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.

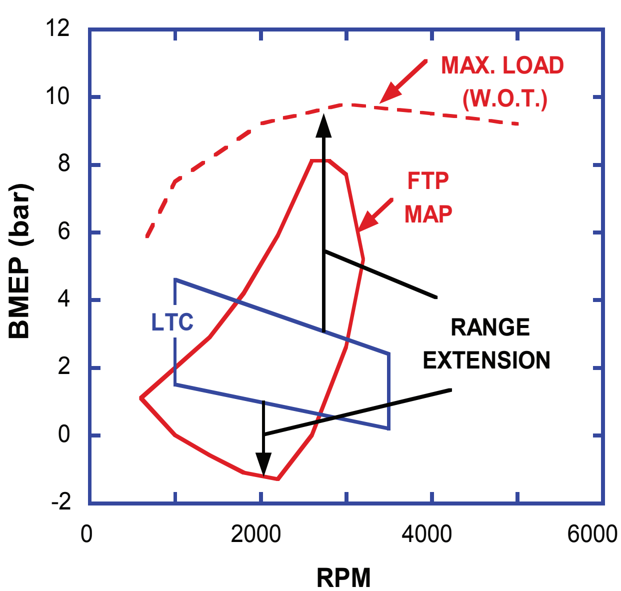

FIGURE 1. Performance map showing limited current achievable LTC range relative to a typical automotive range for maximum load and over the FTP driving cycle.

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

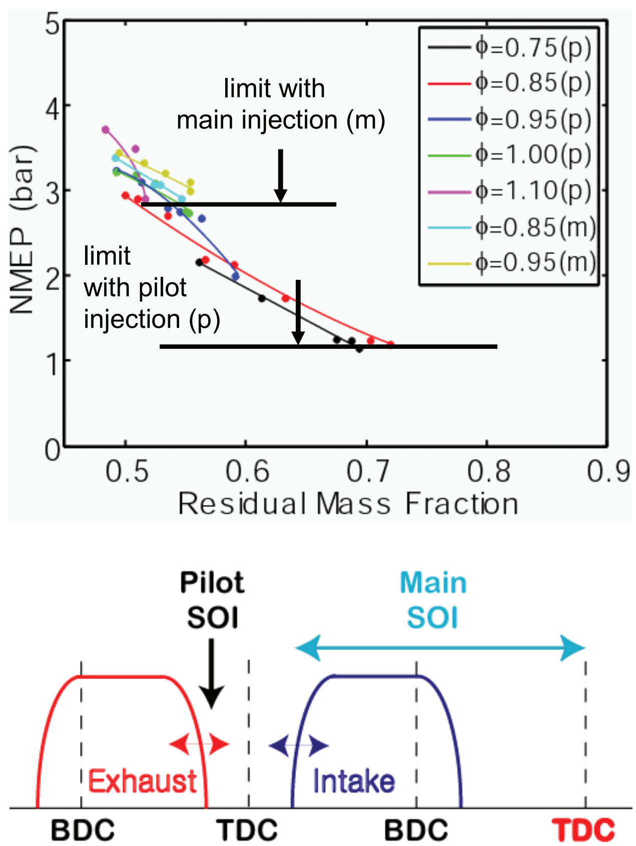

FIGURE 2. Lower load limit extension by pilot injection during negative valve overlap (NVO).

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.

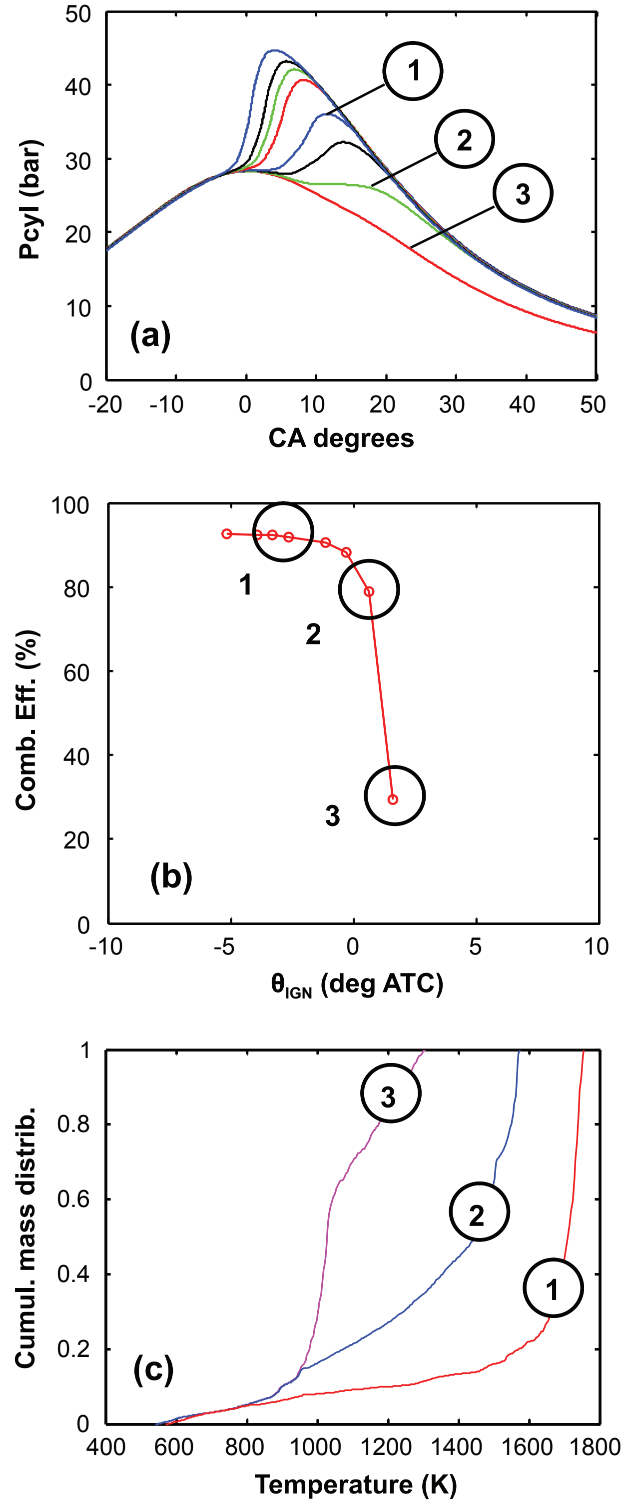

FIGURE 3. Coupled CFD/kinetic results for an HCCI timing sweep; a) pressure traces; b) corresponding combustion efficiencies; c) corresponding maximum in-cylinder temperature distributions. Numbers identify three cycles with high, medium and low efficiency.

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

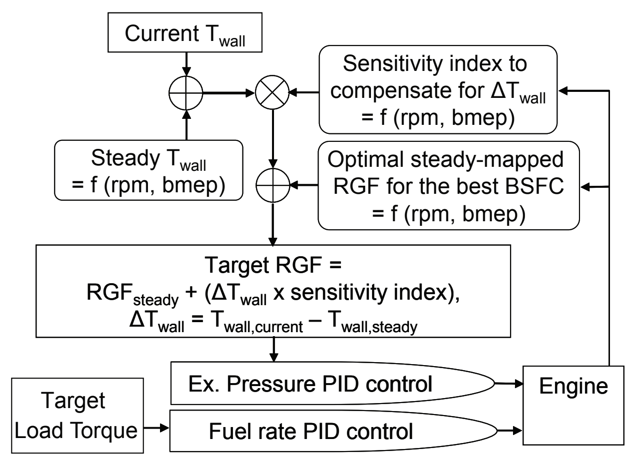

FIGURE 4. Schematic of simulated control strategy to compensate for wall temperature effects.

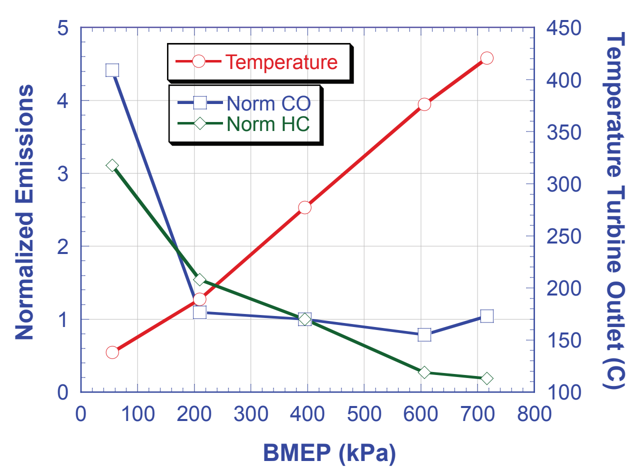

FIGURE 5. Typical rapid increase in CO and HC emissions with decreasing turbine exhaust temperature in a diesel LTC application.

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.

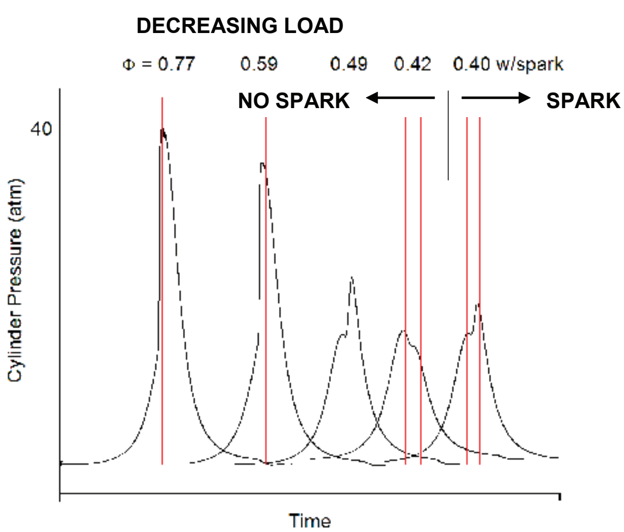

FIGURE 6. Sequence of LTC pressure curves in order of decreasing load (Φ) showing effect of spark at leanest Φ in advancing combustion and increasing stability.

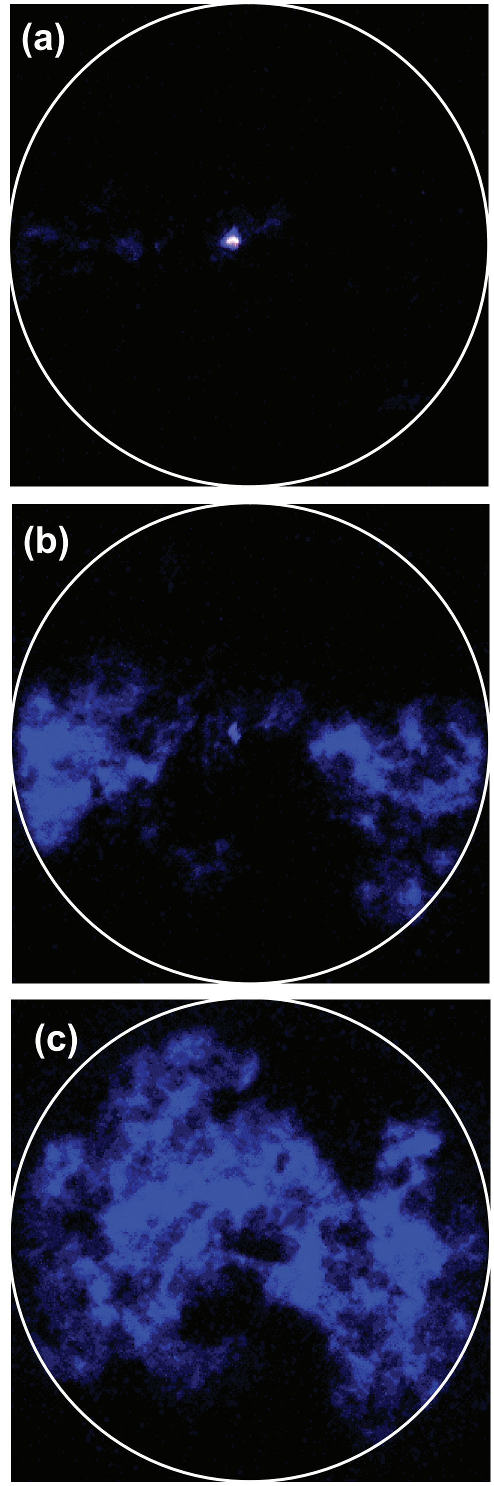

FIGURE 7. Sequence of images from the UM optical engine showing spark assisted HCCI at $\phi = 0.4$ and 700 rpm with Indolene fuel. (a) t =0: shows spark and localized reaction zone, (b) t = 0.67 ms: shows initial ignition occurring at edges of chamber, (c) t = 1.33 ms: main combustion event.

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

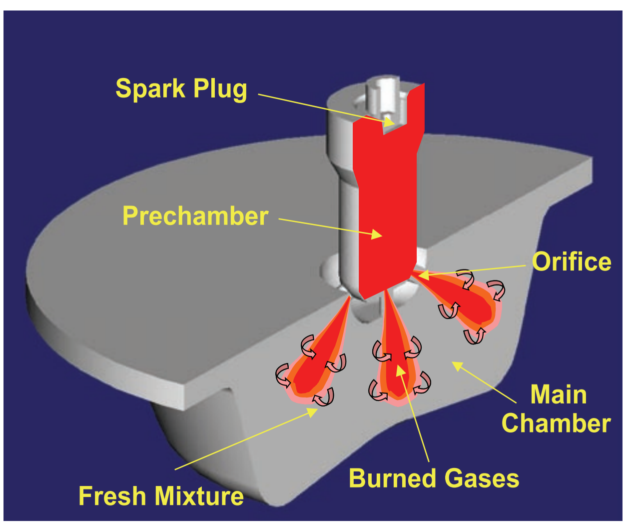

FIGURE 8. Prechamber Concept for Spark Assisted LTC Combustion Control

the fuels each ignited in the same location within the cylinder volume, indicating these areas were zones of preferential thermal gradients.

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.

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

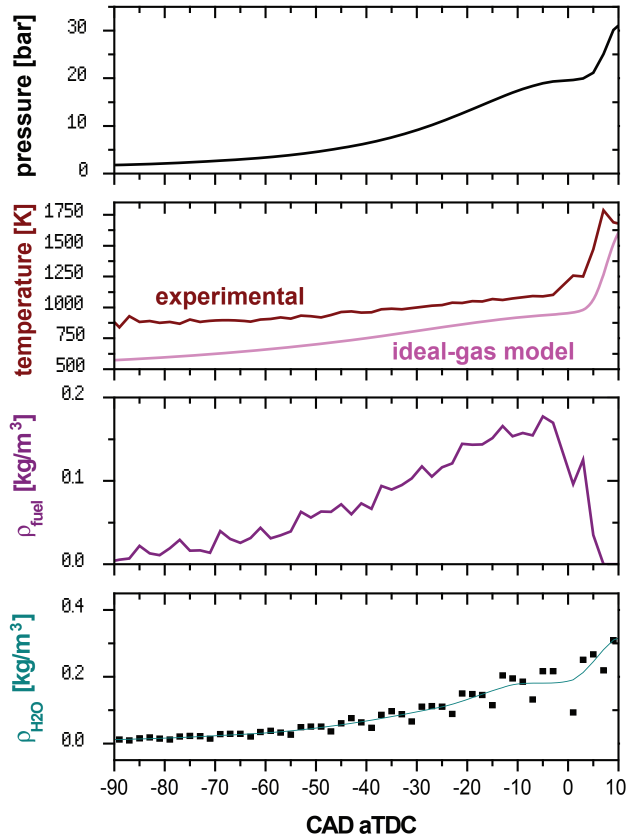

FIGURE 1. Measurements of pressure (by piezoelectric transducer), temperature, fuel, and H_2O vapor (all by absorption spectroscopy of 1600-1850 nm @ 0.75 nm resolution) in a metal engine operating in HCCI mode.

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.

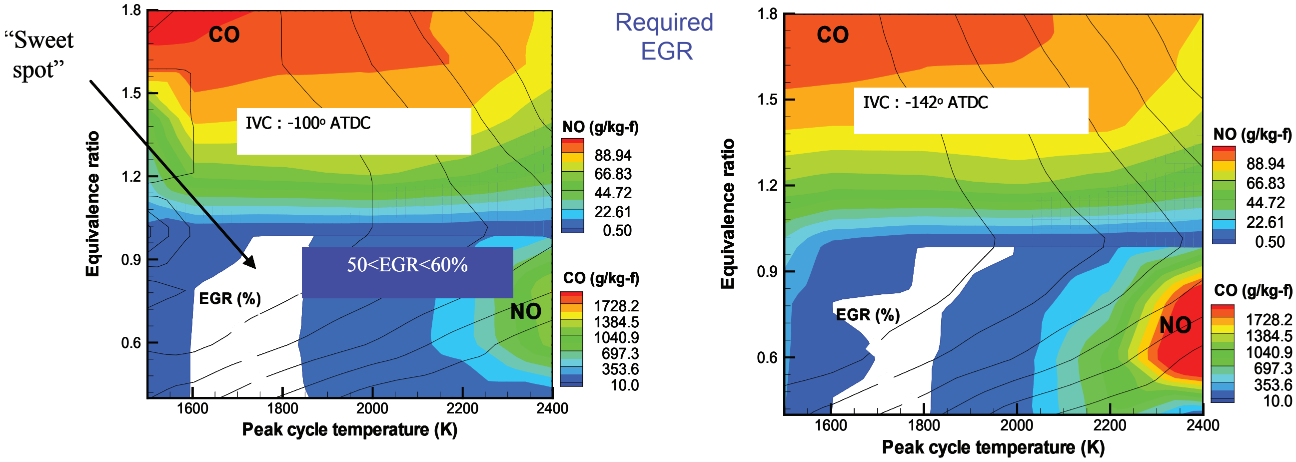

FIGURE 2. Effect of intake valve closure (IVC) timing on CO and NO emissions as a function of EGR. (White region indicates low emission window.)

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 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.

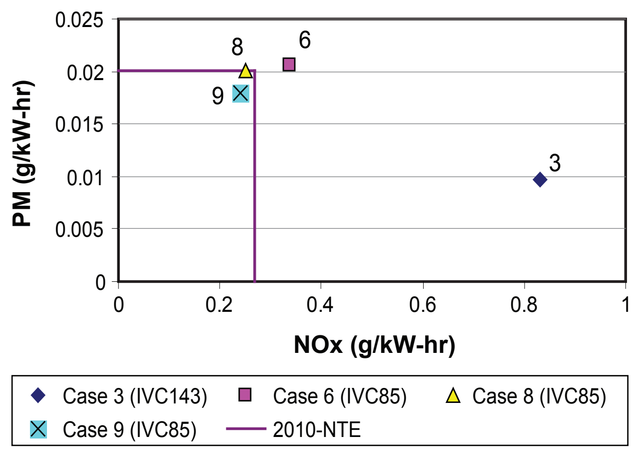

FIGURE 3. NOx vs. PM at SOI 55° BTDC, 40% EGR, with standard IVC timing (143° BTDC) and IVC 85° BTDC. Intake boost pressure is 184, 184, 179, 172 kPa for cases 3, 6, 8, and 9, respectively.

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

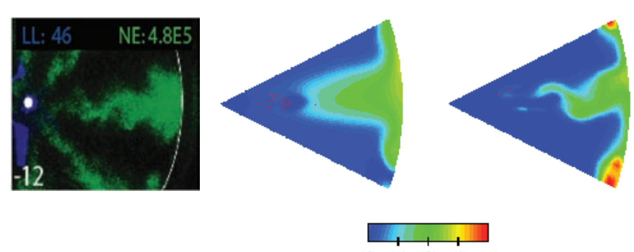

FIGURE 4. Experimental (natural emissions) and simulated temperature contours in diesel combustion using standard RANS and advanced LES turbulence models.

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,

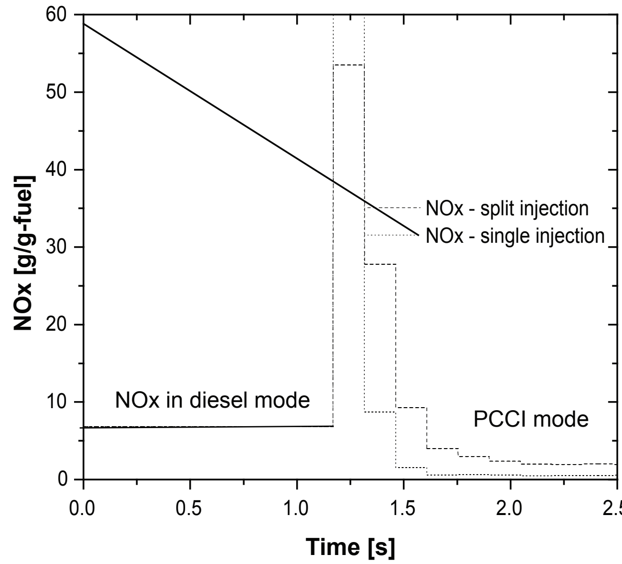

FIGURE 5. NOx emissions for diesel and PCCI combustion modes during a mode transition.

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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- Gas Technology Institute (GTI), Des Plaines, IL (John Pratapas, Lead Investigator)
- 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.

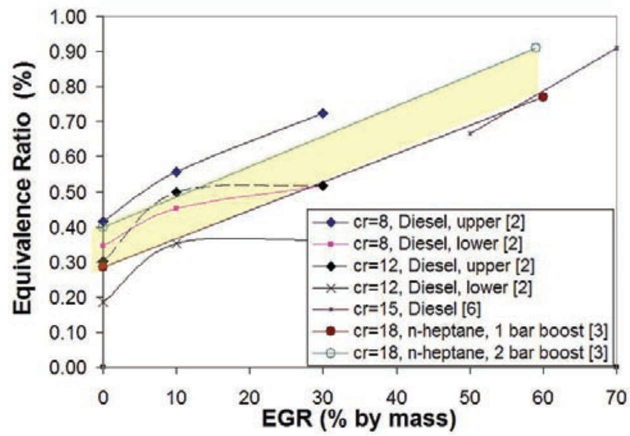

FIGURE 1. Relation between Equivalence Ratio and EGR for LTC Mode

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.

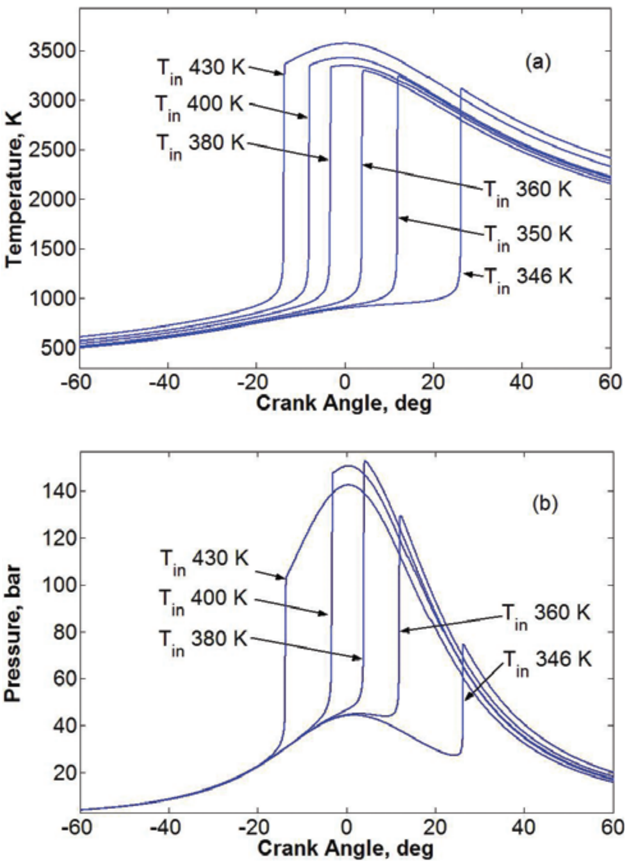

FIGURE 2. Effects of Intake Temperature in Temperature (a) and Pressure (b) Profiles for a CR=18:1

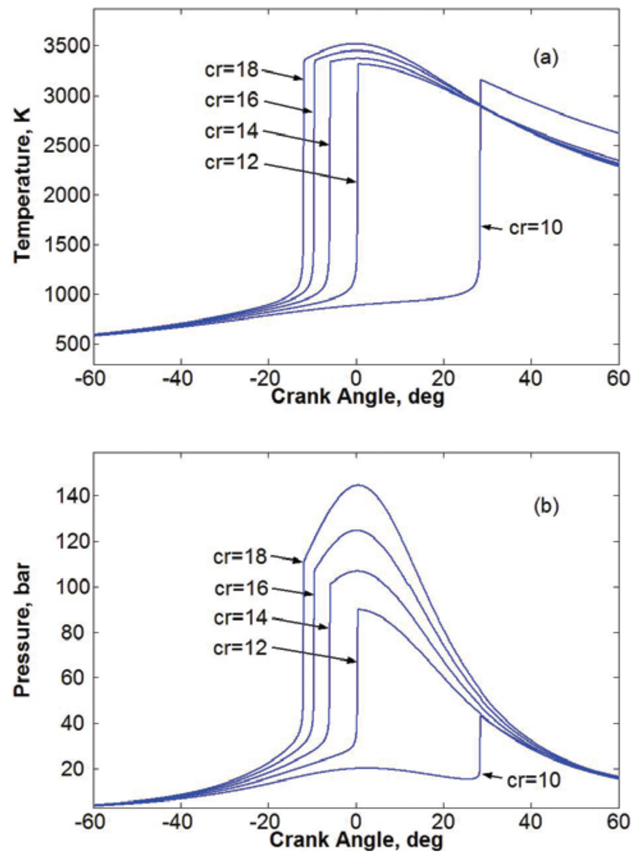

FIGURE 3. Effects of Compression Ratio on In-Cylinder Temperature (a) and Pressure (b) Profiles at T_{in}=420 K.

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.

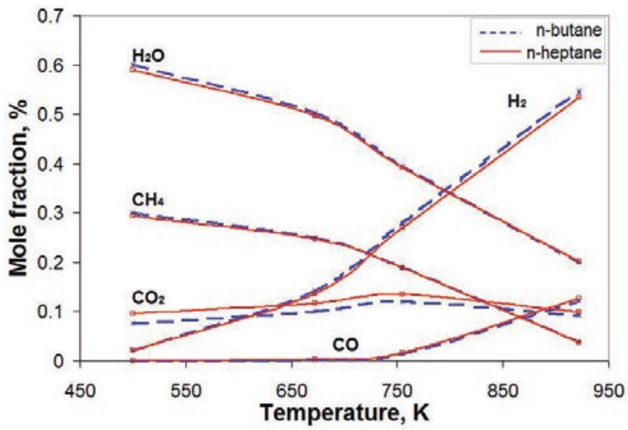

FIGURE 4. Reformed Fuel Composition for N-Heptane and N-Butane (Steam:Carbon ratio 2:1, Pressure 1 atm)

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

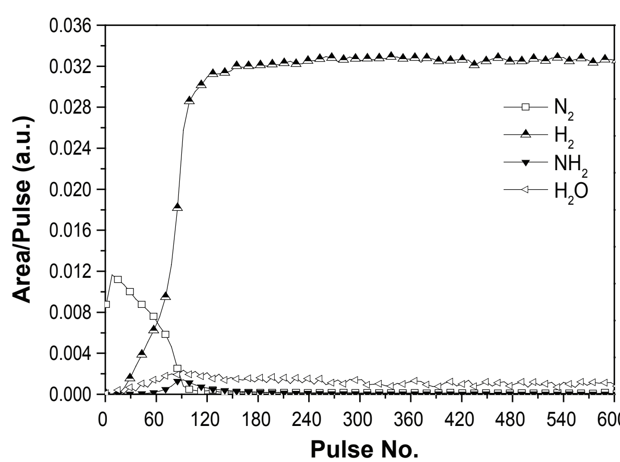

FIGURE 1. Effluent profiles during reduction of pre-nitrated Pt/BaO/Al_2O_3 at 350°C.

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/γ-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

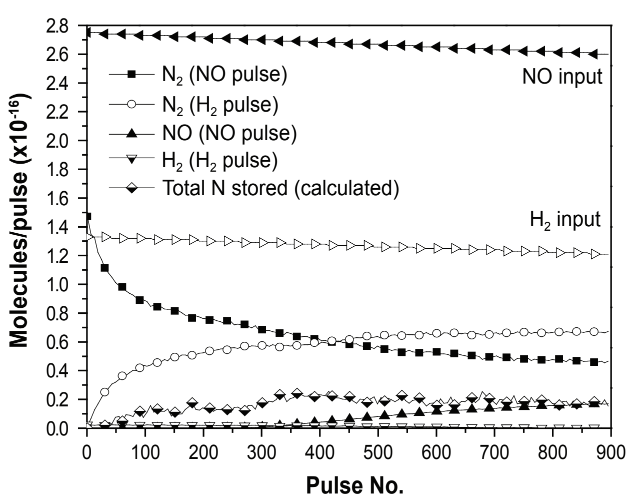

FIGURE 2. NO-H_2 pump probe over pre-reduced Pt/BaO/Al_2O_3 for NO:H_2 = 1:0.5 and 350°C.

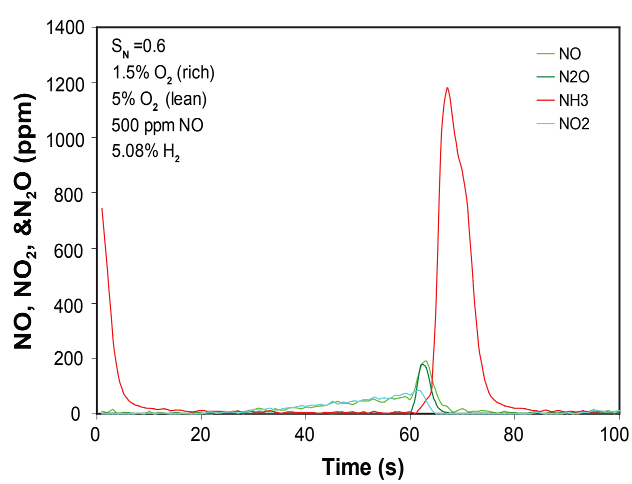

FIGURE 3. Effluent profile of N-containing species during NOx storage and reduction.

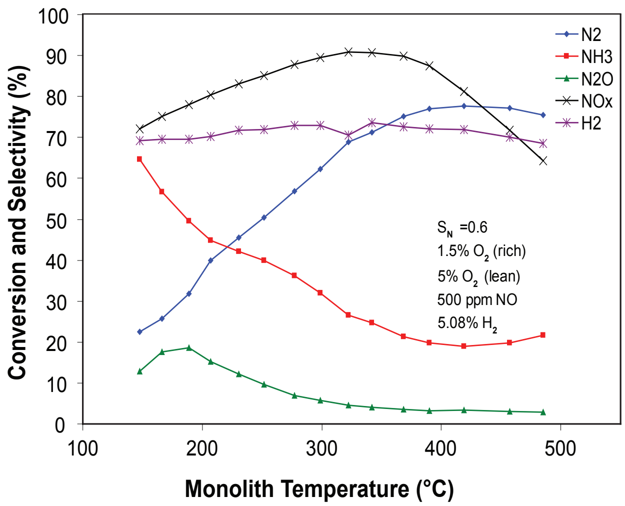

Figure 4. Cycle-averaged conversion and selectivity during NSR on Pt/Ba catalyst.

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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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

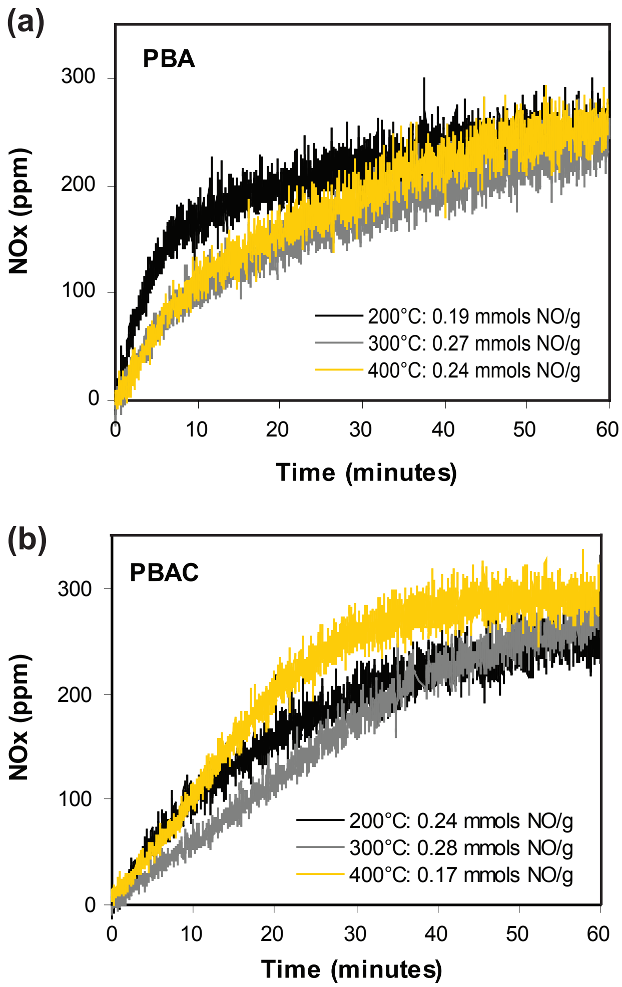

FIGURE 1. Outlet NOx Concentration as a Function of Time During Storage Capacity Measurement A: Pt/Ba/Al_2O_3; B: Pt/Ba/Al_2O_3-Pt/CeO_2 (74 wt%-26 wt%)

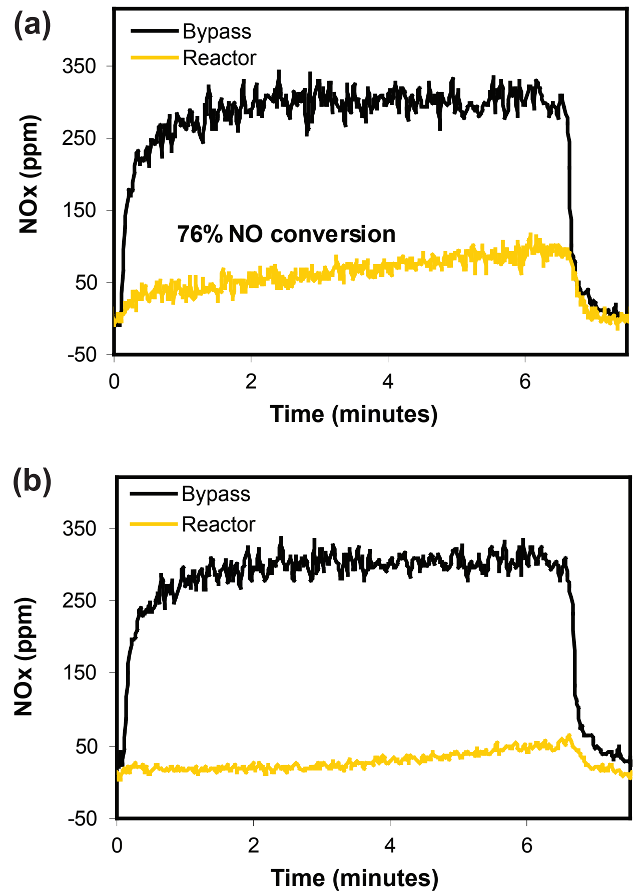

FIGURE 2. Outlet NOx Concentration as a Function of Time during Steady-State Lean-Rich Cycling

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).

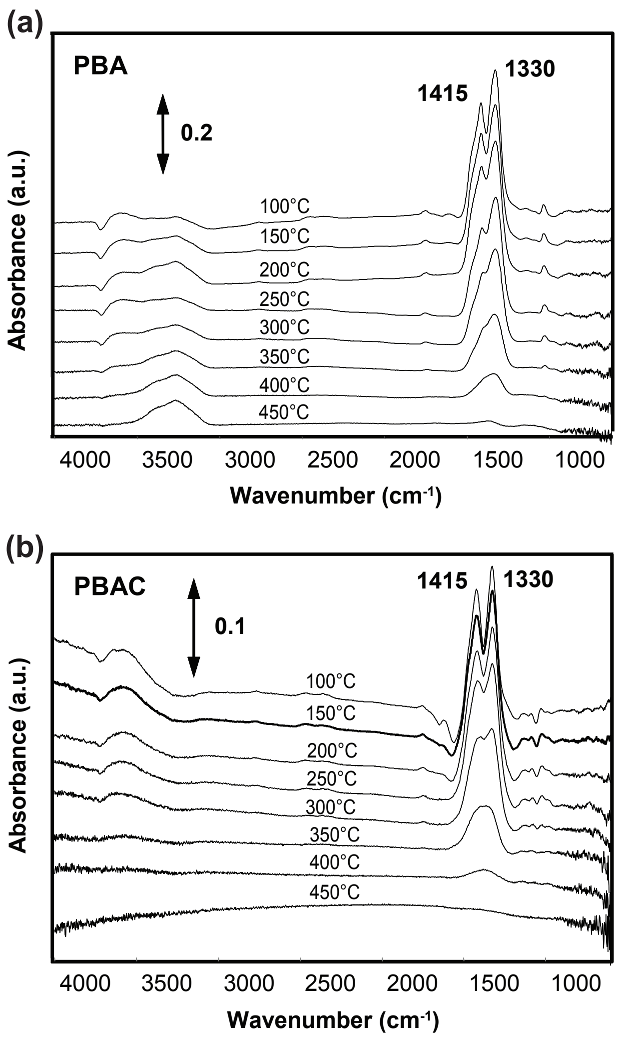

FIGURE 3. DRIFT Spectra of Catalysts PBA and PBAC Loaded with NOx during H_2-TPR

- 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.

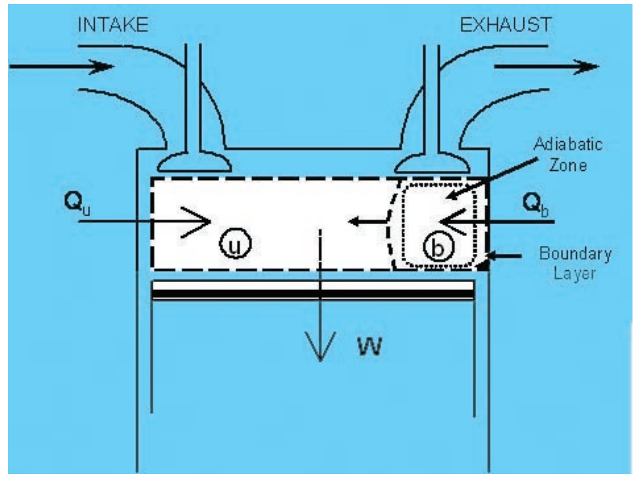

FIGURE 1. Schematic of the Engine Cylinder Depicting the Three Zones During Combustion

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

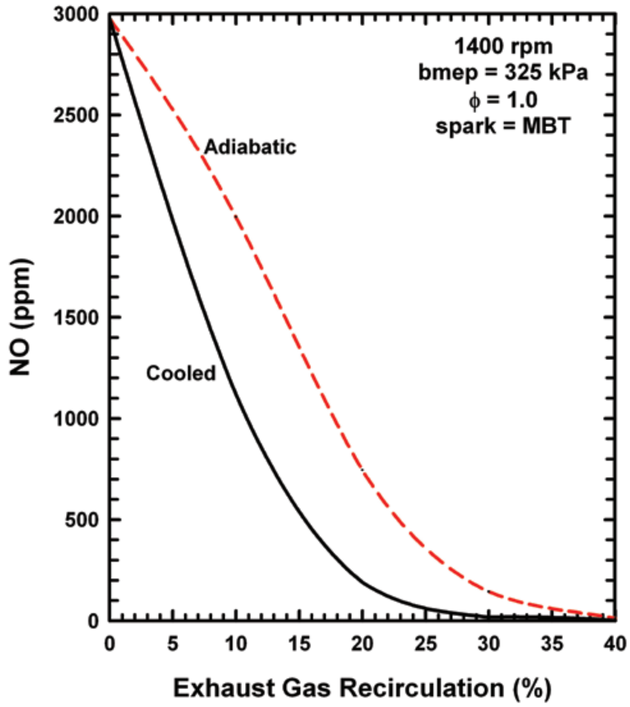

FIGURE 2. Nitric oxide concentration in the exhaust as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

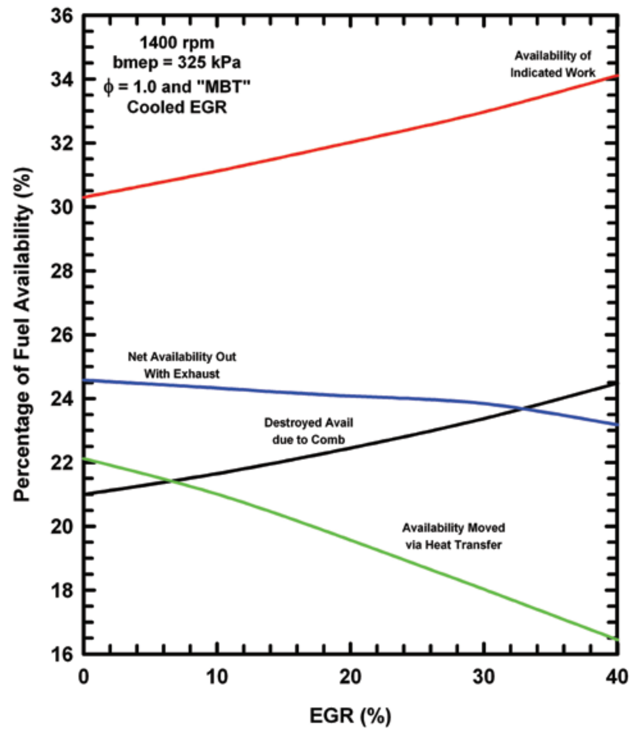

FIGURE4. Four availability terms as functions of the percentage of exhaust gas recirculation for the base case conditions for the *cooled* EGR configuration.

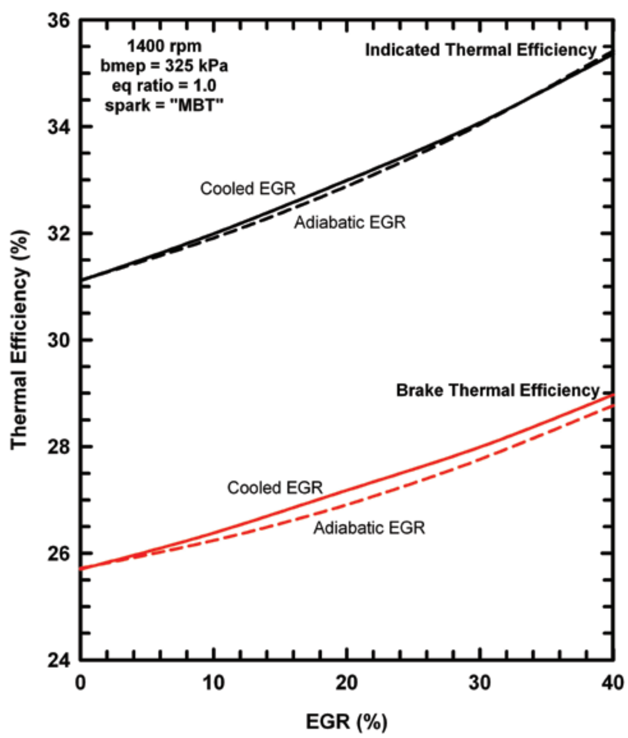

FIGURE 3. Indicated and brake thermal efficiency as functions of the percentage of exhaust gas recirculation for the base case conditions for both cooled and adiabatic EGR configurations.

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

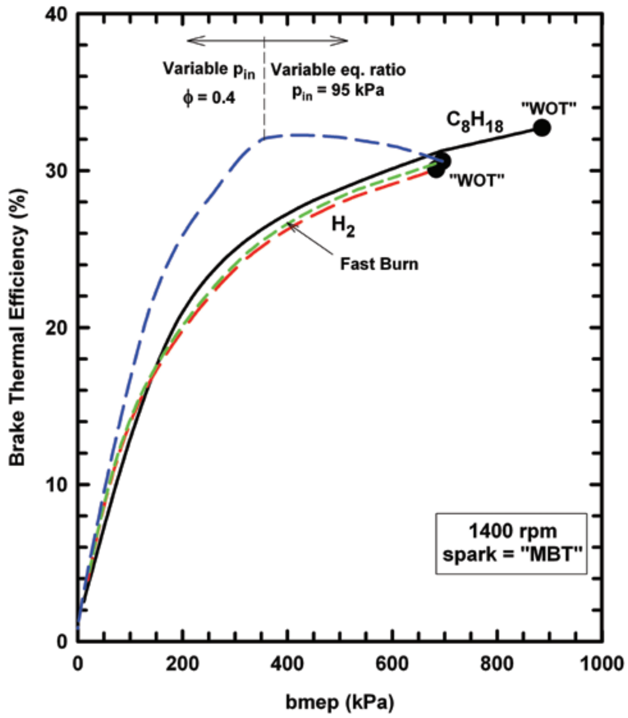

FIGURE 5. Brake thermal efficiency as functions of brake mean effective pressure for the base case using isooctane and three cases using hydrogen.

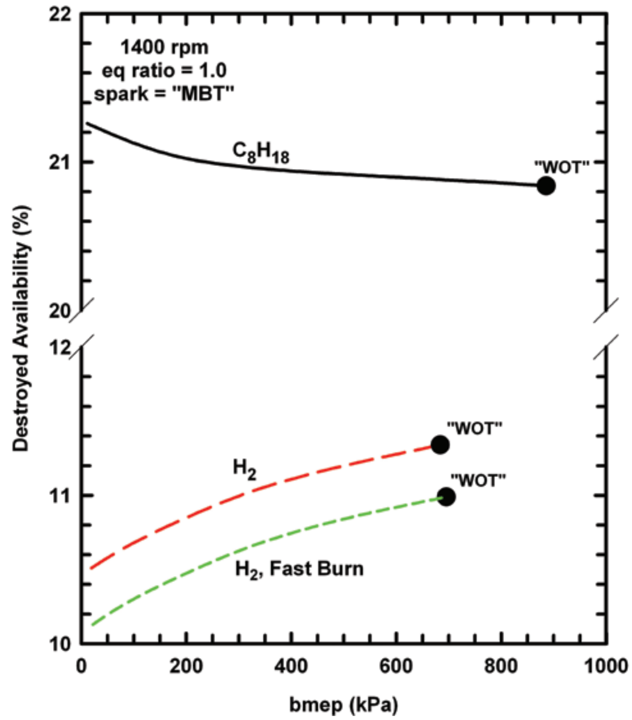

FIGURE 6. The destroyed availability due to combustion as functions of engine load (bmep) for engine operation with hydrogen with a burn duration of 60°, with hydrogen with a burn duration of 30° (fast burn), and with isooctane with a burn duration of 60°, all for an equivalence ratio of 1.0, and 1400 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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1. 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.

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.

FY 2006 Publications/Presentations

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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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.

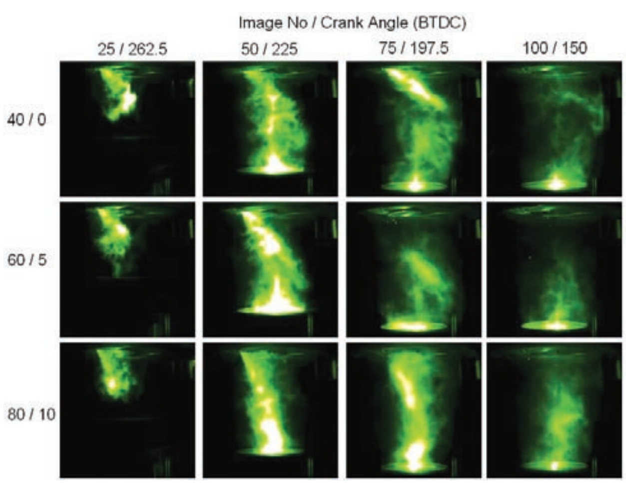

FIGURE 1. In-Cylinder Fuel Mixture Formation at 2,500 rpm/WOT/30 bar Fuel Pressure/SOI at 300° CA BTDC

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

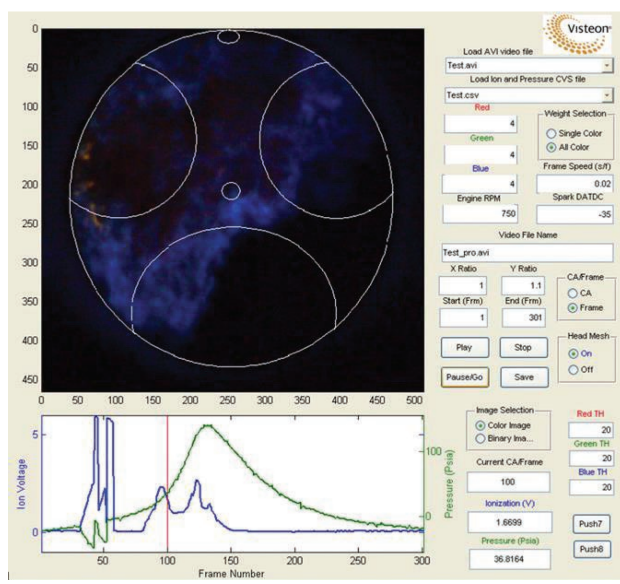

FIGURE 2. Custom-Built GUI Schematic for Flame Image Analysis (The combustion image with its corresponding pressure and ionization voltage data can be evaluated simultaneously.)

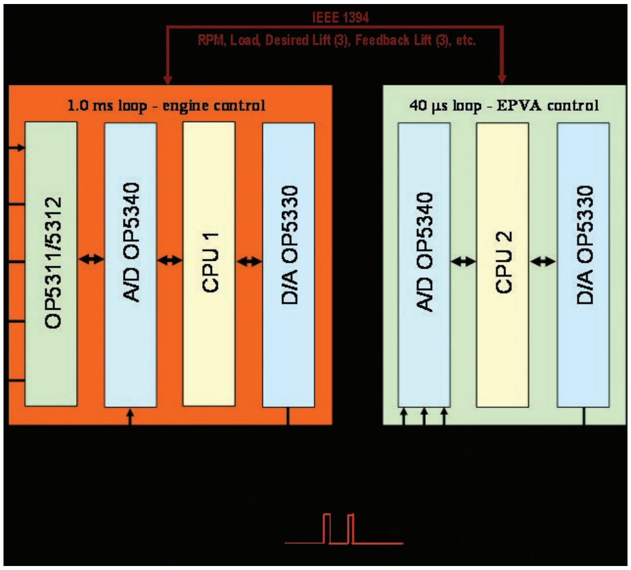

FIGURE 3. Opal-RT Hardware Architecture and System I/O

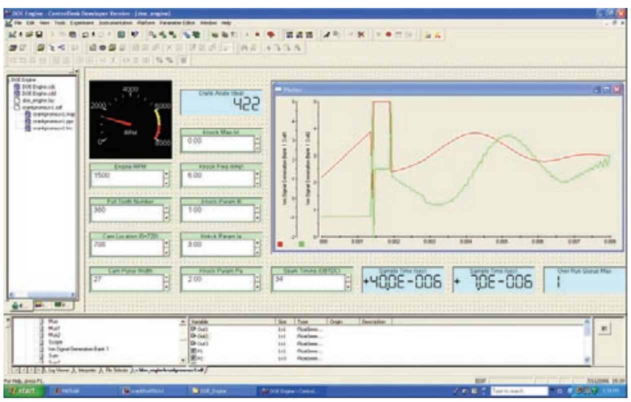

FIGURE 4. dSpace Hardware-In-Loop Simulator

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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