts per million
PRF	Primary Reference Fuels (iso-octane and n-heptane),
PRF80	PRF mixture with an octane number of 80 (i.e., 80% iso-octane and 20% n-heptane)
PRR	Pressure rise rate
psi	Pounds per square inch
psig	Pounds per square inch gauge
Pt	Platinum
PWM	Pulse width modulated
Q	Heat
Q1, Q2, Q3, Q4	First, second, third and fourth quarters
OTR	Over-the-road
QW	Quantum well
R&D	Research and development
RANS	Reynolds Averaged Navier Stokes
RCF	Rapid compression facility
RGF	Residual gas fraction
Rh	Rhodium
ROI	Rate of injection
rpm	Revolutions per minute
RT	Room temperature
S	Entropy
S	Sulfur
SAE	Society of Automotive Engineers
SCF/min	Standard cubic feet per minute
SCI	Stoichiometric compression ignition
SCORE	Sandia Compression-ignition Optical Research Engine
SCOT	Staged combustion with oxygen transfer
SCR	Selective catalytic reduction
sec	Second
SEM	Scanning electron microscopy
Si	Silicon
SI	Spark ignition
SIDI	Spark ignition direct injection
SF	Scaling factor
SFC	Specific fuel consumption
SFTP	Supplemental Federal Test Procedure
SLPM	Standard liters per minute
SMPS	Scanning mobility particle scanner
SMR	Steam reformation
SNL	Sandia National Laboratories
SNR	Signal-to-noise ratio
SO_2	Sulfur dioxide
SOC	Start of combustion
SOI	Start of injection
SOF	Soluble organic fraction
SO_x	Oxides of sulfur
Sp	Mean piston speed
SpaciMS	Spatially resolved capillary inlet mass spectrometer

SR	Steam reforming
SU	Stanford University
SUV	Sports utility vehicle
SV	Space velocity
SwRI	Southwest Research Institute
T	Temperature
TAGS	Tellurium, antimony, germanium and silver
TAP	Temporal Analysis of Products
TCR	Thermo-chemical recuperation
TDC	Top dead center
TDL	Tunable diode laser
TE	Thermoelectric
TEG	Thermoelectric generator
TEM	Transmission electron spectroscopy
TGM	Thermoelectric generator module
THC	Total hydrocarbon
TP	Tailpipe
TPD	Temperature-programmed desorption
TPGME	Tri-propylene glycol monomethyl ether
TPR	Temperature-programmed reduction
TPRX	Temperature-programmed reaction
TPS	Throttle position sensor
TP-XRD	Temperature programmed x-ray diffraction
u	Gas velocity
U	Internal energy
UCB	University of California Berkeley
UEGO	Universal exhaust gas oxygen
UHC	Unburned hydrocarbons
ULSD	Ultra-low sulfur diesel
UM	University of Michigan
UNIBUS	Uniform bulky combustion system
US06	Supplemental Federal Test Procedure (SFTP)
UTM	Universal Transverse Mercator (mapping projection methodology)
UTRC	United Technologies Research Center
UV	Ultraviolet
V	Volt
VAT	Variable admission turbine
VCR	Variable compression ratio
VCT	Variable cam timing
VDC	Volts – direct current
VGC	Variable geometry compressor
VNT	Variable nozzle turbine
VOCs	Volatile organic compounds
VPTNA	Volvo Powertrain North America
VTG	Variable turbine geometry
VVA	Variable valve actuation
VVT	Variable valvetrain
W	Work
WAVE	Ricardo engine and one-dimensional gas dynamics simulation software
W	Watt
WGS	Water-gas-shift
WGSR	Water-gas-shift reaction
WHR	Waste heat recovery
WOT	Wide open throttle
WREL	Watt Road Environmental Laboratory
wt%	Weight percent
XANES	X-ray absorption near-edge spectroscopy
XPS	X-ray photoelectron spectroscopy
XRD	X-ray diffraction
Y	Yttrium
yr	Year
Zn	Zinc
ZT	Dimensionless thermoelectric figure of merit; equal to: (electrical conductivity)(Seebeck coefficient)^2(temperature)/(thermal conductivity)

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