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

A. Combustion and Related In-Cylinder Processes

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

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Objectives

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

Accomplishments

- A collaborative paper between Argonne and Robert Bosch GmbH was published in September 2007, based on X-ray measurements of near-production nozzles.
- Our first single-shot measurements of sprays were performed and published in 2007. These measurements showed that important features of the spray are remarkably reproducible from one spray event to the next.
- In FY 2007, we developed a new data analysis technique that allows us to calculate the average velocity of the fuel in a spray as a function of time. This is one of the few experimental techniques that can measure spray velocity, and can do so in the very-near-nozzle region.
- In FY 2007 we published an article in the Journal of Automobile Engineering's Special Issue on Engine Diagnostics. Our paper was one of only seven chosen for publication in this important special issue.
- FY 2007 saw the continuation of an important collaboration with General Motors (GM) and the Engine Research Center (ERC) at the University of Wisconsin. One week of X-ray measurements in FY 2007 was dedicated to this collaboration.
- In FY 2007, we demonstrated that X-ray measurements of full-production six-hole nozzles can be performed without sacrificing data quality.

Future Directions

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

Introduction

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

Approach

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

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

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

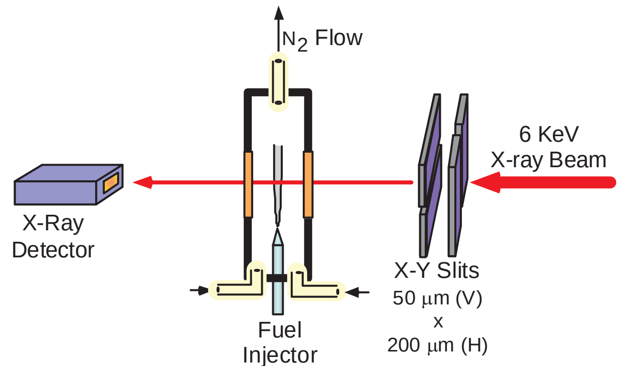

FIGURE 1. Schematic of the Experimental Setup

Results

In 2007 we made significant advances to make measurements of sprays under conditions similar to those in a real engine. For the first time, X-ray measurements were performed using a full-production six-hole nozzle. These measurements demonstrated that we could isolate a single spray from this nozzle, and study it without interference from neighboring sprays. This is a significant step, as most of our previous work has used single-hole nozzles, which may generate sprays that differ in structure from true production nozzles. The measurements of production nozzles enable the results to be directly applied to modern engines and computational models.

A new analysis technique for the X-ray spray measurements was developed in FY 2007 that allows us to calculate the average velocity of the fuel in a spray as a function of time. This is one of the few experimental techniques that can measure spray velocity, and can do so in the very-near-nozzle region. The fuel velocity is an extremely important quantity in spray modeling, as it directly influences aerodynamic breakup. Yet, few reliable measurements of velocity in the spray core have been published, and modelers often must assume or 'tune' the velocity, reducing the reliability of the models. Figure 2 shows the axial velocity of the fuel over the course of the injection event. Note that a significant amount of time is required for the fuel to reach its maximum velocity, while most spray models assume a constant speed over the entire spray event. With this new analysis, we can now provide modelers with

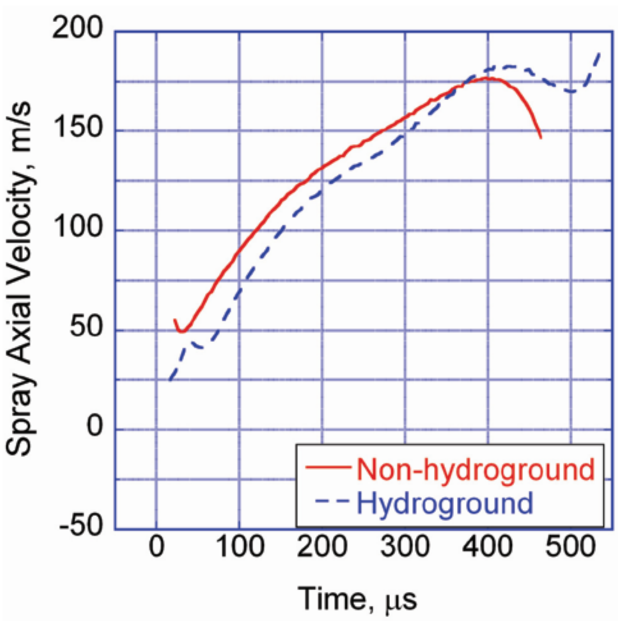

FIGURE 2. Average Spray Axial Velocity as a Function of Time for Two Different Nozzles at 250 Bar Injection Pressure

accurate measurements of the average speed of the fuel, resulting in improved spray modeling.

Our first single-shot measurements of sprays were performed and published in 2007. Previously, all of our published results were averaged over many sprays. The new X-ray monochromator which became operational in FY 2006 increased our X-ray flux by a factor of 50, and enabled us to make meaningful measurements from a single spray event. Figure 3 shows the projected density of fuel as a function of time for four individual spray events (red points) and for the average of 32 spray events (black curve). These measurements showed that important features of the single-shot measurements remarkably reproducible, and are preserved in the average measurements, while the noise is significantly reduced. Therefore, conclusions about spray structure which have been made based on averaged data are likely applicable to single-shot events as well.

Our group's collaboration with Robert Bosch GmbH had another milestone in FY 2007; a joint paper was published based on research completed in FY 2006. This paper detailed the measurements of near-production nozzles at high spray chamber densities. In order to build on the results of this paper, Bosch has requested that additional collaborative measurements be performed in FY 2008, with Bosch providing state-of-the-art injection equipment and technical support. This has all been accomplished based on a handshake agreement with engineers at Bosch Corporate Research, Stuttgart. Bosch has supported our work over the last two years with approximately $50,000 of in-kind contributions, and the work has been freely publishable and available to our memorandum of understanding partners.

FY 2007 saw the continuation of an important collaboration with GM and the ERC at the University of Wisconsin. One week of X-ray measurements in FY 2007 was dedicated to this collaboration. Measurements were performed at ambient pressures up to 30 bar for several different nozzle geometries. The analysis of the results is being performed by students and faculty at ERC with funding from GM. The collaboration will continue in the future, and the experiments and analysis will form the Ph.D. thesis of Amaury Malave at the University of Wisconsin.

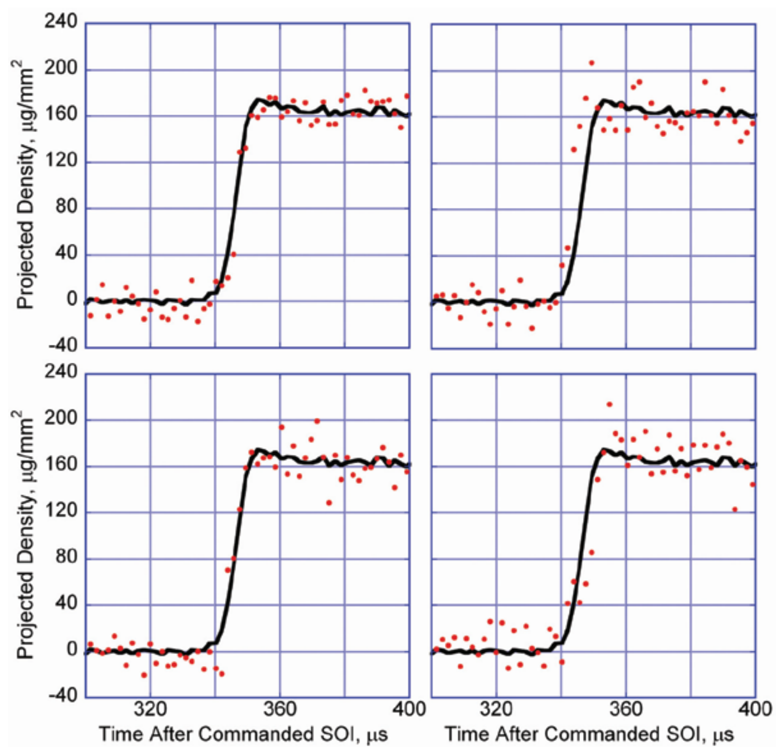

FIGURE 3. Projected Density of Fuel Versus Time at the Apparent Start of Injection for Four Individual Spray Events (Red Points) and the Average of 32 Spray Events (Black Curve)

Conclusions

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

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4. "Improved Method to Determine Spray Axial Velocity Using X-Ray Radiography", A. Kastengren, C. F. Powell, T. Riedel, S. –K. Cheong, Y. Wang, K. –S. Im, X. Liu, J. Wang. 20th Annual Conference on Liquid Atomization and Spray Systems, Chicago, IL, May 2007.

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II.A.2 Low-Temperature Automotive Diesel Combustion

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Objectives

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

Accomplishments

- Completed automotive low-temperature combustion (LTC) facility upgrade incorporating a General Motors (GM) 1.9-liter production diesel head into an optically-accessible, single-cylinder engine. Installed new exhaust gas recirculation (EGR) simulation capabilities permitting simulated EGR with H_2O, CO_2, N_2, O_2, CO, unburned hydrocarbon (UHC)¸ and other trace components.
- Established correspondence between optical and traditional metal engine performance and emissions, through close comparison of pressure-based performance metrics as well as engine-out emissions for a range of combustion system parameters.
- Evaluated optical engine performance and emissions for a wide range of operating conditions characterizing both high-dilution and late-injection LTC operating regimes. Identified operating conditions of interest for future optical studies focusing on the sources of CO and UHC emissions.
- Examined sources of UHC emissions and their cyclic-variability through time-resolved measurements obtained with a fast flame ionization detector.
- Identified a "best-fit" modeling constant that matches the measured turbulent kinetic energy and its dissipation rate to data obtained in a motored engine.
- Demonstrated the ability of multi-dimensional engine combustion models to predict the influence of swirl on soot formation and oxidation in heavy-duty diesel engines, and employed the model to understand asymmetries in soot formation with respect to the fuel jets.

Future Directions

- Develop optical diagnostic technique for visualizing the in-cylinder spatial distribution of CO.
- Apply optical techniques to investigate sources of UHC and CO emissions in highly dilute, LTC regimes.
- Evaluate the effect of engine boost on low-temperature combustion systems and on the fuel conversion efficiency loss typically observed with high dilution levels.
- Examine how trace components in simulated EGR influence the combustion and emissions formation processes.
- Assess the impact of strain and rotation dependent model coefficients on the modeling of the turbulent kinetic energy dissipation in flows with bulk compression.

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Introduction

Direct injection diesel engines have the highest fuel conversion efficiency and the lowest CO_2 emissions of any reciprocating internal combustion engine technology. However, this efficiency often comes at the expense of high NOx or particulate matter (soot) emissions. Through adoption of LTC techniques–relying on lower compression ratios, large quantities of cooled EGR, and unconventional injection timing and/or strategies–soot and NOx can often be dramatically reduced. Unfortunately, the low combustion temperatures beneficial for inhibiting soot and NOx formation can also lead to significant CO and UHC emissions, due to the slower oxidation of these species and to the more stringent mixing requirements imposed by the low O_2 concentration in the intake charge. Failure to rapidly oxidize CO and UHC can also result in a substantial penalty in fuel consumption. Reduction of CO and UHC emissions, and recovery of fuel economy, is imperative if these engines are to achieve widespread acceptance. Only then can they contribute to our energy security and help reduce the CO_2 emissions associated with personal transportation.

Identifying the dominant in-cylinder processes influencing CO and UHC emissions, understanding the relevant physics controlling these processes, and developing a predictive modeling capability are crucial steps toward the development and optimization of clean, fuel-efficient engines utilizing LTC systems. Each of these components is represented in the research described in the following.

Approach

The research approach consists first of establishing an optically-accessible research engine with characteristics and operating conditions that allow it to closely match the combustion and engine-out emissions behavior of traditional, all-metal test engines. Detailed measurements of in-cylinder flows, fuel and pollutant spatial distributions, and other thermo-chemical properties are subsequently obtained, and employed both to identify the dominant physical processes governing combustion and emission formation and to formulate and validate multi-dimensional computer models. These measurements are closely coordinated and compared with engine-out emissions and with the predictions of numerical simulation efforts.

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

Results

Research efforts in this fiscal year were divided among four main areas: completion of the facility upgrades to incorporate a GM production diesel engine head into our optically-accessible engine and to improve our EGR simulation capabilities; careful matching of all-metal test engine performance and emissions data to establish the relevance of the optical engine measurements; benchmarking engine performance and emissions over a broad range of operating conditions to establish the foundation for future optical studies; and assessment of the performance of various aspects of turbulent combustion modeling in engines.

The upgraded optical engine is shown in Figure 1. In addition to incorporating the GM 1.9-liter production head, the optical access was improved significantly. By recessing the upper liner into the cylinder head, a clear view into the squish volume can be achieved even with the piston at top dead center (TDC). The large top-ring land height further allows imaging of the full-bowl depth at crank angles ±30° on either side of TDC. Moreover, a concave surface on the bottom of the optical piston acts as a negative lens, and allows imaging of the squish volume from below to within 3 mm of the cylinder wall.

Because the optical engine is skip-fired, there is no natural source of undiluted exhaust gas and EGR must be simulated. Concurrent with the engine upgrade, we also improved our ability to simulate EGR. The EGR system now incorporates a boiler that allows the addition of H_2O to our previous mixture of CO_2 and N_2. We have also added the capability to include CO and UHC, as well as other trace species in our simulated EGR. These species influence the combustion process through their thermophysical properties, their impact on the chemical kinetics of the ignition process, and through their intrinsic heating value. At high EGR rates, EGR characterized by large CO and UHC mole fractions contains a significant quantity of chemical energy, and impacts the amount of fuel required to obtain a given load significantly.

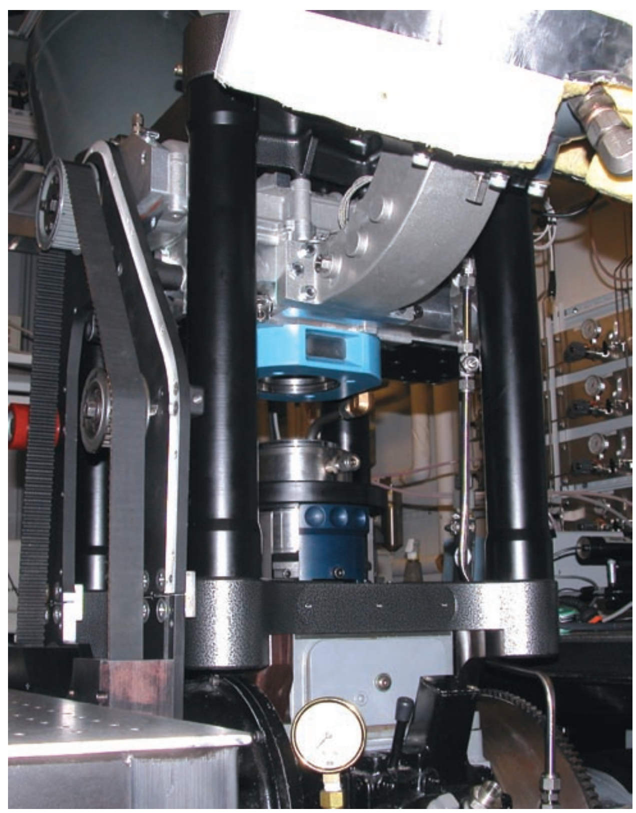

FIGURE 1. The Optically-Accessible Engine Incorporating the GM 1.9-Liter Head

To ensure that the data acquired in the optical engine accurately represents the combustion process occurring in all-metal engines, we have carefully matched the near-TDC thermodynamic conditions of the metal test engine by closely matching the composition of the intake gases, the near-TDC pressure of a motored metal engine trace (obtained with hot combustion chamber surfaces and representative EGR and residual concentrations), and the ignition delay. The same fuel batch was used in both the metal and optical engine tests to ensure that the ignition delay can be used as an accurate thermometer. A comparison of the apparent heat release rate observed in the metal and the optical engines is shown in Figure 2. Note that the timing of the main heat release is quite sensitive to intake temperature. With an intake temperature of 72°C, both the timing and the magnitude of the peak heat release are well matched. The breadth of the heat release measured in the metal engine is greater, however, and the optical engine heat release exhibits greater post-TDC fluctuations. Modeling of the optical engine extended piston as an oscillating spring-mass system suggests that these differences may be attributed to deformation of the optical piston.

A comparison of the UHC and CO emissions measured in both engines for a start of injection (SOI) sweep is presented in Figure 3. The magnitude, the location of the minima, and the trends in the emissions match well when the full complement of EGR gases is employed in the optical engine. When only N_2 and CO_2 are used to simulate EGR the magnitude of the emissions is higher. While running these tests, the injected fuel quantity was held constant. Hence, the differences observed cannot be attributed to reduced fueling when the simulated EGR contains UHC and CO. Away from the minimum, the relative increase in CO emissions is well matched, while the UHC emissions increase more rapidly in the optical engine. We believe this is due to a greater sensitivity of UHC emissions to wall temperature differences between the two engines. The existence of a distinct minimum in UHC and CO emissions (as well as indicated specific fuel consumption) is also noteworthy. A similar minimum was identified in a previous engine build, and shown to be associated with an optimal fuel distribution that best utilizes the available air [1]. The duplication of this behavior demonstrates the general applicability of this earlier work.

We have also investigated the ability of multi-dimensional engine combustion models to duplicate and explain the behavior of soot distributions in swirl-supported, heavy-duty diesel engines. Experimentally, soot observed during the expansion stroke is found to be rotating in a counter-clockwise direction, characterized by a positive vorticity (Figure 4). This vorticity, as well as the temporal evolution of the soot cloud, mark the soot-containing fluid as the remnants of the windward (with respect to swirl) side of the fuel jet head vortex. Because the swirl might be expected to transport fresh air into the windward side–thereby enhancing mixing–higher soot levels in this region are not expected. The predictions of multi-dimensional simulations performed at the University of Wisconsin, also shown in Figure 4, both reproduce and help explain this phenomenon. In the presence of swirl, the initial premixed heat release occurs predominantly on the leeward side of the jet. Combustion-induced flows subsequently lead to better mixing and reduced soot formation in this area. The higher soot concentrations on the windward side of the jet are thus predominantly due to higher rates of soot formation in this region just after the premixed combustion event.

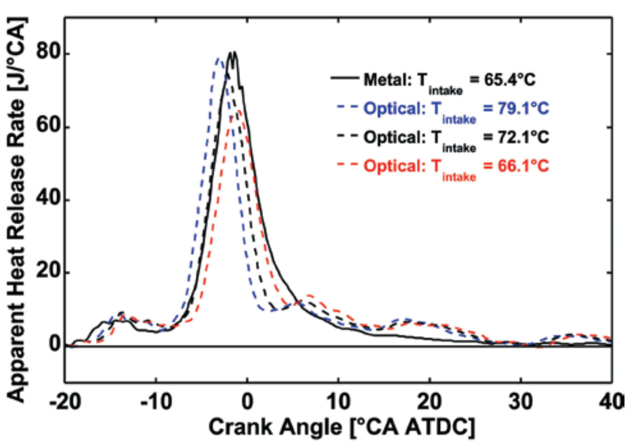

FIGURE 2. A comparison of the apparent heat release rate observed in the optical and the all-metal test engines at 2,000 RPM, a load of 6 bar indicated mean effective pressure, SOI = -41.7°, and a 9% O_2 concentration. Metal engine results courtesy of Prof. David Foster, GM-University of Wisconsin collaborative research laboratory.

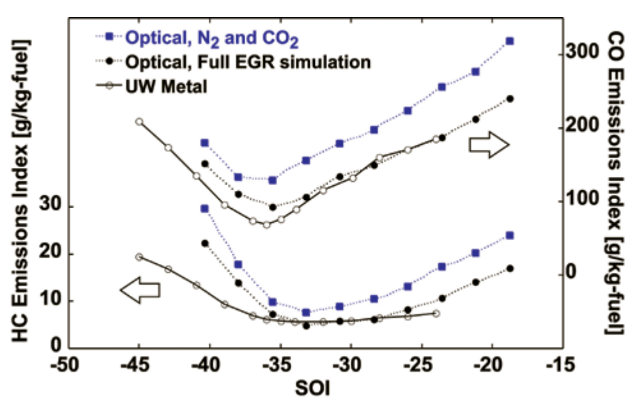

FIGURE 3. UHC and CO Emissions Obtained in an SOI Sweep, for the Same Conditions Identified in Figure 2

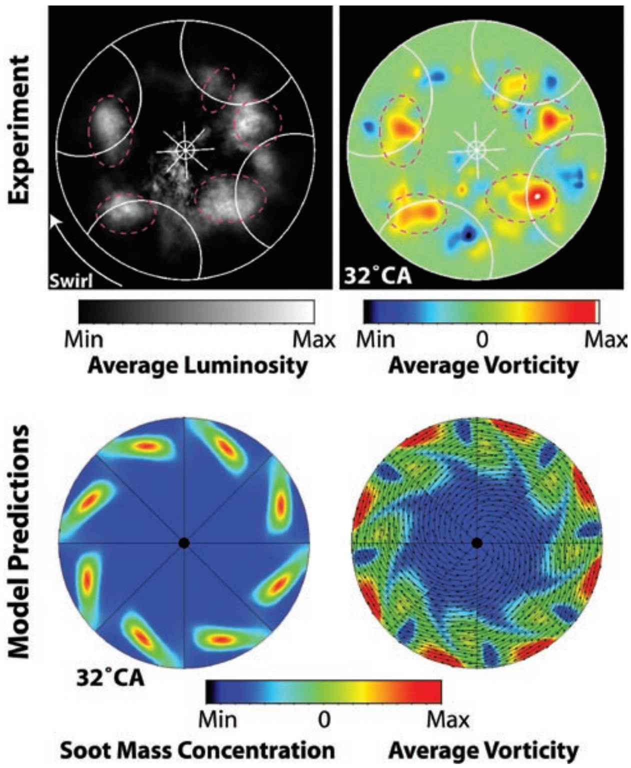

FIGURE 4. The upper row presents the mean distribution of soot luminosity and the axial component of vorticity (flow rotation) measured in a heavy-duty diesel engine with a swirl ratio of 1.7. Model predictions of these quantities are shown in the lower row. The model correctly predicts the approximate location of the soot and its correlation with positive vorticity.

Conclusions

- An upgrade to the optical engine and improved EGR simulation facilities have been completed and offer new capabilities for investigation the sources of emissions and inefficiencies in LTC systems.
- Careful matching of operating conditions allows both the combustion performance and the emissions behavior to be well-matched between optical and traditional metal engines, ensuring the relevance of data obtained from the optical engine.
- Performance and emission behavior has been mapped over a wide range of operating conditions, providing the foundation for future optical studies of emission sources and their mitigation in LTC regimes.
- The ability of multi-dimensional simulations to predict and explain the soot distributions observed in swirl-supported heavy-duty engines has been examined. The simulations reproduce the experimental results and show that enhanced mixing during the premixed heat release on the leeward side of the jet reduces the formation of soot as compared to the windward side of the jet.

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Special Recognitions & Awards

Invited Lecture: *2007 SAE Homogeneous Charge Compression Ignition Combustion Symposium*, Sept. 12–14, Lund.

II.A.3 Heavy-Duty Low-Temperature and Diesel Combustion Research and Heavy-Duty Combustion Modeling

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Objectives

The overall FreedomCAR and Vehicle Technologies (FCVT) goal for this project is to develop fundamental understanding of advanced low-temperature combustion (LTC) technologies. The specific goals for FY 2007 include:

- Understand LTC unburned hydrocarbon (UHC) emissions (Sandia)
  - This is a response to a specific industry request to understand why UHC emissions increase dramatically when ignition occurs after the end of fuel injection.
  - It is also consistent with the overall FCVT goal of understanding UHC emissions for low-load LTC.
- Improve LTC diesel computer models (Sandia and University of Wisconsin)
  - Improve predictions of diesel flame lift-off and soot formation at LTC conditions.
  - Understand how mixing, combustion, and pollutant formation are affected by engine design parameters, including 1) piston bowl geometry, 2) swirl ratio, and 3) spray targeting.
  - Validate/improve modeling of LTC mixing, combustion, and pollutant formation processes.
- Continue to refine conceptual model for LTC conditions (Sandia)
  - This is a long-term goal with continuous effort to update our understanding of in-cylinder LTC processes as more data becomes available.

Accomplishments

- Optical experiments showed conclusively that over-mixed fuel near the injector yields significant UHC emissions when ignition occurs after the end of injection because it does not achieve complete combustion.
  - Persistent formaldehyde fluorescence and absence of OH fluorescence shows that near-injector mixtures do not burn to completion when ignition occurs after the end of injection.
  - Direct equivalence ratio measurements by toluene fluorescence show that the mixtures *rapidly* become fuel lean, and that they are stagnant, remaining near the injector late in the cycle.
  - The total amount of over-mixed fuel in the near-injector region that does not achieve complete combustion follows trends and magnitude of measured UHC emissions.
- After refinement to include cool-flame reactions, computer models show improved agreement with experiments at LTC conditions.
  - Skeletal chemical kinetics mechanisms were modified to include cool-flame reactions to better simulate flame lift-off at LTC conditions.
  - With better lift-off simulation, prediction of soot formation was also improved.
- Initiated a parallel experimental and modeling study of effects of bowl geometry, spray angle, and swirl ratio on in-cylinder LTC processes
  - Preliminary computer models predict that spray targeting is the most significant factor affecting LTC performance and emissions, though swirl is important as well.
  - Will acquire large optical dataset of mixing, combustion, and pollutant formation with ranges of bowl diameter, spray angle, and swirl ratio to understand effects of design factors and to validate model predictions of in-cylinder phenomena.

Future Directions

- Apply optical diagnostics for other LTC conditions
  - Compare single and split/pilot injection schemes for conventional and LTC combustion using multiple imaging diagnostics.
- Maintain modeling collaboration with the University of Wisconsin to improve computer model performance for LTC conditions.
  - Analyze large optical dataset of parametric variation in bowl geometry, injector spray angle, and swirl ratio.
  - Use experimental data to validate and improve computer models.

- Develop simple mixing model of end-of-injection mixing processes.
  - Improve understanding of physical processes affecting liquid- and vapor-fuel mixing after end of injection.
  - Predict effect of injection rate shapes on mixture formation.
- Continue to extend the conceptual model of diesel combustion to LTC conditions.

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Introduction

Although LTC strategies can achieve very low emissions of nitrogen oxides (NOx) and particulate matter (PM) at high efficiency, they typically have increased emissions of other pollutants, including UHCs. The UHC emissions often increase with longer ignition delays (ID) [1,2], particularly when the ID exceeds the injection duration. As part of a specific request for insight into in-cylinder processes causing high UHC emissions, Cummins Inc. provided UHC data from a wide range of diesel engine operating conditions. Figure 1 shows that the UHC emissions become very high for conditions with positive "ignition dwell," defined as the time between the end of injection (EOI) and the start of combustion. UHC emissions for LTC conditions with large, positive ignition dwells are likely dependent on in-cylinder phenomena occurring near or after EOI.

The primary goal of this project for FY 2007 is verify the existence of over-lean mixtures near the injector that do not achieve complete combustion when the ignition dwell is positive, and to assess the importance of these mixtures to UHC emissions. This primary goal is consistent with the overall FCVT goal of understanding UHC emissions for low-load LTC conditions. A second goal is to improve LTC diesel computer models (in collaboration with the University of Wisconsin) to better predict diesel flame lift-off and soot formation at LTC conditions, as well as to understand the influence of engine design parameters on mixing, combustion, and pollutant formation.

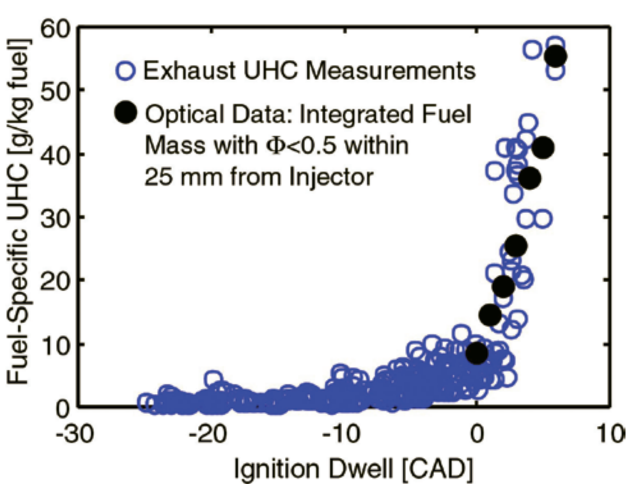

FIGURE 1. Exhaust UHC for a wide range of diesel engine operating conditions (open blue circles) and in-cylinder fuel mass in mixtures with $\Phi<0.5$ within 25 mm of the injector (filled black circles) at various ignition dwells. Exhaust emissions data is from Cummins Inc.

Approach

This project uses an optically-accessible, heavy-duty, direct-injection diesel engine (Figure 2). Imaging access is through a window in the bowl of an extended piston. Windows in the cylinder wall and in the piston bowl-wall are for the laser diagnostics. Figure 2 also shows the setup of the optical diagnostics, which use three cameras. The progress of vapor-fuel combustion is inferred from simultaneous images of planar laser-induced fluorescence (PLIF) of formaldehyde (H_2CO) and hydroxyl radical (OH) under LTC conditions with varying ignition dwells. Quantitative measurements of the in-cylinder vapor-fuel concentration using PLIF of a toluene fuel-tracer are compared to engine-out UHC emissions. The engine operating condition simulates exhaust gas recirculation dilution to 12.6% intake oxygen (by volume), and the engine load is near 4 bar indicated mean effective pressure, with injection near top-dead center.

The modeling work uses a version of the Los Alamos KIVA computer code that has been improved at the University of Wisconsin. Instead of using full detailed chemistry, the model uses a reduced kinetic mechanism for n-heptane ignition and combustion so that solutions can be completed in a reasonable time. Based on sensitivity analysis of a more complex full chemistry mechanism [3], the reduced mechanism was recently improved to include cool-flame reactions that are important for predicting the diesel flame lift-off length at LTC conditions. Also, a multi-objective genetic algorithm [4] was implemented in the KIVA computer model to predict an optimal set of piston bowl designs and spray geometries, which will be studied and validated experimentally in FY 2008.

Results

Simultaneous images of H_2CO fluorescence (red) and OH fluorescence (green) under conditions with ignition dwells that are short (top row) and long (bottom row) are shown in Figure 3. The images were acquired (1) near the peak in the first-stage ignition heat release, (2) near the peak in the second-stage ignition heat release, and (3) late in the cycle, when combustion was essentially complete. For each image in Figure 3, the

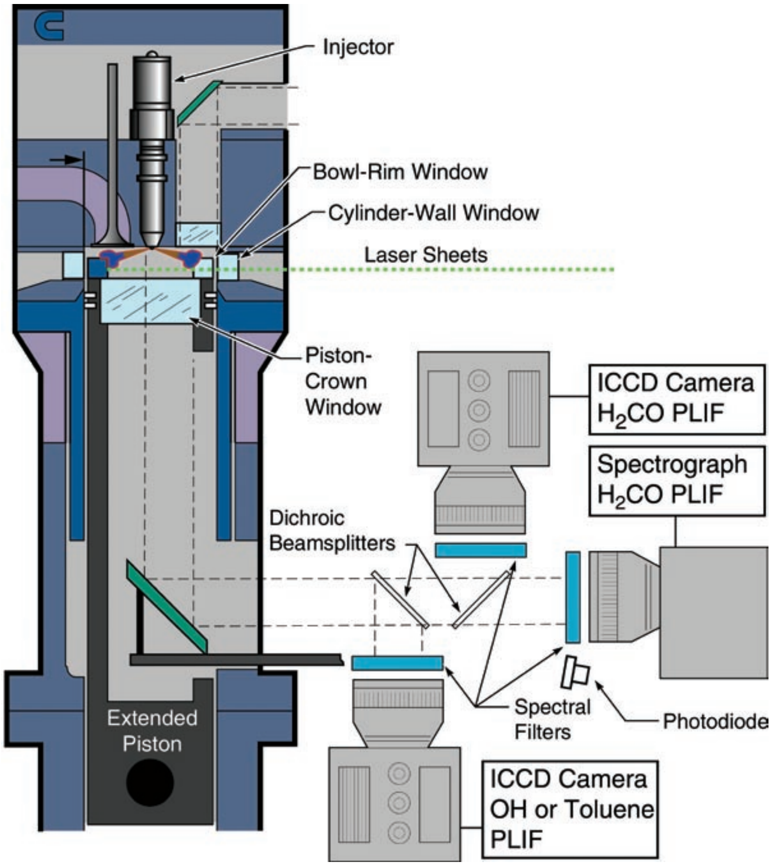

FIGURE 2. Schematic Diagram of the Optically Accessible Direct Injection Diesel Engine and Optical Setup

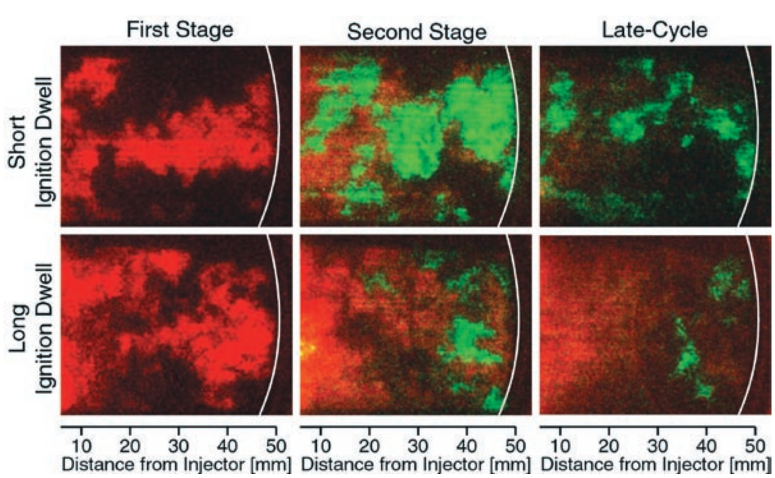

FIGURE 3. Representative composite images of H_2CO PLIF (red) and OH PLIF (green) for the shorter-ID (top row) and longer-ID (bottom row) operating conditions. Images were acquired shortly after first-stage ignition (left column), second-stage ignition (middle column), and late in the cycle (right column). The curved white line represents the piston bowl, and the distance from the fuel injector is indicated below the images.

view is through the piston-crown window (see Figure 2), and the curved white line represents the piston bowl-rim. One of the eight fuel jets, which penetrates horizontally from left to right from the perspective of the camera, is captured in the images. The injector is about 6 mm to the left of the field of view, as indicated by the scale at the bottom of the images.

For both operating conditions, H_2CO PLIF first appears throughout the horizontal jet during the first stage of ignition, and the OH initially appears during the second stage of ignition, in the downstream region of the jet, near the piston bowl-rim. H_2CO fluorescence indicates regions that have completed the first stage of ignition, but have not yet reached complete combustion, while OH indicates regions that have transitioned to the second stage of ignition, where combustion is largely complete.

For the shorter ignition dwell condition (top row), OH fluorescence also appears upstream, near the injector. Late in the cycle, some OH fluorescence (green) is apparent in pockets throughout the combustion chamber, while H_2CO fluorescence (red) is very weak or absent. By contrast, for the long ignition dwell, OH fluorescence almost never appears upstream, and H_2CO fluorescence persists late in the cycle. Although some H_2CO fluorescence is detectable downstream, the strongest fluorescence is typically upstream, within about 25 mm from the injector. The persistent H_2CO fluorescence indicates that combustion is incomplete, and chemical kinetics simulations predict that over-mixing of the fuel to overly lean mixtures is the most likely cause for incomplete combustion.

Figure 4 shows direct measurements of the in-cylinder vapor-fuel equivalence ratio using toluene fluorescence, and the data confirms that the mixtures near the injector indeed become very fuel-lean shortly after the end of injection. In Figure 4, the injector was rotated from its orientation in Figure 3, so that one of the jets that intersected the laser sheet penetrated upward and to the right (2 o'clock position), and another penetrated down and to the right (4 o'clock position).

At EOI, which is 0° after the end of injection (AEI), the mixtures on the jet centerline are fuel-rich throughout the jet, with the richest mixtures near the injector, as is typical of conventional quasi-steady diesel jets. But rapidly after the end of injection, the mixtures near the injector become fuel-lean. By only 0.25° AEI, the axial equivalence ratio distribution is relatively flat. By 1° AEI, the upstream mixtures, near the injector, are clearly leaner than the downstream mixtures. By 3.5° AEI, the mixtures are near stoichiometric within 25 mm from the injector. At 5° AEI, which is the start of the main combustion, the mixtures near the injector are very fuel-lean, which is consistent with the predictions of over-lean mixtures by the chemical kinetics simulation to explain the persistent H_2CO fluorescence. Also, downstream mixtures that showed strong OH fluorescence (Figure 3) are near-stoichiometric (Figure 4), and should achieve complete combustion. At later times, the jets become indistinct, and the residual jet momentum does not carry the fuel-lean mixtures downstream; rather, they stagnate near the injector, do not achieve complete combustion, and go on to contribute to UHC emissions. Indeed, as shown in Figure 1, the total in-cylinder fuel in mixtures with equivalence ratios less than 0.5 within 25 mm from the injector (filled black circles) agrees very well with exhaust UHC measurements (open blue circles). This agreement indicates that incomplete combustion in over-lean mixtures near the injector is likely responsible for much of the UHC emissions for conditions with long positive ignition dwell.

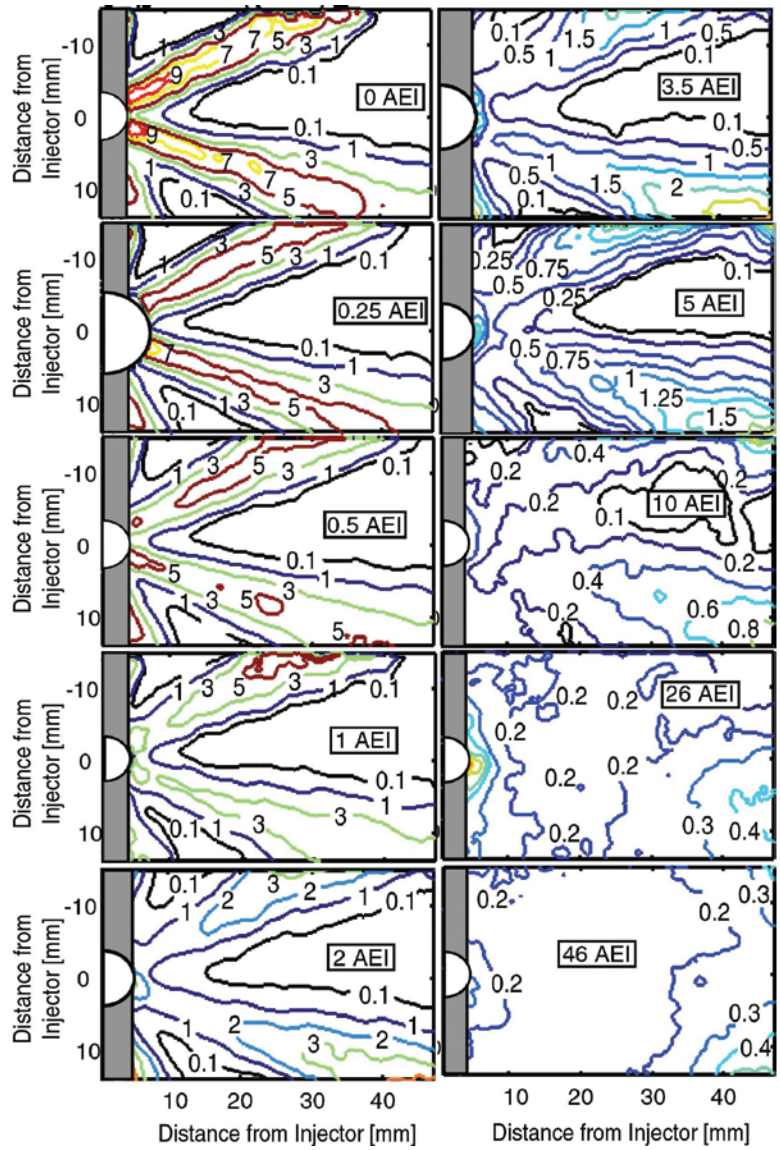

FIGURE 4. Equivalence ratio contours measured by toluene fluorescence. The time in crank-angle degrees after the end of injection (AEI) is indicated in each of the plots. The injector is on the middle left edge of each image, and two of the eight fuel jets fall within the field of view (see Figure 3 for field of view). The white half circle and vertical gray rectangle masks represent areas of residual laser flare off the injector and firedeck surface, respectively, where fuel vapor measurements are not viable.

Figure 5 shows a comparison of diesel jet lift-off lengths under LTC conditions from measurements in a constant-volume combustion vessel (squares), predictions from the KIVA computer model using the original chemical kinetics mechanism with no cool flame reactions (circles), and predictions with several critical cool-flame reactions added to the mechanism (triangles). Addition of the cool-flame reactions that were identified through a sensitivity analysis of a complex detailed chemistry mechanism [3] clearly improves the agreement between the model predictions (triangles) and experimental measurements (squares). These improved predictions of flame lift-off translate to better prediction of soot formation in the diesel jets under LTC conditions (not shown here).

Finally, Figure 6 shows the results of a design optimization using genetic algorithms with the KIVA computer model. The technique [4] identifies a set of optimum designs (the Pareto citizens, in blue triangles) that have the best performance over a range of emissions and efficiency criteria, plotted on the axes. The "Pareto surface" of the blue triangles is useful because rather than producing only a single optimum design as in previous optimization approaches, different optimal engine designs may be selected from the Pareto surface depending on the relative importance of the performance criteria to the engine designer.

Conclusions

- This project uses an optical engine to study in-cylinder phenomena coupled with modeling collaborations to improve simulation capabilities for LTC conditions.
- Multiple imaging diagnostics showed that over-mixed fuel near the injector yields significant UHC emissions because it does not achieve complete combustion when ignition occurs after the end of injection.
- Using experimental data for validation, the accuracy of computer model predictions was improved.
- FY 2007 activity transfers results to industry to address a specific request for information about dramatic increase UHC emissions for LTC conditions.
- Future work will explore multiple injection strategies and combustion chamber design parameters with both experiments and simulations.

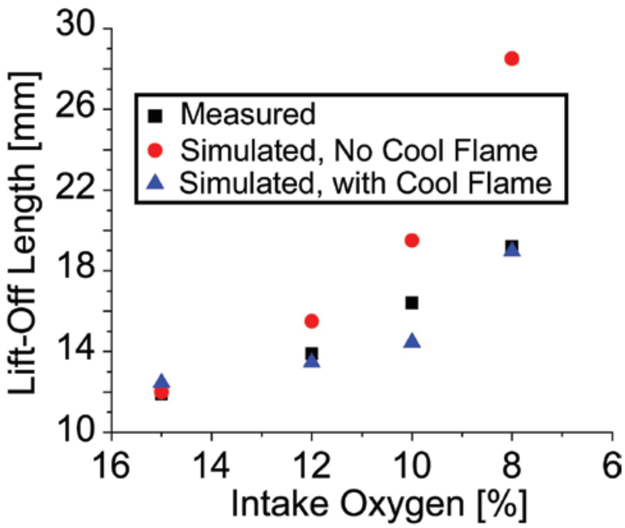

FIGURE 5. Lift-Off Measurements (Black Squares) and Predictions with (Blue Triangle) and without (Red Circle) Cool-Flame Reactions in the n-Heptane Reduced Mechanism

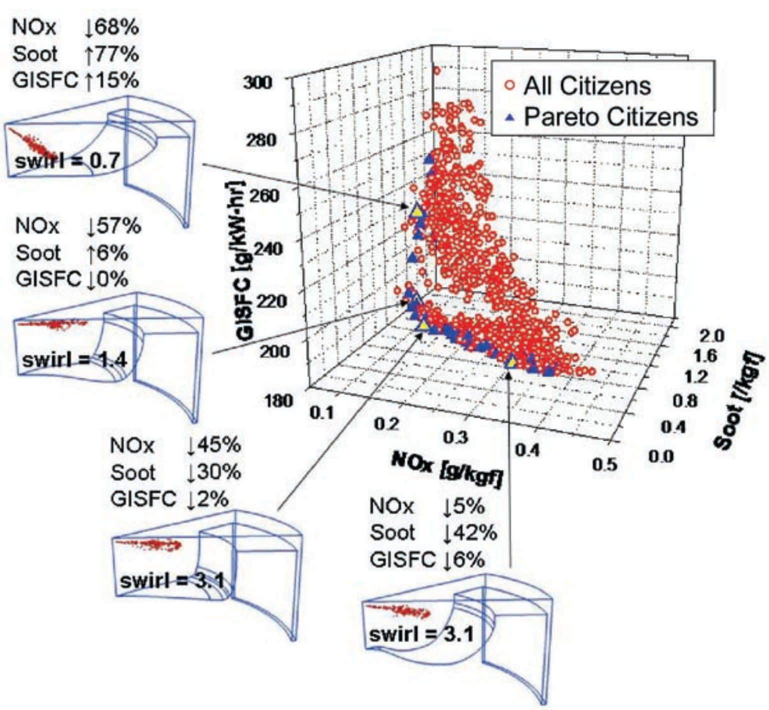

FIGURE 6. Predicted emissions and fuel consumption performance for simulations with different piston bowl geometry, fuel spray angle, and swirl ratio at a LTC condition. The optimal "Pareto surface" citizens (blue triangles) are a subset of the full set of configurations tested (red circles).

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FY 2007 Publications/Presentations

Publications

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2. "In-Cylinder Unburned Hydrocarbon Visualization During Low-Temperature Compression-Ignition Engine Combustion Using Formaldehyde PLIF," T. Lachaux and M. Musculus, Proceedings of the Combustion Institute Vol. 31, pp. 2921-2929, Presented August 2006, Published late 2006.

3. "A Computational Investigation into the Effects of Spray Targeting, Swirl Ratio

and Bowl Geometry for Low-Temperature Combustion in a Heavy-Duty Diesel Engine," C. Genzale, D. Wickman and R.D. Reitz, SAE paper 2007-01-0119, 2007 SAE International Congress and Exposition, April 2007.

4. "Numerical Predictions of Diesel Flame Lift-off Length and Soot Distributions under Low Temperature Combustion Conditions," G. Vishwanathan and R.D. Reitz, Submitted SAE Congress, 2008.

5. "Evaluation of the Equivalence Ratio-Temperature Region of Diesel Soot Precursor Formation Using a Two-Stage Lagrangian Model," L. Pickett, J. Caton, M. Musculus, and A. Lutz., International Journal of Engine Research Vol. 7, No. 5, pp. 349-370, December 2006.

6. "Validation of Engine Combustion Models Using Detailed In-Cylinder Optical Diagnostics Data for a Heavy-Duty Compression-Ignition Engine," S. Singh, R. Reitz, M. Musculus and T. Lachaux, International Journal of Engine Research, Vol. 8, No. 1, pp. 97-126, Jan. 2007.

7. "Two-Stage Ignition and Unburned Fuel Emissions for Heavy-Duty Diesel Low-Temperature Combustion of Neat n-Heptane," M. Musculus and T. Lachaux, 5th US Combustion Meeting, San Diego, March 25-28, 2007.

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

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

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11. Invited by Woodhead Publishing of Cambridge to contribute book chapter to "Direct Injection Combustion Engines and Their Fuels for Automotive Applications in 21st Century".

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1. "Quantitative Laser Diagnostics Issues in Transient, High-Pressure Environments of Engines," M. Musculus, L. Pickett, P. Miles, Third International Conference on Lasers and Diagnostics, City University, London, UK, May 23, 2007.

2. "Diesel Jet Mixing in Conventional and Low-Temperature Diesel Combustion," M. Musculus, J. Dec, and T. Lachaux, presented at 10th International Conference on Present and Future Engines for Automobiles, Rhodes Island, Greece, May 30, 2007.

3. "Liquid-Phase Fuel Penetration in Diesel Sprays at the End of Injection," M. Musculus and T. Lachaux, Advanced Engine Combustion Working Group Meeting, June 2006.

4. "Vapor-Phase Fuel-Air Mixing in Diesel Jets at the End of Injection," T. Lachaux, M. Musculus, L. Pickett and C. Idicheria, Advanced Engine Combustion Working Group Meeting, June 2006.

5. "Visualization of UHC Emissions for Low-Temperature Diesel Engine Combustion," M. Musculus and T. Lachaux, Diesel Engine-Efficiency and Emissions Reduction Conference, Detroit MI, August 21, 2006.

6. "Unburned Hydrocarbon Emissions from End-of-Injection Over-Mixing for LTC Diesel Combustion," M. Musculus, T. Lachaux, L. Pickett, and C. Idicheria, Advanced Engine Combustion Working Group Meeting, February 2007.

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

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Objectives

- Determine the history of liquid penetration at conditions typical of early-injection low-temperature diesel combustion.
- Investigate the timing and amount of soot formation for short-injection events at high-exhaust gas recirculation (EGR) low-temperature combustion (LTC) conditions.
- Show how multiple injections affect liquid-phase penetration.

Accomplishments

- Quantified the extent of liquid-phase penetration for typical early-injection LTC conditions with various injection durations, nozzle sizes, injection pressures and number of injections. Provides an understanding needed to prevent liquid wall impingement and its negative impacts on emissions and combustion efficiency.
- Showed that the extent of liquid penetration depends upon the injected mass for short injections less than the steady-state liquid length, rather than the nozzle size or injection pressure.
- Demonstrated that small nozzles actually form more soot than larger nozzles when the injection duration is adjusted such that the mass injected is constant.

Future Directions

- Investigate the location of evaporation for end-of-injection mixing near the nozzle and its impact on unburned hydrocarbons.
- Determine how multiple injections can be used to affect ignition timing and minimize unburned hydrocarbons (UHC) at LTC conditions.
- Perform direct measurements of mixing (equivalence ratio) at the time of the premixed burn in constant-injection-duration diesel fuel jets for various EGR levels and multiple injection strategies. This investigation will show how mixing between injections affects the equivalence ratio and location of the premixed burn.

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Introduction

Avoiding liquid impingement upon the cylinder liner and preventing excessive impingement on the piston bowl are considered to be key technologies for successful implementation of diesel LTC combustion. Cylinder-liner impingement causes oil dilution and piston impingement may cause high UHC emissions, poor fuel-air mixing, and low combustion efficiency. Unfortunately, prevention of liquid impingement is difficult because the early-injection timing (-50° to -20° crank-angle degrees, CAD), required to induce sufficient fuel-air premixing, also creates charge-gas conditions where liquid impingement is likely (i.e., low charge-gas temperature and density). A low charge-gas temperature will result in little fuel evaporation, and a low density will allow rapid penetration with little momentum and mass exchange with the spray. Alternatively, if injection phasing is retarded closer to top dead center (TDC), there will be less time available for mixing prior to ignition and fuel-rich mixtures forming both nitrogen oxides and soot may be produced. Overall, there is a strong need to understand the effects of injector variables such as nozzle size, injection pressure, injection duration, and number of injections on liquid phase penetration and combustion in LTC engines.

Approach

With the ability to carefully control the charge-gas temperature and density, a constant-volume vessel was utilized to quantify the extent of liquid penetration and soot formation while the thermodynamic and injector conditions were varied. Experiments using a Bosch second-generation common-rail injector with various single-hole nozzles of the same shape (KS1.5/86) are reported here. A more detailed description of the facility may be found in [1].

Mie-scattering and shadowgraph images were simultaneously acquired using high-speed cameras to define the spray liquid and vapor phases, respectively, for a given set of conditions as shown in Figure 1. Mie-scatter images were acquired at a rate of 50 kHz. A survey of the literature shows typical premixed compression-ignition timing ranges from (-40° to -20° CAD) *for conventional spray included angles and nozzle sizes*. Table 1 shows the expected thermodynamic conditions for these injection timings with other

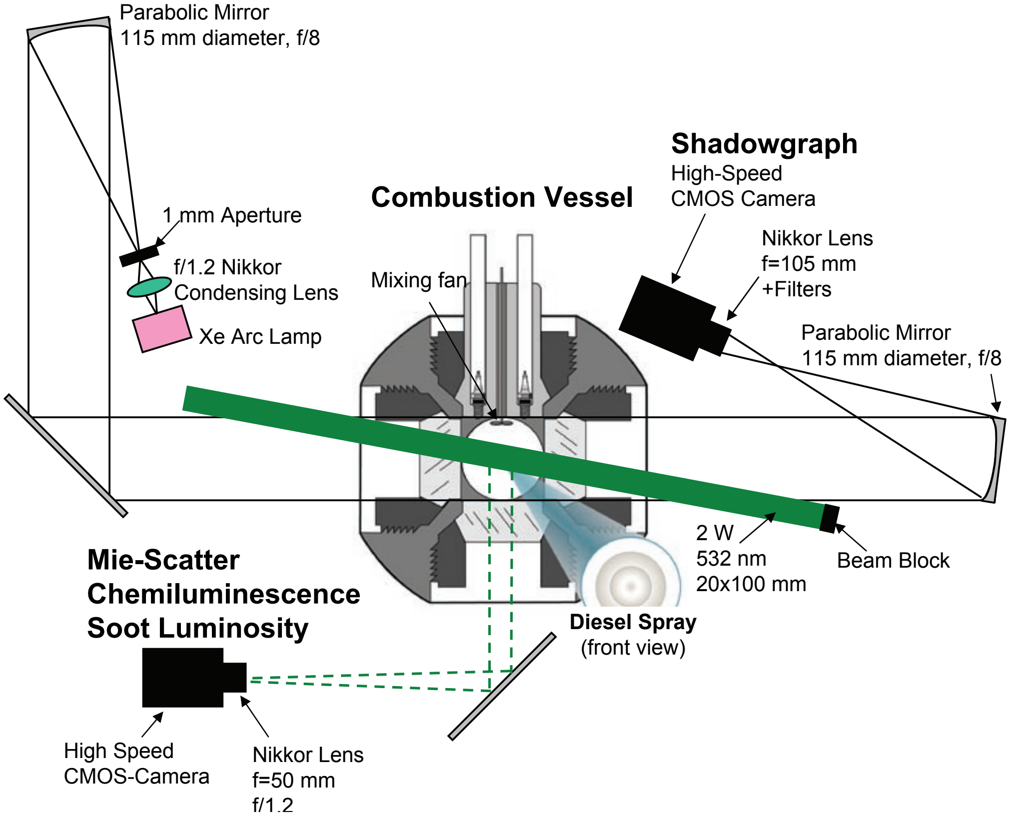

FIGURE 1. Combustion Vessel and High-Speed Imaging Setup (Mirror spacing not to scale.)

assumptions listed on the table. Finally, a #2 diesel fuel (T_{90} = 573 K) and kerosene fuel (T_{90} = 523 K) were compared to assess the effect of fuel type.

TABLE 1. Calculated Charge-Gas Conditions for a Given Crank-Angle (CA)

Assumptions: T_{BDC} = 340 K; P_{BDC} = 1 atm; Compression Ratio = 16; γ = 1.35;					
CAD [°ATDC]	-40	-35	-30	-25	-20
Temperature [K]	601	637	677	721	768
Density [kg/m^3]	5.2	6.2	7.3	8.8	10.5

Results

Figure 2 shows the transient liquid penetration for a long-injection event (solid) and a short-injection event with a 250 μs injection duration (dotted). The liquid length is the longest axial distance of any measurable elastic scatter from droplets, defining the axial boundary between liquid and vapor phases of the spray. The long-injection event shows the expected trend of decreased liquid penetration with injection timing retarded towards TDC. The long-injection-duration sprays eventually reach a "steady-state" liquid length as has been demonstrated in the past [2]. The -40 CAD timing has a steady liquid length of approximately 90 mm, which would likely impinge liquid on the cylinder liner. However, shortening the injection duration to 250 μs

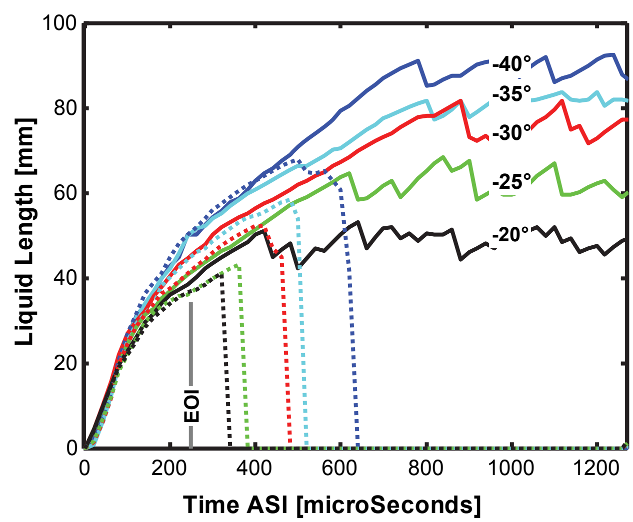

FIGURE 2. Transient Liquid Penetration for Long (Solid) and Short (Dashed) Injection Durations (Thermodynamic conditions for the simulated crank-angle of injection given in Table 1. Fuel, kerosene; T_{fl} = 373 K; d = 0.180 mm; DP_{inj} = 110 MPa.)

significantly decreases the maximum liquid penetration, particularly for the problematic, earlier injection timings. These findings suggest that short injection durations are less likely to experience wall impingement, and therefore could be used for successful LTC operation. However, the amount of fuel injected is small, which would limit the operating load. This is consistent with known trends for LTC operation in engines.

Figure 3 compares the effect of fuel type on the transient liquid history. A lower boiling-point fuel is shown to be effective in reducing the maximum liquid penetration, as well as shortening the time before the fuel completely evaporates after the end of injection. This behavior is expected to be favorable for LTC operation.

An alternative to the use of a lower-boiling point fuel to limit the liquid penetration is to use multiple short injections, as demonstrated in Figure 4. Shadowgraph images, marking the vapor phase, are shown at the right of Figure 4. Blue lines overlaid on the image mark the boundary of the liquid phase obtained from Mie-scatter images. The image sequence shows the first two injections of a four-injection event (equal injection durations). During the first injection, the liquid and vapor phases overlap, indicating low evaporation rates. After the end of injection (0.411 ms), liquid and vapor coincide at the head of the jet, but a vaporized fuel region remains near the nozzle. The second injection begins as liquid vaporizes at the head of the jet. This new injection quickly reaches the vapor region at the head of the jet as it flows through the "wake" left behind by the first injection.

The maximum penetration distance of the liquid and vapor phases is shown at the left of Figure 4 for the entire four-injection event. The vapor phase separates from the liquid phase after the end of the first injection and continues to penetrate across the chamber. The maximum penetration of the liquid phase of the second injection is longer than the first because of mixing with cooler gas vaporized by the first injection and faster penetration by moving through the wake of the first injection. Following injections (second and third) penetrate approximately the same as the second injection. In addition, the maximum liquid penetration remains much less than that of a single, continuous injection with a long injection duration (red curve). Therefore, pulsation of the injector is shown to be effective in limiting liquid penetration and possibly preventing wall wetting.

The dependency of the maximum liquid penetration distance upon injection duration was investigated further by examining the effects nozzle diameter and injection duration with the same total mass injected. It is well known that reducing the injection pressure or nozzle size will reduce the rate of liquid penetration, but the injection duration must be increased in order to reach the same injected mass. For short, transient injections, the question is which strategy minimizes

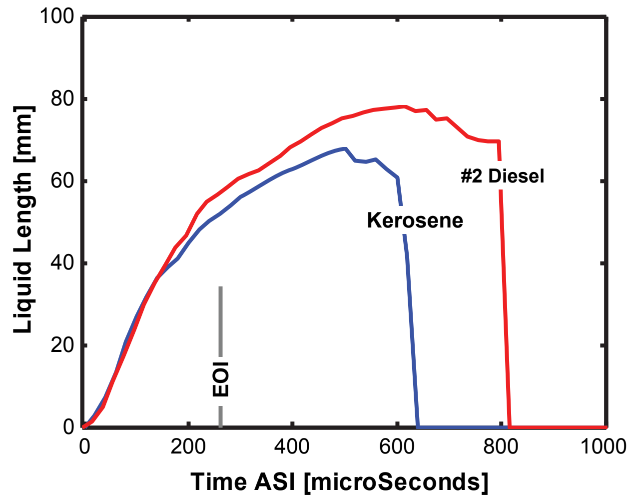

FIGURE 3. Transient Liquid Penetration for Diesel Fuel Compared to Kerosene at -40 CAD Thermodynamic Conditions and a 250 µs Injection Duration (Other conditions the same as Figure 2.)

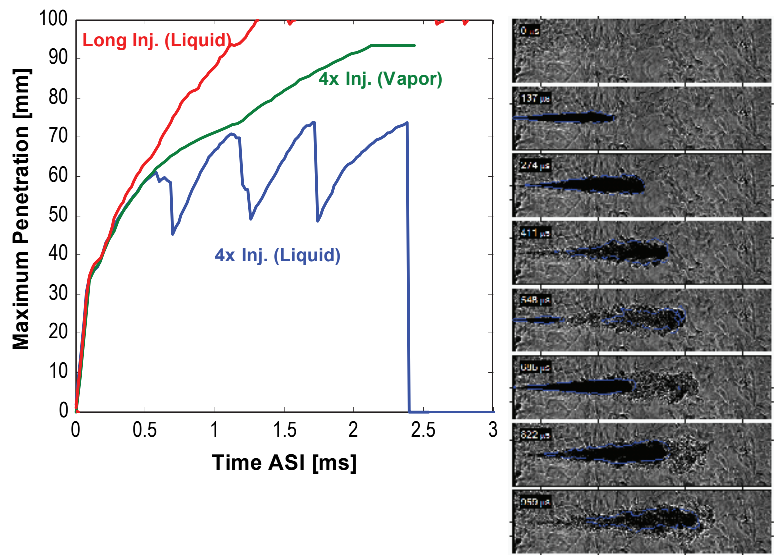

FIGURE 4. Transient Penetration of Liquid (Blue) and Vapor (Green) Phases for a Four-Injection Event (Injection duration for each injection is 0.2 ms. A long injection duration [2 ms] is shown for reference [red]. -40 CAD simulated conditions, Fuel = #2 diesel; T_{fl} = 373 K; d = 0.110 mm; DP_{inj} = 110 MPa.)

liquid penetration. Figure 5 shows the maximum measured liquid penetration for a range of nozzle sizes with the same injection pressure. The major conclusion is that nozzle size does not affect the maximum liquid penetration, indicating that the maximum liquid penetration tends to collapse for given injection mass. Note that this result is restricted to transient injections where the maximum liquid penetration is less than a steady-state value. For example, the steady-state liquid length scales linearly with nozzle diameter and this would eventually dominate if smaller nozzle diameters were used. A study of injection pressure effects confirmed the result that the maximum liquid was the same when the same mass was injected. The collapse of maximum liquid penetration with injection mass may be one contributing factor that limits LTC combustion to low-load conditions.

Similarly, it is well known that reducing the nozzle diameter increases the rate of mixing relative to the fuel injection rate, but again the injection duration must be increased to deliver the same total amount of fueling. Figure 6 shows that the longer injection duration actually causes *more* soot formation for smaller nozzles compared to larger nozzles. The timing of the injection event relative to the ignition delay appears to be important. When injection ends after ignition (negative ignition dwell), the luminosity rise is severe, indicating strong soot luminosity. However, when the injection ends prior to ignition (positive ignition dwell), the luminosity rise is mild, indicating only chemiluminescence from high-temperature combustion (confirmed by other diagnostics). This concept is similar to that explained for the success of MK combustion [3]. With fixed injection pressure, smaller nozzles tend to produce soot because of the required longer injection duration. Figure 6 shows that a solution to remove soot formation is to use both a small nozzle and higher injection pressure, thereby shortening the injection duration for a given injected mass.

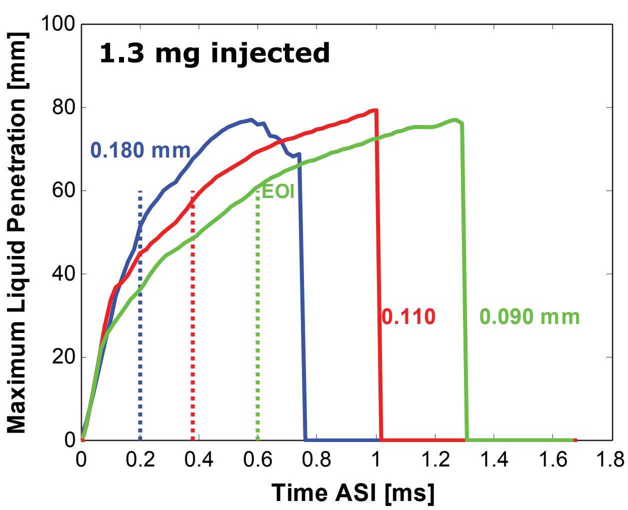

FIGURE 5. Transient Liquid Penetration for Various Nozzle Sizes, each with 1.3 mg Total Injected Mass (Thermodynamic conditions and fuel are the same as Figure 4.)

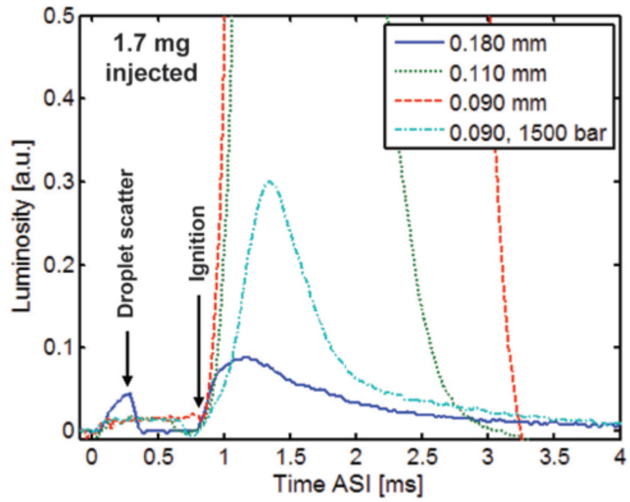

FIGURE 6. Luminosity Rise (Chemiluminescence and/or Soot Formation) for Various Nozzle Sizes, each with 1.7 mg Total Injected Mass (LTC ambient conditions: 900 K, 60 bar, 15% O_2. Injector conditions: #2 diesel; T_{fl} = 373 K; DP_{inj} = 110 MPa unless otherwise specified.)

Conclusions

The effects of injector variables such as nozzle size, injection pressure, injection duration, and number of injections on liquid phase penetration and combustion were investigated this year. Liquid-phase transients were investigated at conditions typical of early-injection LTC engines. Shortening the injection duration and applying multiple injections limits the liquid penetration to be much less than that of a steady-state spray. Results also show that variation in nozzle size and injection pressure while maintaining the same injection mass produces the same maximum liquid penetration. In addition, small nozzles actually form more soot than larger nozzles when the injection duration is adjusted such that the mass injected is constant.

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3. Kimura, S., Aoki, O., Kitahura, Y., Aiyoshizawa, E., "Ultra-Clean Combustion Technology Combining a Low-Temperature and Premixed Combustion Concept for Meeting Future Emissions Standards," SAE Paper 2001-01-0200, 2001.

FY 2007 Publications/Presentations

1. Musculus, M.P.B, Lachaux, T., Pickett, L.M., and Idicheria, C.A. "End-of-Injection Over-Mixing and Unburned Hydrocarbon Emissions in Low-Temperature-Combustion Diesel Engines," SAE paper 2007-01-0907.

2. Idicheria, C.A. and Pickett, L.M. "Quantitative Mixing Measurements in a Vaporizing Diesel Spray by Rayleigh Imaging," SAE paper 2007-01-0647.

3. Pickett, L.M. and Idicheria, C.A. "Effects of Ambient Temperature and Density on Soot Formation under High-EGR Conditions," THIESEL 2006.

4. Idicheria, C.A. and Pickett, L.M. "Formaldehyde Visualization Near Lift-Off Location in a Diesel Jet," SAE Powertrain and Fluid Systems Conference, SAE 2006-01-3434.

Special Recognitions & Awards/Patents Issued

1. 2006 SAE Russell S. Springer Award to Cherian Idicheria for best technical paper by author less than 36 years of age. (SAE 2006-01-3434).

II.A.5 Achieving High Efficiency Clean Combustion (HECC) in Diesel Engines

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Objectives

- Increase speed-load operation range in HECC modes for improved emissions and efficiency.
- Investigate mixed-source exhaust gas recirculation (EGR) methods for improved control of dilution composition and temperature.
- Develop computer simulations for improved guidance for, and interpretation of, experiments.
- Commission modern light-duty diesel engine which is representative of state-of-the-art engine technology.

Accomplishments

- Demonstrated increase in speed-load range for HECC operation of a light-duty diesel engine.
- Characterized mixed-source EGR for controlling intake temperature and, correspondingly, emissions and efficiency.
- Explored relationship between brake specific fuel consumption (BSFC) and combustion noise for HECC operation.
- Commissioned and mapped modern light-duty diesel engine.

Future Directions

- Explore advanced combustion operation on a General Motors (GM) 1.9-L engine including efficiency, emissions, noise, and stability with a high-pressure loop (HPL) EGR system.
- Characterize effect of intake mixture temperature and composition on advanced combustion operation.
- Investigate acoustic and vibration energy transmission paths for diagnostics and control of conventional combustion and advanced combustion modes.

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Introduction

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

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

Approach

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

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

The MB engine also has a low-pressure loop (LPL) EGR system which is used in coordination with the original equipment HPL EGR system to achieve mixed-source EGR as shown in Figure 1. The potential of mixed-source EGR is explored using LPL EGR as a "base" for dilution rather than as a sole source. HPL EGR provides the "trim" for controlling mixture temperature and has the potential for enabling more precise control of dilution set points. The mixed-source approach is also useful for conditions when LPL EGR does not provide sufficient dilution for achieving HECC operation. Additional dilution is achieved with the HPL EGR system, mitigating the need for throttling or a LPL EGR pump.

Results

Four speed-load conditions which were originally defined by an industry working group to be representative of light-duty diesel engine operation were selected for use in this study. While this approach does not take into account cold-start or other transient phenomena, the metric has been successfully used by others for comparison purposes and to demonstrate potential improvements from one technology to another.

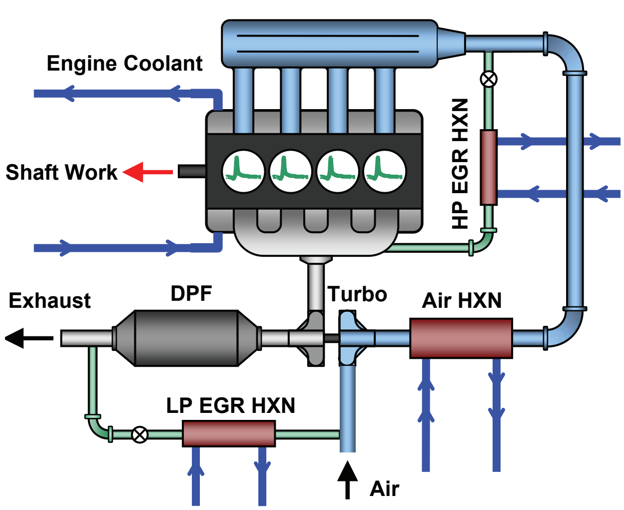

FIGURE 1. Schematic of Mixed-Source EGR System Showing HPL and LPL EGR Loops

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

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

The four modes used in this study are summarized in Table 1. ORNL is also working with the Advanced Combustion & Emissions Control Technical Team to propose a new set of operating conditions for use in characterizing efficiency and emissions improvements from advanced engine technologies. A well-defined set of operating conditions would allow improved comparisons across the DOE light-duty diesel activities.

Experiments were performed on a MB 1.7-L diesel engine using HPL, LPL, and mixed-source (combination of HPL and LPL) EGR to achieve HECC operation for the modal conditions in Table 1. The recipe used for HECC in these experiments is a PCCI approach which makes use of high dilution, high fuel injection pressure, and proper combustion phasing to achieve efficient LTC operation. An example comparison of the heat release profiles for conventional and HECC operation is shown in Figure 2 for 1,500 rpm, 2.6 bar brake mean effective pressure (BMEP). The heat release profile for HECC operation is consistent with more premixed combustion as compared to conventional operation. This strategy may also lead to higher combustion noise levels as shown in Figure 3 for the 1,500 rpm, 2.6 bar BMEP condition. A significant increase in combustion noise was observed for HECC operation to achieve BSFC values similar to those for conventional operation.

The mixed-source EGR approach allows for the control of the intake air-EGR mixture temperature independent of overall dilution level. As an example, the relationship between PM and NOx is shown in Figure 4 for several EGR scenarios and engine conditions of 2,300 rpm, 4.2 bar BMEP. Shown are conventional combustion results for the original equipment EGR rate, HECC operation with HPL EGR, and HECC operation with mixed-source EGR where intake mixture temperature is held constant at 50°C. Intake mixture temperature was held constant by adjusting the ratio of LPL and HPL EGR and overall dilution. Although not shown, this trend was also observed for 1,500 rpm, 2.6 bar BMEP modal condition. The existence of this NOx-PM relationship within the HECC regime may have important implications for matching emissions (*i.e.*, the combustion process) to aftertreatment. Mixed-source EGR is a reasonable method for achieving the

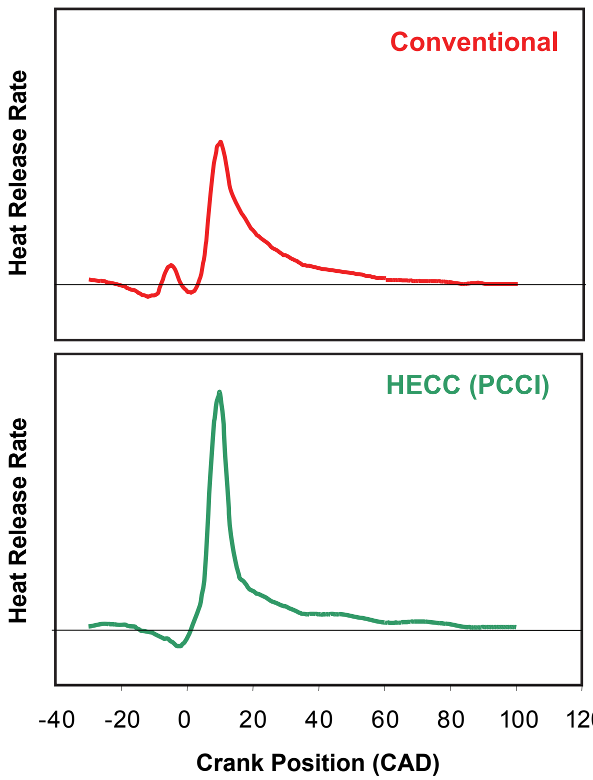

FIGURE 2. Example Heat Release Profiles for Conventional and HECC Operation at 1,500 RPM, 2.6 bar BMEP

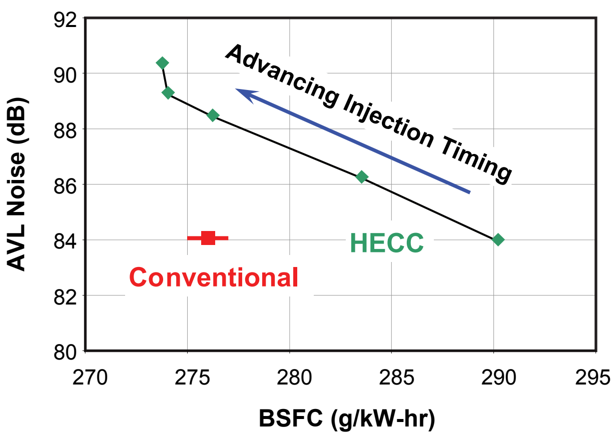

FIGURE 3. Combustion Noise and BSFC Relationship for Conventional and HECC Operation at 1,500 RPM, 2.6 bar BMEP

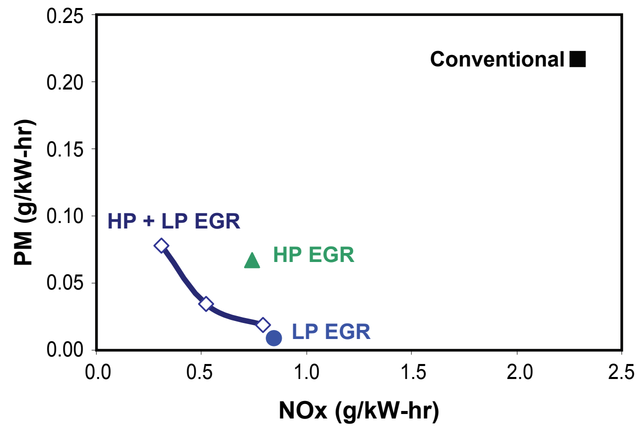

FIGURE 4. Comparison of NOx and PM Emissions with Intake Mixture Temperature Maintained Constant at ~50°C for HECC Operation at 2,300 RPM, 4.2 bar BMEP

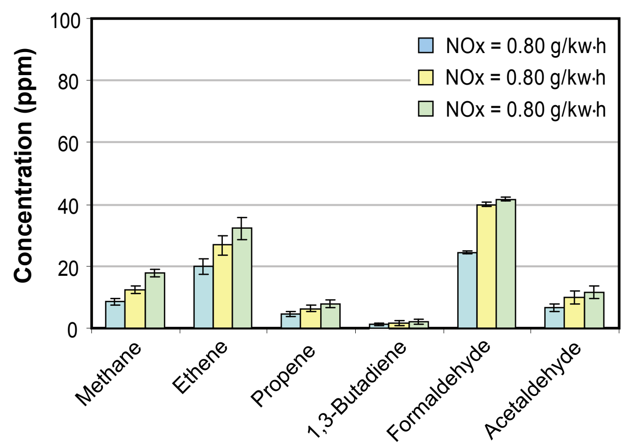

FIGURE 5. Light HC Species and Aldehyde Compounds with Intake Temperature Maintained Constant at ~50°C for HECC Operation at 2,300 RPM, 4.2 bar BMEP

necessary precise control of dilution in real-world applications to take advantage of this NOx-PM relationship. Light hydrocarbon (HC) species and aldehyde compounds were also measured for the mixed-source EGR experiments and are shown in Figure 5. The results indicate an increase in methane, alkenes, and aldehyde compounds accompany a reduction in NOx emissions. This is consistent with a decrease in overall combustion temperature due to higher dilution of the combustion charge. A similar trend was observed for the 1,500 rpm, 2.6 bar BMEP condition.

Mixed source EGR was also used to investigate the effect of intake mixture temperature on PM emissions while maintaining a constant NOx emissions level. An example of this is shown in Figure 6 for the 2,300 rpm, 4.2 bar BMEP condition. An analysis of the accompanying heat release data indicates the reduction in PM with decreasing intake mixture temperature is most likely the result of a longer ignition delay and correspondingly a larger premixed burn fraction. Light HC species and aldehyde compounds are summarized in Figure 7 for theses experiments. An increase in these compounds was observed for decreasing intake mixture temperature. The higher concentrations at lower intake temperatures are most likely the result of lower bulk cylinder temperature which results in a larger quenching

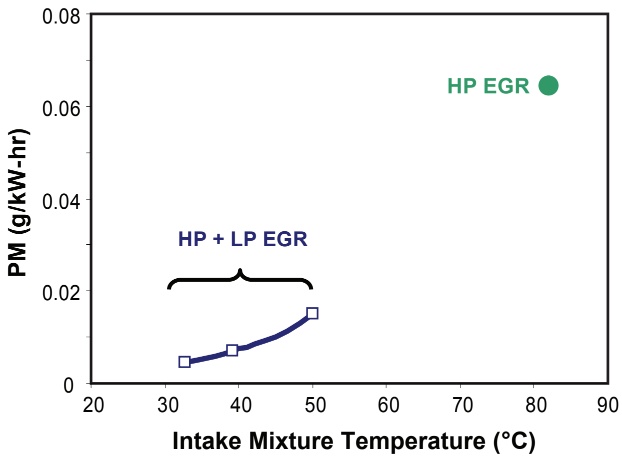

FIGURE 6. PM Emissions as a Function of Intake Mixture Temperature for Constant Engine-Out NOx of ~77 ppm for HECC Operation at 2,300 rpm, 4.2 bar BMEP

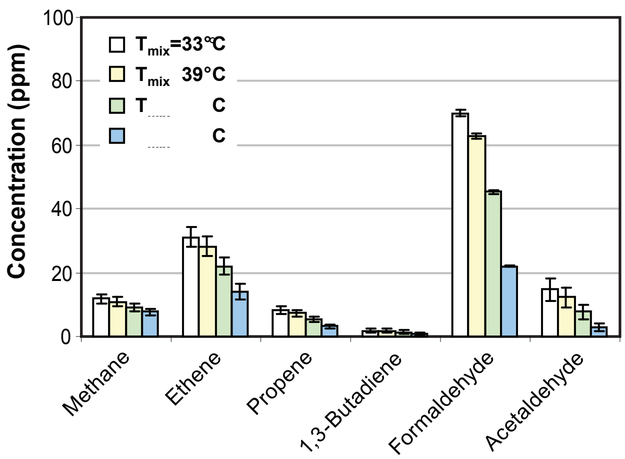

FIGURE 7. Light HC species and aldehyde compounds as a function of intake mixture temperature for constant engine-out NOx of ~77 ppm for HECC Operation at 2,300 RPM, 4.2 bar BMEP

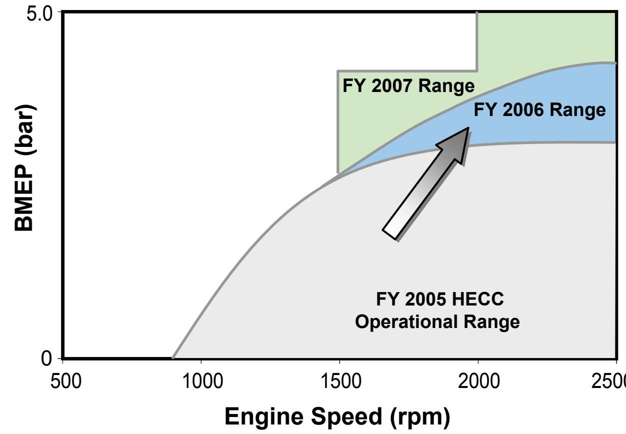

FIGURE 8. Speed-Load Range Expansion of HECC Operation Accomplished with Improved Control of Intake Mixture Temperature

volume. A similar trend was observed for the 1,500 rpm, 2.6 bar BMEP condition.

The mixed-source EGR HECC data summarized in the previous discussion does not always adhere to the strict definition of HECC used by ORNL. The LPL EGR method often has a BSFC penalty which is mostly dominated by the increase in backpressure (and corresponding increase in pumping losses) associated with the catalyzed diesel particulate filter (cDPF). The cDPF was not regenerated between each experiment and therefore the exhaust backpressure on the engine was not constant across the experimental matrix. The effect on BSFC is discussed in more detail in an upcoming SAE paper which has been submitted for the 2008 SAE Congress.

Expansion of the speed-load range for HECC operation is important for reducing aftertreatment requirements and ultimately increasing the overall engine system efficiency. To this end, an effort was undertaken to investigate expansion of the HECC operational range with increased heat rejection of the HPL EGR system. This allowed for an extension of the upper range of the HECC operating envelope which is shown in Figure 8. BSFC values for the HECC conditions represented in this figure are similar to those observed for the original equipment factory conditions.

Due to the concise nature of this report, we were not able to discuss all of the research performed during this activity in FY 2007. Please see the publications/presentations list for more information.

Conclusions

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

- Characterized relationship between combustion noise level and BSFC for HECC operation. Increases in noise level make efficient operation a challenge in LTC modes.
- Improved cooling (*i.e.*, heat rejection) of the HPL EGR systems allows for an incremental improvement in expanding the HECC speed-load operational range.
- Mixed-source EGR has the potential for precise control of intake mixture temperature and dilution for more robust HECC operation and improved matching with aftertreatment systems.

- A GM 1.9-L engine with a flexible control system was commissioned at ORNL and will be the primary research platform for subsequent HECC research. This engine geometry is being used at Sandia National Laboratories (optical single-cylinder engine), Lawrence Livermore National Laboratory (modeling), and the University of Wisconsin (metal single- and multi-cylinder engines) and has resulted in improved collaboration in DOE funded activities in support of meeting FreedomCAR efficiency and emissions milestones.

FY 2007 Publications/Presentations

1. *Submitted.* K. Cho, M. Han, R. M. Wagner, C. S. Sluder, " Mixed-Source EGR for Enabling High Efficiency Clean Combustion Modes in a Light-Duty Diesel Engine", 2008 SAE Congress & Exposition (Detroit, MI; April 2008).

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

3. R. M. Wagner et al., "Modeling and Experiments to Achieve High-Efficiency Clean Combustion (HECC) in LD Diesel Engines", Advanced Combustion & Emissions Control Technical Team meeting (Southfield, MI; July 2007).

4. R. M. Wagner et al., "Modeling and Experiments to Achieve High-Efficiency Clean Combustion (HECC) in LD Diesel Engines", 2007 Department of Energy (DOE) Advanced Combustion Engines Merit Review (Washington, D.C.; June 2007).

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

Special Recognitions & Awards/Patents Issued

1. FreedomCAR Technical Highlight in 2007.

2. J. B. Green, C. S. Daw, R. M. Wagner, "Combustion Diagnostic for Active Engine Feedback Control"; United States patent number 7,277,790 B1.

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

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Gurpreet Singh

Objectives

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

Approach

- Adhere to strict algorithmic and implementation requirements for LES with emphasis placed on accuracy and application of science-based subgrid-scale models.
- Focus on state-of-the-art engine systems and geometries with emphasis placed on establishing an enhanced understanding of turbulence-chemistry interactions.
- Provide scientific foundation for advanced model development with emphasis placed on local, unsteady, intricately coupled in-cylinder processes, i.e.,
  - Flame structure, stability and effects of stratification,
  - Local extinction, re-ignition and auto-ignition, and
  - Pollutant emissions and soot formation.

Accomplishments

- Completed infrastructure and preprocessor modifications to make calculations routine.
  - Computational Combustion and Chemistry Laboratory for IC-engine research installed, tested and operational (256 processor Beowulf cluster).
  - Commercial grid generation capability established (ANSYS ICEM) and interfaced with the CRF LES code.
  - Implementation of tension-splines designed and tested to provide an efficient mesh movement capability in full IC-engine geometries (ports, valves, piston).
- Performed systematic model validation of two fundamental combustion models in collaboration with the DOE Office of Science (see Barlow et al., www.ca.sandia.gov/tnf).
  - Stochastic Reconstruction Model ("science-based").
  - Tabulated Linear Eddy Model ("engineering-based").
- Continued sequence of calculations focused on CRF optical hydrogen internal combustion engine (H_2-ICE) in collaboration with C. White and S. Kaiser (see related annual report).
  - Moved to treatment of direct-injection processes (several prerequisite tasks required to achieve this goal).
  - Initiated studies focused on H_2-injector pattern optimization (Collaboration with Ghandhi et al., University of Wisconsin).
- Systematically extended effort toward treatment of LTC engine processes.
  - Simulation of the effect of spatial fuel distribution using the Linear Eddy Model.
  - LES of direct injection processes for diesel and LTC engine applications (see Pickett et al., www.ca.sandia.gov/ecn).

Future Directions

- Continue high-fidelity simulations of the optical H_2-ICE.
  - Direct-injection with new head, match experimental activities.
  - Validation through comparison of measured, modeled results.
    - Chemiluminescence imaging and particle image velocimetry (PIV)
    - Planar laser induced fluorescence (PLIF)

- Joint analysis of data extracted from validated simulations.
  - Enhance basic understanding
  - Improve engineering models
  - H_2-injector pattern optimization
- Systematically extend to homogeneous charge compression ignition (HCCI) engine experiments.
  - Perform detailed studies of LTC processes.
  - Work toward treatment of complex hydrocarbon processes.
- Continue leveraging between DOE Office of Science (OS) and Energy Efficiency and Renewable Energy (EERE) activities.
  - Detailed validation, analysis of key combustion phenomena.
  - Access to high-performance "leadership-class" computers.

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Introduction

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

To establish a scientific foundation for technology breakthroughs in transportation fuel utilization, the DOE Office of Basic Energy Sciences (BES) convened a workshop entitled "*Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels"* from October 30 to November 1, 2006 (www.sc.doe.gov/bes/reports/files/CTF_rpt.pdf). Execution of the workshop involved advance coordination with the DOE Office of EERE, FreedomCAR and Vehicle Technologies (FCVT) program, which manages applied research and development of transportation technologies. Results provide the collective output from over 80 leading scientists and engineers representing academia, industry, and national laboratories in the United States and Europe. Panels were convened to identify priority research directions in the area of novel combustion for new engine technologies, utilization challenges of alternative fuels in these systems, crosscutting science themes and gaps in our understanding of combustion processes related to 21st century fuels. Panel leads distilled the collective output to produce eight distinct targeted research areas required to advance the single overarching grand challenge of developing "*a validated, predictive, multiscale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications*." This project targets the research issues identified for multiscale simulation and modeling of IC-engine processes.

Approach

As part of the *Reacting Flow Research* and *Advanced Engine Combustion* programs at the CRF, we have developed a high-fidelity, massively-parallel simulation framework that is capable of performing both direct numerical simulation (DNS) and LES of reacting flows in complex geometries. Two complementary projects have been established. The first is funded under the DOE OS, BES program, and focuses on LES of turbulence-chemistry interactions in reacting multiphase flows. The second is funded under the DOE Office of EERE, FCVT program, and focuses on the application of LES to low-temperature and hydrogen engine combustion research. Objectives and milestones for both projects are aimed at establishing high-fidelity computational benchmarks that match the geometry and operating conditions of key target experiments using a single unified theoretical-numerical framework. The projects are complementary in that the OS-BES activity provides the basic science foundation for detailed model development and the EERE-FCVT activity provides the applied component for advanced engine research.

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

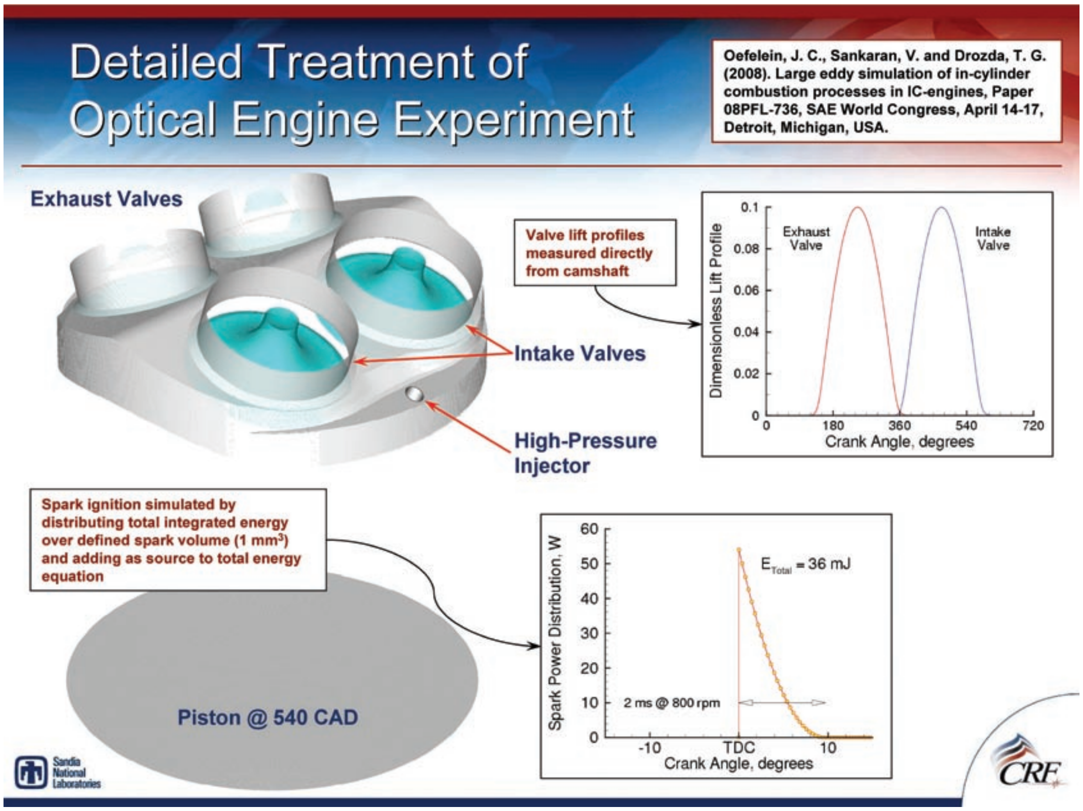
Results

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

LES of the CRF Optically Accessible Hydrogen-Fueled IC-Engine: Objectives related to this milestone are to perform benchmark simulations of the CRF optically accessible H_2-ICE shown in Figure 1a. Our primary goal is to provide a detailed understanding regarding optimal injection strategies and the three-dimensional characteristics of in-cylinder combustion processes. A series of staging studies in FY 2006 and FY 2007 have established our baseline capability for performing the simulations. The time-dependent grid has been designed and optimized, preliminary validation of the combustion models has been established, and initial comparisons with available experimental data have been performed. We have now advanced to the treatment of direct-injection (DI) processes, which is the operational mode of choice for development of a highly efficient engine cycle using hydrogen as the fuel. The LES calculations currently in progress will provide the most resolved high-fidelity results of in-cylinder combustion processes to-date. Our analysis is focused on multidimensional turbulence-chemistry interactions and related cycle-to-cycle variations. The simulations are coordinated with the experimental campaign at the CRF, which has similar goals using advanced imaging techniques in the optical engine but is limited to two-dimensional planes. Results from these calculations will provide a clear understanding of the power density limitations associated with hydrogen-fueled engine cycles, maximum fuel efficiency, NOx emissions, turbulent mixing characteristics, and the effects of mixture stratification as a function of local processes over full engine cycles.

LES of Direct Injection Processes for Hydrogen and Low-Temperature Combustion Applications: As a subset of the task outlined above, we have established an initial benchmark series of simulations aimed at understanding high Reynolds number, high-pressure, direct-injection processes for hydrogen and low-temperature engine applications (see Figure 1b). High-fidelity representations of direct injection processes in IC-engines are an essential component toward the development a validated predictive modeling capability. Direct injection of hydrogen at high-pressure conditions, for example, has emerged as a promising option for improving fuel economy and emissions in H_2-ICEs. Gaseous injection technology, however, is relatively new and there is only limited information on optimal configurations. Similarly, direct-injection of liquid fuels for low-temperature engine applications such as HCCI has many advantages, but detailed time-accurate models are still lacking. To address these issues, we have initiated a series of benchmark calculations that identically match key experimental efforts. Data from these experiments are being used for validation. Figure 1b shows an example result from LES compared to the shadowgraph data of Petersen and Ghandhi (University of Wisconsin). This represents the initial starting point to study a series high-pressure gas injectors designed for use in H_2-ICEs. We will also focus on issues related to liquid jet breakup using the case studies provided by Pickett et al. (www.ca.sandia.gov/ECN).

LES of In-Cylinder Homogeneous-Charge Compression-Ignition Engine Processes: The potential benefits of HCCI engine cycles and key technical barriers have been well established. Ignition timing must be controlled over a wide range of speeds and loads. The rate of heat release due to combustion must be limited to allow high-load operation. Smooth operation through rapid transients must be maintained. A robust cold-start capability must be developed. Finally, hydrocarbon and carbon monoxide emissions standards must be met. Overcoming these barriers requires an improved understanding of in-cylinder HCCI processes



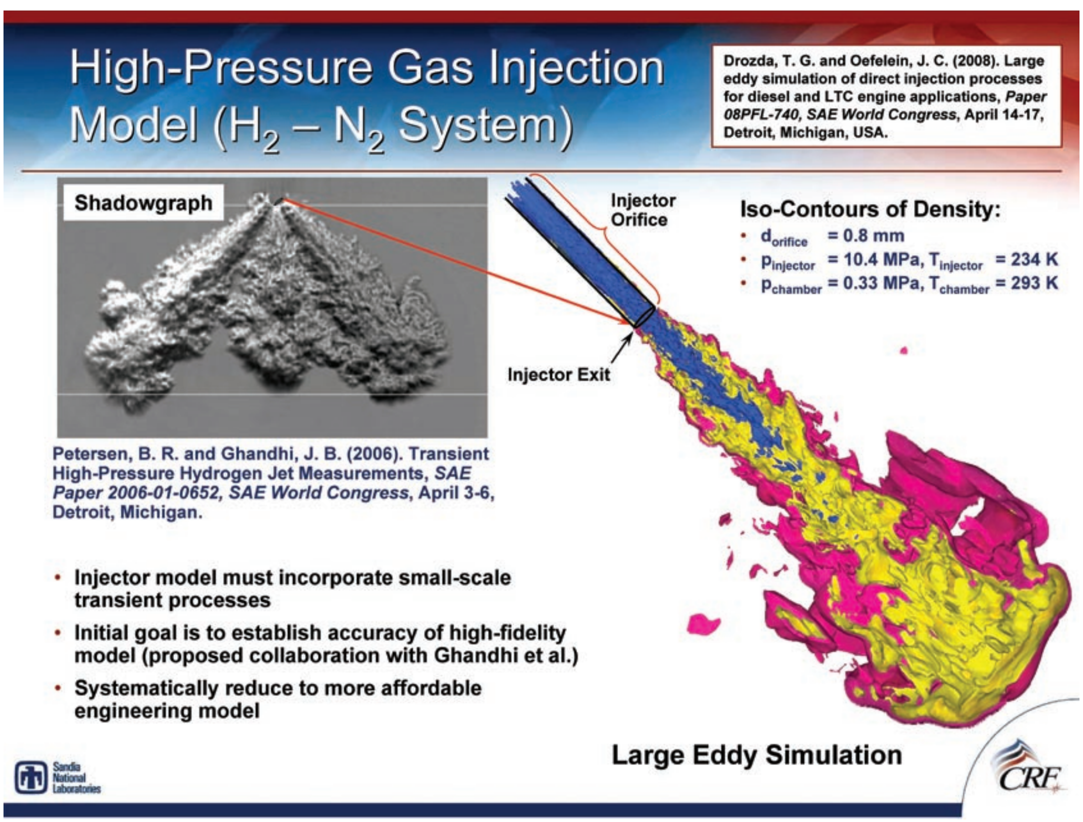


FIGURE 1. Images (top) show the LES grid surface topology and related details for calculations of the CRF optically accessible hydrogen-fueled IC-engine. Images (bottom) show the corresponding high-pressure injector dynamics simulated in this engine, with results compared to the shadowgraph data of Peterson and Ghandhi (University of Wisconsin).

combined with an understanding of how the coupled effect of these processes can be favorably altered using appropriate control mechanisms. Using the same approach as that described above for the H_2-ICE, we have begun a series of LES calculations that complement ongoing HCCI engine research. Initial emphasis has been placed on the optically accessible research engine developed at the CRF. Research conducted by Steeper et al. (see FY 2007 Publications) has provided an initial baseline for implementation of our combustion models using n-heptane as the fuel.

Conclusions

Future work will be focused both on hydrogen fuel injector pattern optimization and on the critical needs and challenges associated with the use of hydrogen as a fuel. These needs include obtaining a clearer understanding of power density limitations, maximum fuel efficiency, in-cylinder NOx formation, turbulent mixing characteristics, turbulence-chemistry interactions, and the effects of mixture stratification as a function of local in-cylinder processes over full engine cycles. Information from the simulations, combined with detailed laser-based experiments at well-defined target conditions, will provide the science-base needed by engine companies to develop fuel efficient, low-emissions H_2-ICEs. Through interdisciplinary leveraging with other projects, we will continually perform assessments of the base model and select chemical kinetics mechanisms to: 1) verify that the chemical mechanisms selected for the IC-engine work are capable of representing important phenomena such as ignition and extinction, and 2) build a validated level of confidence in the overall accuracy of the coupled LES model framework.

FY 2007 Publications/Presentations

1. J. C. Oefelein, V. Sankaran and T. G. Drozda (2008). Large eddy simulation of in-cylinder combustion processes in IC-engines, *paper 08PFL-736, SAE World Congress*, April 14–17, Detroit, MI.

2. T. G. Drozda and J. C. Oefelein (2008). Large eddy simulation of direct injection processes for diesel and LTC engine applications, *paper 08PFL-740, SAE World Congress*, April 14–17, Detroit, MI.

3. T. G. Drozda, G. Wang, V. Sankaran, J. R. Mayo, J. C. Oefelein and R. S. Barlow (2007). Scalar filtered mass density functions in nonpremixed turbulent jet flames, *Submitted to Combustion and Flame*.

4. R. R. Steeper, V. Sankaran, J. C. Oefelein and R. P. Hessel (2007). Simulation of the effect of spatial fuel distribution using a linear eddy model, *paper 07FFL-186, SAE Powertrain & Fluid Systems Conference and Exhibition*, October 29-November 1, Chicago, IL.

5. P. K. Tucker, S. Menon, C. L. Merkle, J. C. Oefelein and V. Yang (2007). An approach to improved credibility of CFD simulations for rocket injector design, *paper 2007-5572, 43rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit*, July 8-11, Cincinnati, OH.

6. T. G. Drozda, G. Wang, V. Sankaran, J. R. Mayo, J. C. Oefelein and R. S. Barlow (2007). Scalar filtered mass density functions in nonpremixed turbulent jet flames, *Proceedings of the 5th US Joint Meeting of the Combustion Institute*, March 25-28, San Diego, CA.

7. V. Sankaran and J. C. Oefelein (2007). Advanced preconditioning strategies for chemically reacting flows, *Paper 2007-1432, 45th AIAA Aerospace Sciences Meeting & Exhibit*, January 8-11, Reno, NV.

8. T. C. Williams, R. W. Schefer, J. C. Oefelein and C. R. Shaddix (2007). Idealized gas turbine combustor for performance research and validation of large eddy simulations, *Review of Scientific Instruments*, 78(035114): 1-9.

9. J. C. Oefelein, V. Sankaran and T. G. Drozda (2006). Large eddy simulation of swirling particle-laden flow in a model axisymmetric combustor, *Proceedings of the Combustion Institute*, 31: 2291-2299.

10. J. C. Oefelein (2006). Large Eddy Simulation of mixing and combustion for direct-injection operation. *European Commission HyICE Program: Optimization of a hydrogen powered internal combustion engine*, Project 506604, Chapter D4.3.G: 1-18.

11. J. C. Oefelein, T. G. Drozda and V. Sankaran (2006). Large Eddy Simulation of Turbulence-Chemistry Interactions in Reacting Flows: The Role of High-Performance Computing and Advanced Experimental Diagnostics, *Journal of Physics*, 46: 16-27.

12. J. C. Oefelein (2006). Large eddy simulation of turbulent combustion processes in propulsion and power systems. *Progress in Aerospace Sciences*, 42: 2-37.

Presentations at Conferences and Project Meetings

1. BES 27th Annual Combustion Research Meeting, Wintergreen, VA, Jun. 06.

2. SciDAC 2006, Denver CO, Jun. 06.

3. 42nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Sacramento, CA, Jul. 06.

4. 8th TNF Workshop, Heidelberg, Germany, Aug. 06.

5. 31st International Symposium on Combustion, Heidelberg, Germany, Aug. 06.

6. Penguin Computing Advisory Board Meeting, San Francisco CA, Sep. 06.

7. AFOSR Contractors Meeting, Annapolis, MD, Sep. 06.

8. AFRL Rocket Modeling Workshop, Annapolis, MD, Sep. 06.

9. CRF Advisory Board, Livermore, CA, Nov. 06.

10. 45th AIAA Aerospace Sciences Meeting, Reno NV, Jan. 07.

11. Advanced Engine Combustion and HCCI Working Group Meeting, Livermore, CA, Feb. 07.

12. CRF Diagnostics and Reacting Flow Peer Review, Livermore, CA, Mar. 07.

13. SERDP Project Meeting on Predicting the Effects of Fuel Composition and Flame Structure on Soot Generation in Turbulent Nonpremixed Flames, San Diego, CA, Mar. 07.

14. 5th US Joint Sections Meeting of the Combustion Institute, San Diego, CA, Mar. 07.

15. Multi-Agency Workshop on Next Steps in Development of a Cyber Infrastructure for Combustion, San Diego, CA, Mar. 07.

16. Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security, 1st Town Hall Meeting, LBL, Apr. 07.

17. DOE Merit Review of Advanced Combustion, Emissions & Fuels Research, Washington, D.C., Jun. 06.

II.A.7 Detailed Modeling of Low Temperature Combustion and Multi-Cylinder HCCI Engine Control

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DOE Technology Development Manager: Gurpreet Singh

Subcontractors:
- University of California, Berkeley, CA
- University of Wisconsin, Madison, WI

Objectives

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

Accomplishments

- Developed methodologies for experimental measurement of 40 hydrocarbon species in HCCI engine exhaust.
- Demonstrated high fidelity modeling of the Sandia HCCI engine (John Dec), including unprecedented prediction of 40 measured intermediate hydrocarbon species.
- Demonstrated innovative control strategies and applied them to the Caterpillar 3406 experimental HCCI engine, demonstrating optimum engine performance and fast transient response.

Future Directions

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

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Introduction

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

Approach

Our approach is to collaborate with national laboratories and universities conducting experimental work as a part of DOE's Advanced Combustion in Engines (ACE) Program. Our role in these collaborations is to provide analytical support that complements the very high quality experimental work being conducted at other locations. Although most collaboration to date is HCCI/PCCI centric due to the great importance of these combustion modes, we are working on extending our work to other areas of interest to the DOE ACE Program, such as low-temperature combustion and hydrogen engines. We have also performed key experiments described in this report: exhaust speciation and advanced engine control.

Results

Engine experiments are typically limited to measurement of pressure and emissions of nitrogen oxide, carbon monoxide, and hydrocarbons. Hydrocarbon emissions are typically reported as "total," even though instruments (i.e., flame ionization detectors) do not detect, or only partially detect, oxygenated hydrocarbons.

Recently we teamed up with John Dec from Sandia Livermore to conduct very careful HCCI experiments at low- to mid-loads [1]. In addition to the typical engine measurements, we determined the exhaust composition by measuring the concentration of 40 hydrocarbon species in the exhaust.

Detailed measurement of exhaust composition is a complex process that starts with the collection of exhaust gases in Tedlar® bags that have previously been prepared by three successive evacuations and purgings with dry nitrogen. Two separate bag samples were collected for each operating condition: one for the C1-C2 hydrocarbons, and the other for the remaining species. The C1-C2 hydrocarbons were analyzed by direct injection of exhaust gases into an Agilent 6890 gas chromatograph and detected with a flame ionization detector. Fixed gas standards were used for calibration. All other hydrocarbons and oxygenated hydrocarbons were analyzed using an HP5890/5972MSD gas chromatography mass spectrometry (GC/MS). A Tedlar® bag sample and a 25 ml gas-tight syringe were first heated in an oven to 60°C. A 25 ml sample was drawn into the syringe and subsequently injected directly into a heated glass tube purged with a 25 cc/min high purity helium flow. The helium swept the sample onto an adsorbent comprising a mixture of Carbopak B and carboxen (Supelco VOCARB 3000). After 20 minutes the trap was heated to 250°C and the adsorbed species were concentrated onto the head of the GC column using the helium flow. Compound separation was facilitated using a DB-502 capillary column heated from 35°C to 250°C at 5°C/min and held for 10 minutes. Injector temperature and detector temperature were held at 225°C and 250°C, respectively. Standards were prepared by injecting 1-5 microliters of authentic standards into a Tedlar® bag filled with dry nitrogen and analyzed using the same method. Formaldehyde and acetaldehyde are not properly detected by the GC/MS, and therefore separate samples were collected using a dinitrophenylhydrazine derivatizing solution. After careful sample preparation, aldehyde concentration was measured with a ThermoFinnigan Survey high performance liquid chromatograph.

Detailed measurement of hydrocarbon species in the exhaust of HCCI engines is important for the design of low-temperature oxidizing catalysts and for determining optimum strategies for low power or idle engine operation. In addition to their practical importance, speciation experiments represent a unique opportunity to put our HCCI models to the test. We are confident in the ability of our models to accurately characterize the combustion event. However, trying to predict exhaust composition down to the small hydrocarbon species is a challenge, because these species are intermediate products of combustion that are generated and then consumed as the fuel breaks apart in a chemical kinetic cascade that starts with fuel and (ideally) ends with carbon dioxide. Accurately predicting these small species requires a good characterization of both the formation as well as the destruction of these species in a transient temperature field continuously modified by chemical heat release and turbulent fluid mechanics.

We analyzed the Sandia exhaust speciation experiments with our multi-zone parallel version of the KIVA code (KIVA-MZ-MPI) [2]. We took on the difficult challenge of accurately predicting exhaust composition by making a very detailed mesh that includes cylinder features seldom modeled, such as the gasket crevice and the space behind the top ring (Figure 1). We took advantage of the careful engine measurements to determine appropriate initial conditions (pressure and temperature at intake valve

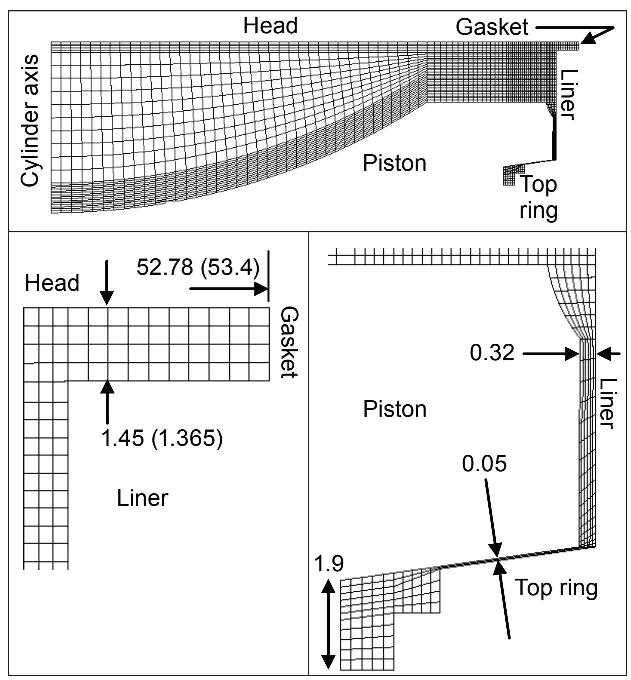

FIGURE 1. Top: Mesh of Computational Domain at Top Dead Center; Left: Head Gasket Volume; Right: Piston/Liner Crevice (Dimensions are mm)

closing) and boundary conditions (wall temperatures) as a function of equivalence ratio.

As expected, our model demonstrates good agreement with experimental pressure traces and heat release rates. In addition to this, we were also able to accurately calculate exhaust composition as a function of equivalence ratio. Figure 2 shows predicted and measured values of the main hydrocarbon species.

This year we also demonstrated the application of advanced control technology for optimizing HCCI engine efficiency. These experiments were conducted in our Caterpillar 3406 engine previously converted to HCCI mode, and were recently reported in *Mechanical Engineering* magazine [3].

Engine operation is typically optimized with a mapping procedure. At each operating point, multiple spark timings (or fuel injection timings for a diesel engine) are tried. The optimal combustion timing is then determined from the mapping data. This procedure is time and labor intensive, because many engine runs are required for mapping the desired region of operation. The process is even more involved for HCCI engines that lack an ignition trigger and require tuning of intake temperature and pressure to achieve the desired combustion timing.

We applied an innovative method to speed up this process: extremum seeking, which is a non-model-based real-time optimization method that iteratively modifies the input of a system such that a desired performance metric reaches a local optimal value. Extremum seeking differs from conventional optimization methods; it performs a non-model based parameter search, which is independent of whether the system is linear or has significant nonlinearities.

For the engine application, extremum seeking determines the combustion timing that minimizes the HCCI engine's fuel consumption. Figure 3 shows that extremum seeking delays the combustion timing from 3 degrees to approximately 9 crank angle degrees after top dead center while simultaneously reducing fuel consumption by more than 10%.

Conclusions

- We have contributed to unprecedented characterization of HCCI engine performance by measuring concentration of 40 hydrocarbon species in the exhaust.
- We have applied our parallel multi-zone KIVA code (KIVA-MZ-MPI) to make accurate predictions of exhaust composition as a function of equivalence ratio.
- Experiments conducted on our Caterpillar 3406 HCCI engine demonstrated the applicability of advanced control methodologies for fast optimization of engine performance.

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1. Analysis of Homogeneous Charge Compression Ignition (HCCI) Engines for Cogeneration Applications, Salvador M. Aceves, Joel Martinez-Frias, Gordon M. Reistad, Proceedings of the ASME Advanced Energy Systems Division, 2004, Journal of Energy Resources Technology, Vol. 128, pp. 16-27, 2006.

2. Gaseous Fuel Injection Modeling using a Gaseous Sphere Injection Methodology, Randy P. Hessel, Salvador M. Aceves, Daniel L. Flowers, SAE Paper 2006-01-3298, 2006.

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

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

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

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

7. Overview of Modeling Techniques and their application to HCCI/CAI Engines, Salvador M. Aceves, Daniel L. Flowers, Robert W. Dibble, Aristotelis Babajimopoulos, in HCCI and CAI Engines for the Automotive Industry, Edited by Hua Zhao, CRC Press, Woodhead Publishing Limited, Chapter 18, pp. 456-474, 2007.

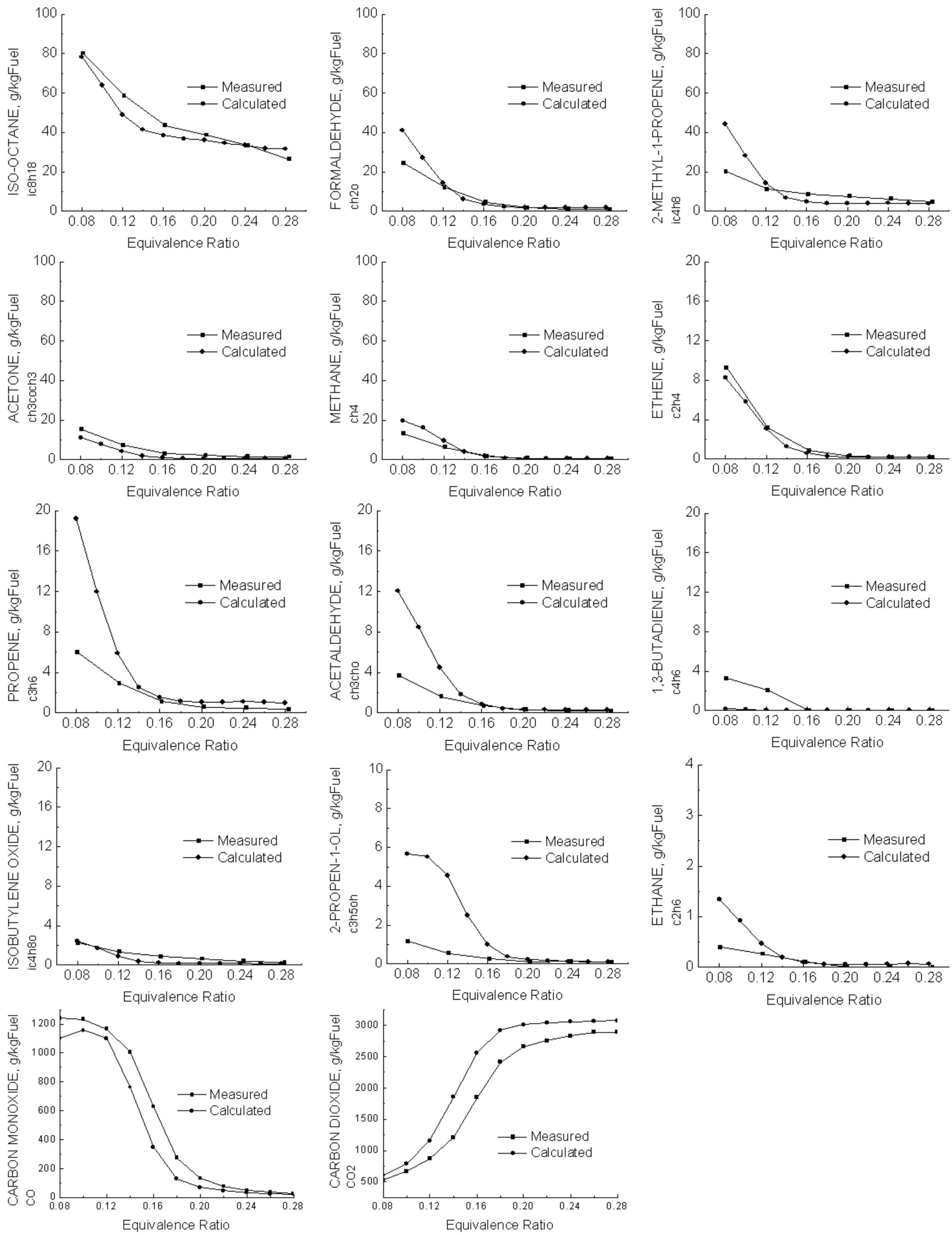

FIGURE 2. Measured and Calculated Species Concentrations as a Function of Equivalence Ratio for the Sandia HCCI Engine

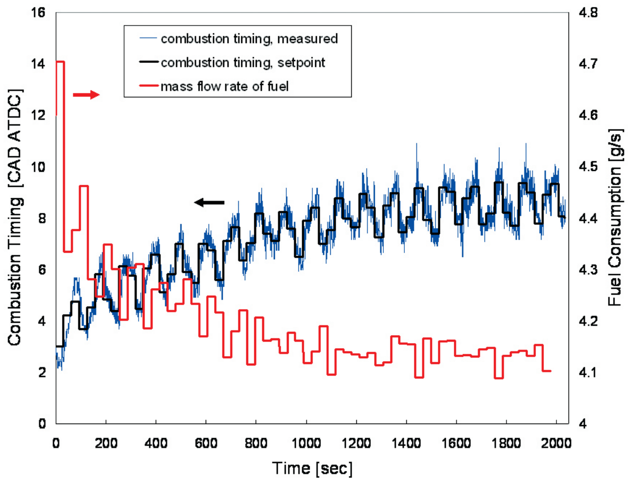

FIGURE 3. Use of extremum seeking for minimization of HCCI engine fuel consumption. Extremum seeking delays combustion timing from 3 degrees to 9 degrees after top dead center, reducing fuel consumption by more than 10%.

8. Improving Ethanol Life Cycle Energy Efficiency by Direct Utilization of Wet Ethanol in HCCI Engines, Joel Martinez-Frias, Salvador M. Aceves, Daniel L. Flowers, Paper IMECE2005-79432, Proceedings of the ASME International Mechanical Engineering Congress and Exhibition, 2005, Accepted for Publication, Journal of Energy Resources Technology.

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

10. Extremum Seeking Tuning of an Experimental HCCI Engine Combustion Timing Controller, Nick Killingsworth, Dan Flowers, Salvador Aceves, Miroslav Krstic, Proceedings of the American Control Conference, New York, NY, July 2007.

11. In Pursuit of New Engine Dynamics, Daniel Flowers, Nick Killingsworth and Robert Dibble, Mechanical Engineering, pp. 20-21, July 2007.

12. A Numerical Investigation into the Anomalous Slight NOx Increase when Burning Biodiesel: A New (Old) Theory, George A. Ban-Weiss, J.Y. Chen, Bruce A. Buchholz, Robert W. Dibble, Fuel Processing Technology, Vol. 88, pp. 659-667, 2007.

Special Recognitions & Awards/Patents Issued

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

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

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

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DOE Technology Development Manager:
Gurpreet Singh

Objectives

Project Objective:

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

FY 2007 Objectives:

- Investigate the effects of exhaust gas recirculation (EGR)/residuals and its constituents on combustion phasing for single- and two-stage-ignition fuels (*i.e.* gasoline-like and diesel-like fuels, respectively).
- Apply chemiluminescence spectroscopy and chemical-kinetic analysis to investigate how HCCI progresses through the autoignition/combustion event, for both one- and two-stage fuels.
- Investigate various techniques to improve fuel/air mixture formation for stratified HCCI at low loads to increase combustion efficiency.
- Support chemical-kinetics and computational fluid dynamics (CFD) modeling work at Lawrence Livermore National Laboratory (LLNL) to help develop improved kinetic mechanisms and advance the understanding of in-cylinder processes.

Accomplishments

- Determined the effects of EGR/residuals and its constituents on combustion phasing for single- and two-stage fuels.
- Showed how HCCI combustion progresses through various phases of autoignition, main combustion, and burnout using a combination of chemiluminescence spectroscopy and chemical-kinetic analysis.
- Investigated several fuel-stratification techniques to improve combustion efficiency at low loads, using a combination of metal-engine performance data and fuel planar laser induced fluorescence (PLIF) imaging.
  – Demonstrated 92.5% combustion efficiency at an idle fueling of $\phi = 0.12$.
- Initiated an improved, detailed exhaust-speciation study to determine the effects of changes in fueling rate, and fuel-stratification at low loads, on emissions (with LLNL).
- Supported chemical-kinetic and CFD modeling work at LLNL, and CFD modeling at the University of Wisconsin by providing data, analysis, and discussions for 1) improving primary reference fuel (PRF) kinetic mechanisms and 2) CFD/kinetic modeling of performance and emissions.

Future Directions

- Conduct an investigation of the potential of EGR/residuals for slowing the pressure-rise rate (PRR) at high loads to further extend the upper-load limit of HCCI.
  – Eliminate the combustion-phasing effects of EGR to correctly evaluate its effect on PRR.
- Investigate the development of thermal stratification and its distribution in the bulk gases during the latter-compression and early-expansion strokes using PLIF imaging.
- Complete detailed exhaust-speciation study over a range of fueling rates and for mixture stratification at low loads for iso-octane and gasoline (with LLNL).
- Determine the effects of ethanol and/or ethanol-gasoline blends on HCCI performance for well-mixed and mixture-stratified operation.
- Complete development and validation of an electro-hydraulic variable valve actuation system, and begin studies of techniques to control HCCI such as late intake valve closing and negative valve overlap.
- Work cooperatively with LLNL on CFD modeling to better understand the sources of HCCI emissions, and continue to support chemical-kinetic model development at LLNL.

Introduction

HCCI engines have significant efficiency and emissions advantages over conventional spark-ignition and diesel engines, respectively. However, several technical barriers must be addressed before it is practical to implement HCCI combustion in production engines. As outlined under the accomplishment bullets above, studies have been conducted over the past year that provide new understanding related to overcoming three of these technical barriers: combustion-phasing control, fuel effects, and poor combustion efficiency at low loads. Addressing these respective barriers, our main studies for FY 2007 included: 1) the use of EGR to control combustion phasing over the load-speed map, 2) an improved understanding of the steps of HCCI autoignition and combustion for various fuels, and 3) techniques for improving combustion efficiency at low loads and reducing CO and HC emissions.

Approach

These studies were conducted in our dual-engine HCCI laboratory using a combination of experiments in both the all-metal and optically accessible HCCI research engines. This facility allows operation over a wide range of conditions, and can provide precise control of operating parameters such as combustion phasing, injection timing, intake temperature and pressure, and mass flow rates of supplied fuel and air. The laboratory is also equipped to meter N_2, CO_2 and H_2O vapor into the intake stream to simulate the addition of combustion products, *i.e.* EGR.

To study the effects of EGR and its constituents on combustion phasing, simulated EGR or its individual constituents were metered into the intake air, while engine performance and emission data were acquired using conventional cylinder-pressure and exhaust-emissions diagnostics. In addition, a cooled EGR loop was added to allow comparison of real and simulated EGR, as a method to determine the effects of trace species in the real EGR.

The investigation of the phases of HCCI autoignition and combustion for various fuels involved metal engine performance experiments followed by detailed studies of the combustion event in the optical engine. Calibrated chemiluminescence spectroscopy provided information on the key chemiluminescence species and the nature of the reactions. A chemical-kinetic analysis was also conducted to better understand the key reactions of each phase of autoignition and combustion, and the differences between single- and two-stage-ignition fuels.

Several fuel-stratification techniques were investigated to improve HCCI combustion efficiency at low loads. A combination of metal-engine performance data and PLIF imaging of the fuel distributions in the optical engine was used to determine the combustion efficiencies and to understand the reasons for the improvements or lack of improvements for the various techniques. As part of this investigation, a new PLIF image analysis technique was developed to account for the local cooling effect of fuel stratification, which can cause errors of up to 40% in the fuel concentration if no correction is applied.

In addition to these investigations, other efforts involved working cooperatively with external organizations. These efforts included: providing data to and working with both chemical-kinetic and CFD modeling groups at LLNL, CFD modelers at the University of Wisconsin, an analytical chemistry group at LLNL for detailed exhaust-species measurements, and continued interactions with the International Truck and Engine Co. on the development of a variable valve actuation system.

Results

EGR and high levels of retained residuals are widely used in HCCI engines to help control combustion phasing. However, the underlying causes are not well understood because exhaust gases can affect HCCI autoignition in multiple ways, and these effects vary with fuel-type. Therefore, an investigation was conducted into the effects of EGR and its constituents for representative single-stage-ignition fuels, iso-octane and gasoline, and two-stage-ignition fuels, PRF80 and PRF60 (80-20% and 60-40% blends of iso-octane and *n*-heptane, respectively) whose autoignition behavior is characteristic of diesel fuel. EGR addition was accomplished both by using real EGR gases and by simulating EGR with complete stoichiometric products (CSP): N_2, H_2O, and CO_2.

Figures 1a and 1b show the effects of CSP addition on the ignition timing for iso-octane and PRF80, respectively. Also shown are the individual CSP components and "dry CSP" which consists of only N_2 and CO_2, simulating complete water condensation. In these figures, the 10% burn point is used as a measure of the ignition point, and the amount of EGR gases added is shown in terms of the intake oxygen mole fraction. As can be seen, the ignition-retarding effect of CSP is similar for both fuels, but the effect of the individual components is substantially different for the two fuel-types. This occurs because these fuels have different sensitivities to the two main effects of EGR, which are a thermodynamic "cooling" effect on the compressed-gas temperature and changes to the autoignition chemistry.

For iso-octane, the effect on autoignition chemistry is limited to a rather weak sensitivity to the O_2 concentration. This is evident by the effect of N_2, which is thermodynamically almost the same as air, yet retards the autoignition slightly. However, this effect is weak, and the ignition timing of iso-octane is much more affected by the thermodynamic-cooling effect of the other CSP constituents. This effect results from the higher heat capacity of these constituents, which reduces the compressed-gas temperature relative to that of air alone. CO_2 has the highest heat capacity followed by H_2O, then CSP, and finally dry CSP. Since the cooling effect of CO_2 is the largest, it causes the most timing retard for a given air displacement, with the timing retard caused by the other diluents following in the order of their specific-heat capacities. The behavior of gasoline (not shown) is similar to iso-octane.

In contrast, for PRF80, the effect of CSP addition is dominated by chemical effects. The strongest is the retarding effect of reduced O_2 concentration, as can be seen by comparing the slope of the N_2 curve with that of CSP. Another chemical effect for PRF80 is the autoignition enhancement by H_2O. The H_2O curve in Figure 1b falls right on top of the N_2 curve despite the thermodynamic cooling effect of H_2O (discussed above). This occurs because H_2O lowers the autoignition temperature for PRF80, almost perfectly counteracting the "cooling" effect of H_2O addition. This ignition-enhancing effect of H_2O explains why dry CSP causes more timing retard for PRF80 than does CSP. For iso-octane the opposite is observed. CO_2 addition adds thermodynamic cooling to the effect of reduced O_2 concentration, further increasing the timing retard. The effect of CSP addition with PRF60 (not shown) is similar to that of PRF80.

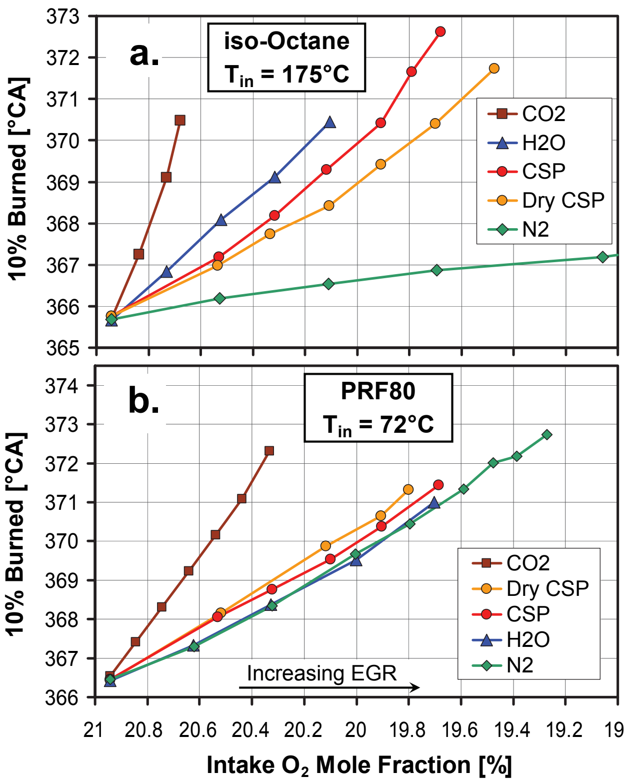

FIGURE 1. Combustion-Phasing (10% Burn Point) Retard with Diluent Addition for Iso-Octane (a) and PRF80 (b) (The amount of CSP or CSP constituent added is shown on the x-axis in terms of intake O_2 mole fraction, which decreases as diluent is added. Charge/fuel mass ratio = 37.8, corresponding to ϕ = 0.4 for no diluent.)

The effect of trace species in real EGR was examined by comparing the ignition-retarding effect of real EGR with that of CSP. The data showed real EGR advanced the combustion phasing relative to CSP for the single-stage-ignition fuels, iso-octane and gasoline, but to retarded it slightly for the two-stage fuel, PRF80. A complete discussion of this study can be found in Ref. [1].

A combined investigation in the metal and optical engines shows that the HCCI autoignition/combustion process occurs in three phases for single-stage-ignition fuels. Initially, a slow temperature rise above the compressed-gas temperature begins when the charge reaches 950–1050 K. This intermediate-temperature heat-release (ITHR) then progressively increases the charge temperature up to the thermal-runaway point, beyond which the temperature rises rapidly due to the high-temperature heat-release (HTHR) reactions. After the main combustion event, a weak burnout phase is observed. For two-stage ignition fuels, low-temperature heat-release (LTHR) or "cool-flame" reactions occur as an initial stage of ignition prior to reaching the ITHR phase. To better understand how the key reactions vary between these combustion phases, and why reaction rates vary with fuel type, spectra of the natural chemiluminescence emission were acquired in the optical engine for both iso-octane and PRF80. The example in Figure 2 shows that the emission spectrum varies significantly between the ITHR

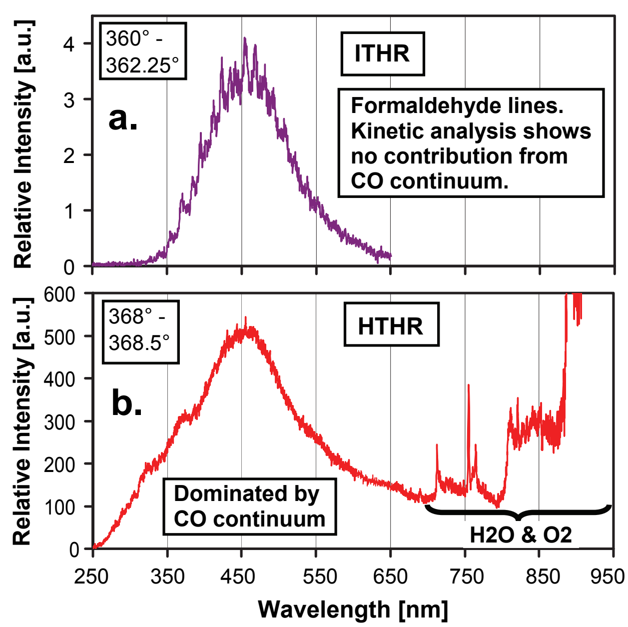

FIGURE 2. Chemiluminescence Spectra During the ITHR (a) and HTHR (b) Combustion Phases for Iso-Octane (The CO-continuum emission is from the CO + O → CO_2 reaction.)

and HTHR phases, indicating significant differences in the key reactions. The ITHR phase is dominated by formaldehyde emission (note the regularly spaced formaldehyde lines in Figure 2a), while the main combustion is dominated emission from the CO-continuum with contributions from OH and HCO, as well as H_2O and O_2 emission to the red and infrared (Figure 2b). A full discussion of this study is given in Ref. [2].

Poor combustion efficiency at low loads, and the associated high emissions of CO and HC, is one of the significant challenges for practical HCCI engines. Previous work has shown that fuel-stratification can significantly improve low-load combustion efficiency by increasing the local combustion temperatures. However, the amount of allowable stratification is limited when the richest regions become sufficiently close to stoichiometric that NOx emissions exceed allowable levels. To improve this combustion-efficiency/NOx tradeoff, various mixture-formation techniques were investigated, including: using two different types of gasoline-direct injection (DI) fuel injectors (hollow-cone spray and 8-hole), varying the injection pressure, and varying the intake-air swirl. For each technique, the amount of stratification was increased by delaying the start of injection (SOI) from early in the intake stroke (well-mixed) until well up the compression stroke (highly stratified) at an idle fueling rate corresponding to $\phi = 0.12$.

Figure 3 summarizes the key findings. As can be seen, the combustion efficiency improves with increased stratification, but eventually the NOx emission rise above the allowable limit. For the base condition of the hollow-cone injector with 120 bar injection pressure, stratification improved the combustion efficiency from 64% for the well-mixed case to 89% at the NOx limit. Switching to the 8-hole injector provided the single largest improvement, increasing the NOx-limited combustion efficiency to 92%. Increasing the injection pressure to 170 bar gave a small additional improvement to 92.5%, which is approaching high-load HCCI combustion efficiencies.

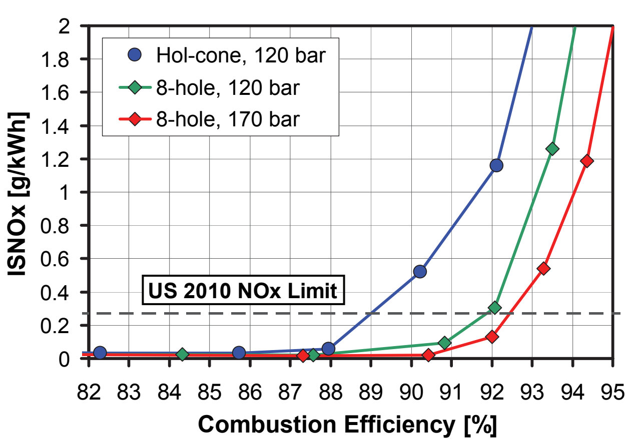

FIGURE 3. Combustion-Efficiency/NOx Tradeoff for Fuel Stratification at Low Loads ($\phi = 0.12$, Idle Fueling) for Iso-Octane (For each curve, the amount of stratification increases from left to right.)

To better understand the reasons for the observed changes in performance, and to gain insight into ways to further improve the mixture, a PLIF imaging investigation of the fuel distributions was also conducted. Figure 4 shows SOI sequences of ϕ-map images (derived from PLIF images) for the hollow-cone and 8-hole injectors. As can be seen, the amount of stratification increases for both injectors as SOI is delayed, resulting in higher local equivalence ratios. For each injector, the image outlined by the red box shows the fuel distribution corresponding to the data point just below the NOx limit in Figure 3. In agreement, these red-boxed images show maximum ϕ values of about 0.6, corresponding to combustion temperatures at which the onset of NOx formation would be expected. As indicated by the crank angles below each image, the NOx limit occurs at a later injection timing for the 8-hole injector (315° crank angle, CA) compared to the hollow-cone injector (300° CA). However, aligning the images sequences relative to the NOx limit shows that the changes in the ϕ distribution with increasing stratification are similar for the two injectors. Also, at the NOx limit, the fuel distribution pattern is similar, with no indication of multiple fuel pockets for the 8-hole injector as might have been expected. Based on these observations, the improved combustion-efficiency/NOx tradeoff with the 8-hole injector must result from fewer low-ϕ regions being present. Although the reason for this improvement is not fully understood, we believe that it is related to the faster mixing with the 8-hole injector, which allows a later SOI at the NOx limit. Considering all the techniques examined to improve the combustion-efficiency/NOx tradeoff, the data consistently showed that a later SOI at the NOx limit resulted in a higher combustion efficiency. We hypothesize that with a later SOI, there is less time for the in-cylinder flows and turbulence (*i.e.* mixing not produced by the injection process) to form overly lean regions by transporting fuel out of the main fuel pockets produced by the fuel-injection process. A complete discussion can be found in Ref. [3].

Conclusions

- EGR is very effective for suppressing the autoignition reactivity of both single- and two-stage ignition fuels, providing a means of controlling combustion phasing over the load-speed map.
- EGR retards the combustion phasing by both a thermodynamic "cooling" effect on the compressed-gas temperature and by changing the autoignition chemistry. For single-stage (gasoline-like) fuels,

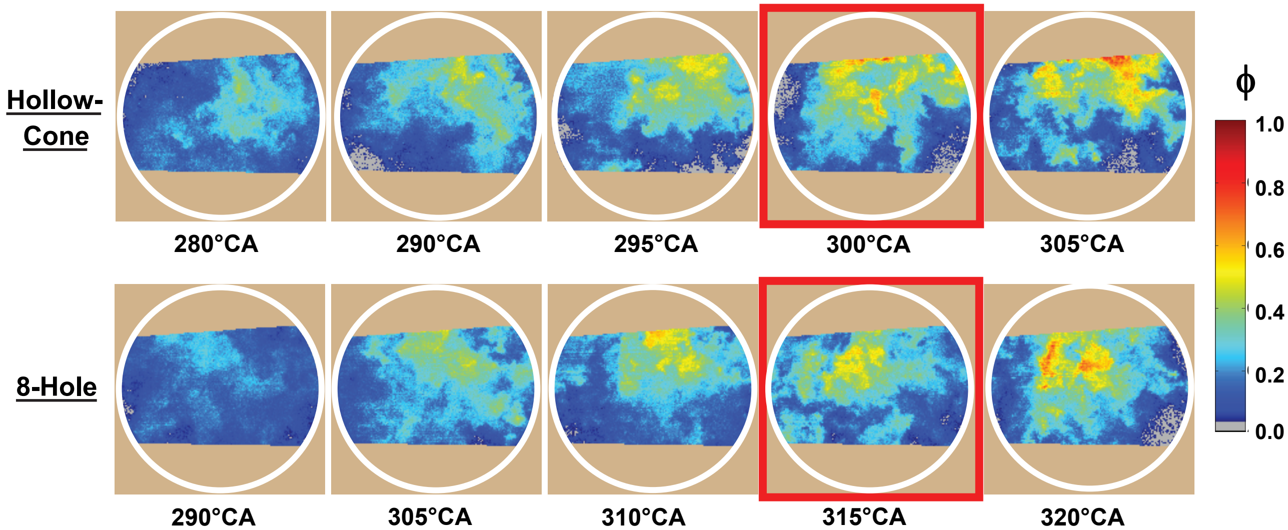

FIGURE 4. Equivalence-Ratio Image Sequences Showing the Changes in Fuel Stratification with Delayed Injection Timing for Both the Hollow-Cone and 8-Hole Injectors with 120 Bar Injection Pressure (The SOI is given below each image. All images were acquired at 365° CA [5° after top dead center].)

the thermodynamic effect is dominant, while for two-stage (diesel-like) fuels, the chemical effect dominates.

- Chemiluminescence-spectroscopy and chemical-kinetic analysis show that the HCCI autoignition/combustion process occurs in three or four phases for single- and two-stage fuels, respectively. Each phase has distinctly different key reactions. ITHR-phase reaction rates can vary significantly with fuel-type, and these differences are critical to differences in autoignition [2].
- Fuel stratification is very effective for increasing the combustion efficiency of HCCI at low-loads (and reducing CO and HC emissions). However, the amount of stratification allowable is limited by NOx emissions, resulting in a combustion-efficiency/NOx tradeoff.
- Compared to the base case of a hollow-cone injector with 120 bar injection pressure, switching to an 8-hole gasoline-DI injector and 170 bar injection pressure improved the combustion efficiency 3.5% at the NOx limit, for a combustion efficiency of 92.5% at an idle fueling of $\phi = 0.12$. This compares to a combustion efficiency of only 64% for well-mixed operation.
- PLIF imaging of fuel distributions, combined with metal-engine performance data, indicates that the improved combustion efficiency with the 8-hole injector is the result of less fuel in low-ϕ regions, for fuel stratification at the NOx limit.

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11. Dec, J. E., Hwang, W., and Sjöberg, M., "Fuel Stratification to Improve Low-Load HCCI: Engine Performance and Fuel-PLIF Imaging," invited presentation, SAE HCCI Symposium, Lund, Sweden, September 2007.

12. Dec, J. E., "Advantages of Charge Stratification in HCCI Engines," plenary lecture, SAE/NA 8th International Conference on Engines for Automobiles, Capri, Italy, September 2007.

Special Recognitions & Awards/Patents

1. Plenary lecture (John Dec) at the SAE/NA 8th International Conference on Engines for Automobiles, Capri, Italy, September 2007.

2. Invited presentation (John Dec) at the SAE HCCI Symposium, Lund, Sweden, September 2006.

3. SAE Russell S. Springer Award (Magnus Sjöberg), presented at 2007 SAE Congress.

4. SAE Lloyd Withrow Distinguished Speaker Award (John Dec), presented at 2007 SAE Congress.

5. U.S. Patent number 7,128,046 B1, "Fuel Mixture Stratification as a Method for Improving Homogeneous Charge Compression Ignition Operation," Dec, J. E. and Sjöberg, M., issued October 31, 2006.

II.A.9 Automotive HCCI Combustion Research

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Objectives

This project comprises optical-engine investigations designed to enhance our understanding of in-cylinder processes in automotive-scale homogeneous charge compression ignition (HCCI) engines. Objectives for FY 2007 include:

- Establish the capability to operate in advanced HCCI operating modes, specifically recompression or negative-valve-overlap (NVO) mode.
- Continue our investigation of the correlation between fuel-air mixture preparation and combustion/emission processes in HCCI engines. Apply new turbulence-modeling tools to clarify the importance of *spatial* fuel-distribution statistics.
- Continue the development of laser-based temperature diagnostics at Stanford University, and conduct tests of the diagnostics in Sandia HCCI research engines.
- Continue development and application of collaborative HCCI-engine-simulation tools.

Accomplishments

- Installed NVO cams in the automotive HCCI engine. Conducted tests to establish the operating range of recompression operation and tested protocols to allow rapid and safe startup in the optical engine.
- Created a 1-D cycle-simulation model to aid the selection of stable NVO operating conditions.
- Adapted Sandia's linear-eddy model (LEM) to provide detailed, stochastic predictions of turbulent mixing in our HCCI engine. The model provided valuable insights into the effect of spatial fuel distribution on HCCI combustion and emissions.
- Continued development of multiple in-cylinder temperature diagnostics at Stanford University.
- Transported Stanford 2-laser diagnostic to Sandia and installed it in the automotive HCCI laboratory. Characterized performance of the diagnostic for simultaneous temperature/composition measurements in an operating engine. Established ±5% accuracy for temperature measurements during the compression stroke, with a sensitivity better than 10 K.
- Began tests of the planar laser-induced fluorescence (PLIF) diagnostic during fired recompression-HCCI operation.
- Continued development of HCCI simulation tools. The University of Wisconsin-Lawrence Livermore National Laboratory (UW-LLNL) model of the Sandia HCCI automotive engine (KIVA/Multi-zone model) achieved full-cycle simulation of homogeneous fired operation. The KIVA code was also coupled with the LEM to enable our spatial-fuel-distribution study.

Future Directions

- Complete operating-range tests of recompression-HCCI combustion.
- Investigate the use of alternative injection strategies, including injection during the recompression period, to accomplish advanced fuel-air mixing strategies. Apply PLIF diagnostic to characterize engine performance under these conditions.
- Examine spark-assisted HCCI operation to understand its potential role for widening the HCCI operating range.
- Test Stanford wavelength-modulation tunable diode laser (TDL) sensor and wavelength-ratioing laser-induced fluorescence (LIF) sensor in Sandia HCCI engines.
- Modify the automotive HCCI facility to enable more flexible valve timing, wider operating range, and multiple combustion modes.

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Introduction

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

Approach

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

Results

NVO Operation

New cams were installed in the automotive HCCI engine this year to permit operation using recompression, or NVO, strategies. To accommodate these strategies, the cams provide a short lift duration of 145 crank angle degree (CAD), and can be timed for a range of NVO operation. When timed to set EVC = IVO (exhaust valve closing equal to intake valve opening), the operation approximates a conventional motored cycle as shown in Figure 1a. The short-duration valve-lift profile is responsible for a slight pressure rise (recompression) visible at top dead center (TDC) of the exhaust stroke. With the cams timed to set EVC = -90 and IVC = +90 CAD, an NVO of 180 CAD is achieved, producing the large recompression seen in Figure 1b during the exhaust and intake strokes. Plotted along with the experimental pressure traces in Figure 1 are model predictions from a GT Power model of our engine that we have developed. The model reproduces the data closely at all operating conditions, and is a useful tool for planning our experimental operating conditions.

Operating with large negative valve overlap is a challenge for optical engines, since typically such strategies require extended operation to reach steady-

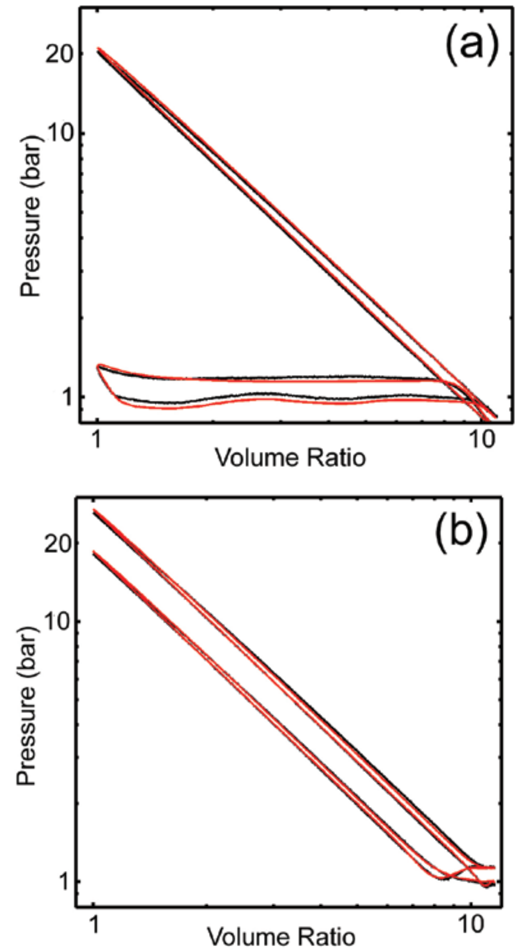

FIGURE 1. Measured and predicted motored engine pressure traces using NVO cams. Black curve = measured data; red curve = predictions from 1-D engine model. 1a: conventional cam timing. 1b: NVO timing with 180 CAD of negative overlap.

state. During this reporting period, we have begun to establish HCCI NVO stable operating regimes for the optical engine as well as strategies for rapid start-up. These strategies employ port injectors with gaseous fuels for warm-up and then transition into HCCI operation with direct-injected PRF90 fuel (primary reference fuel with 90 octane rating). Coupling NVO operation with LIF diagnostics is complicated by high exhaust gas recirculation (EGR) levels, and the possibility of fuel injection during both the compression and recompression strokes. We have successfully demonstrated the ability to make simultaneous temperature/composition measurements during NVO operation (see PLIF measurements in the following).

LEM Modeling

A primary project goal is quantifying the effect of mixture preparation on combustion. LIF measurements of fuel-air mixing provide mixture statistics at the time of ignition, and in previous work we have demonstrated a correlation between LIF-based probability density function (PDF) statistics and engine-out emissions. But PDF statistics are a limited metric since spatial details of the fuel distribution are ignored. This issue was highlighted during an experimental comparison of two fuel injectors in our engine: the injectors produced similar fuel-distribution PDFs, but significantly different NOx emissions. Unlike the PDFs, spatial mixing statistics were distinct: the injector creating a coarser fuel distribution (fewer, larger fuel packets) produced more NOx. Since it is difficult to control mixing statistics experimentally, we have applied a novel combination of modeling tools this year to further examine the question: how do the spatial details of fuel-air mixing affect HCCI combustion?

Collaboration with the UW and LLNL produced a KIVA CFD model of our automotive HCCI engine as part of our project, and we have combined it with Sandia's LEM to capture the necessary turbulent mixing scales. The KIVA model is a full-cycle 3-D simulator with 150,000 grid cells; for computational efficiency, the cells are grouped into 100 zones of common temperature and composition during reaction computations. The 1-D LEM runs in series with the KIVA simulation, solving diffusion/reaction equations on a fine grid and simultaneously simulating turbulence by defining discrete eddy events that randomly rearrange fluid packets much like a physical eddy.

Since we are interested in the effect of fuel distribution on combustion, the LEM is run during the period of combustion (from -30 to +30 CAD after TDC). KIVA provides initial pressure and temperature values for the LEM, averaged over the core region of our engine (roughly corresponding to the measurement volume of our LIF diagnostic). In addition, spatially averaged turbulent kinetic energy and dissipation rate values predicted by KIVA are used at each time step to determine the location, timing, and intensity of the LEM eddy events. Finally, several hypothetical fuel distributions are defined to initialize the LEM simulation at -30 CAD. One such initial distribution, the Coarse distribution, is illustrated in Figure 2a. The LEM predicts the spatial and temporal evolution of temperature, fuel, and products as illustrated in Figure 2b, which is a snapshot of mixture profiles soon after the start of heat release. The visible random structure of the profiles is created by the LEM's turbulence mechanism, and it is an important feature that each cycle simulation produces unique results.

We have simulated initial spatial fuel distributions ranging from very fine to very coarse; Figure 3 presents predicted mean temperature histories for three of these cases, illustrating several insights gained from the work. The Fine distribution corresponding to the results in Figure 3a is similar to the Coarse distribution in Figure 2a, but with twice as many (narrower) fuel

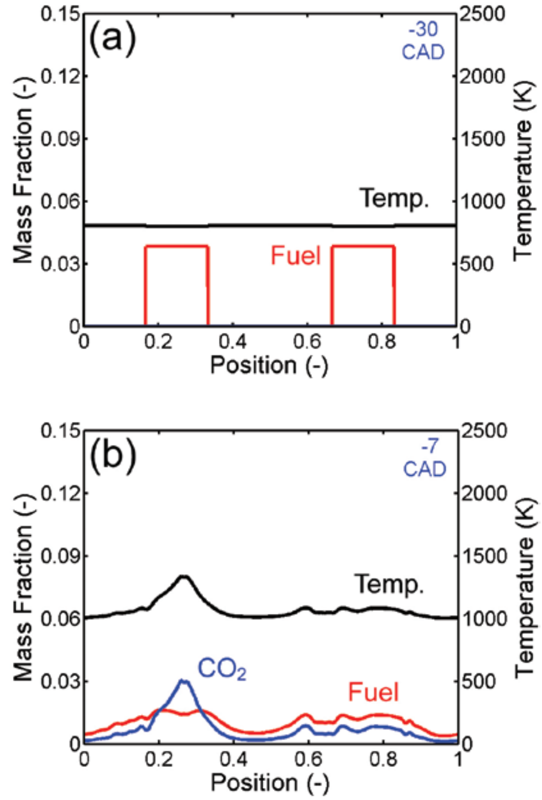

FIGURE 2. LEM predictions for the Coarse fuel distribution: composition and temperature profiles along the LEM's 1-D traverse of the engine core region. 2a: initial conditions at the start of the simulation. 2b: temperature, fuel, and CO_2 profiles soon after the start of heat release.

packets. The dotted line in Figure 3a is KIVA's predicted temperature history for homogeneous-charge operation. The dashed line is averaged temperature from an LEM run in which turbulence has been turned off for comparison purposes. The no-turbulence curve generally follows KIVA's predictions, although the low-temperature heat release (at -22 CAD) is not captured by the LEM's simplified kinetics model. In addition, the LEM main heat release is advanced due to the slight stratification of the Fine distribution. The red (solid) curve in Figure 3a represents LEM results with turbulence activated. There is little difference from the no-turbulence results, and we conclude that for the Fine case, diffusion alone (without turbulence) mixes the initial distribution nearly completely by the start of heat release.

Figures 3b and 3c present the same three curves for the Coarse and the Very Coarse fuel distributions. It is apparent that making fuel distributions more coarse (more stratified) monotonically advances the predicted combustion phasing. Perhaps the most significant results are two trends seen only in the Coarse case, Figure 3b. Here the turbulence (red) curve phasing is retarded with respect to the no-turbulence (dashed) curve, and its maximum rate of temperature rise is reduced as well. These trends are explained by the fact

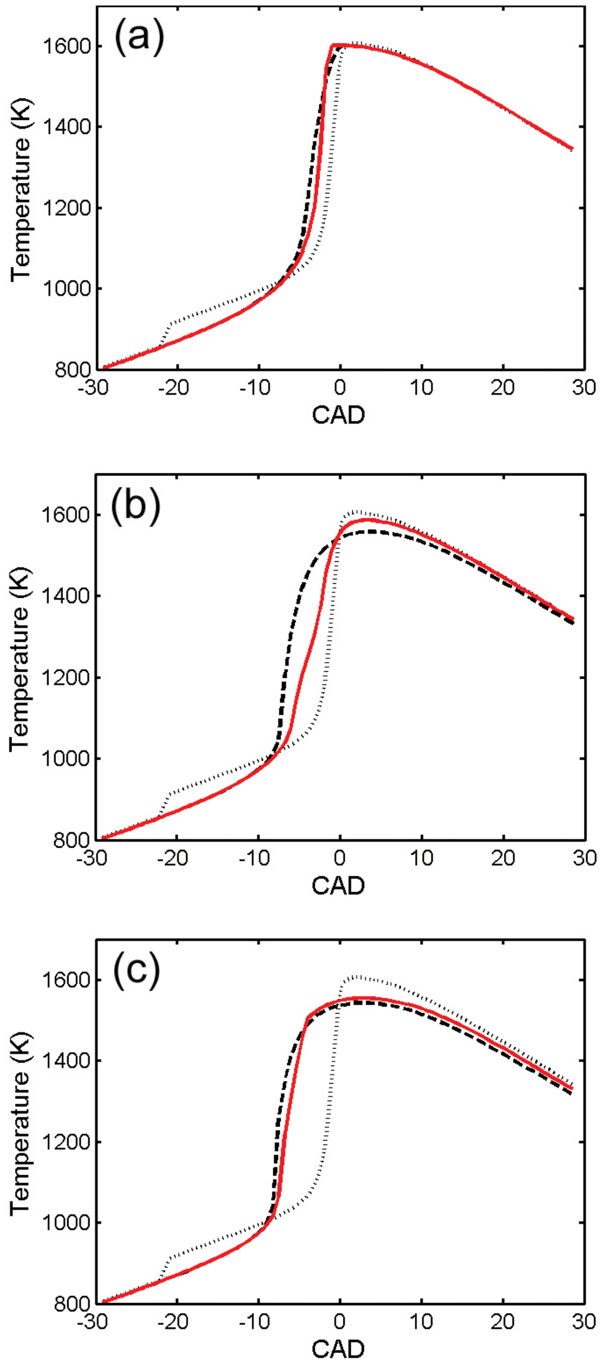

FIGURE 3. Model predictions of mean core-region temperatures: dotted lines = KIVA; dashed lines = LEM with no turbulence; solid red lines = LEM with turbulence. 3a: Fine fuel-distribution case; 3b: Coarse fuel-distribution case; 3c: Very Coarse fuel-distribution case.

that the turbulence integral length scale (estimated by KIVA) happens to match the Coarse fuel distribution length scale. In this case, and only this case, turbulence is effective in homogenizing the charge enough to delay heat release. In addition, the random turbulence mixes some fuel packets more than others, resulting in de-synchronized combustion that produces the more gradual heat release seen in the red curve of Figure 3b. Note that each realization of the LEM produces a unique temperature history: the resulting non-overlapping histories (not shown) allow an assessment of cyclic variation. Finally, the matching LEM temperature histories for the Very Coarse case, Figure 3c, indicate that diffusion and turbulence are ineffective in mixing fuel distributions that are as coarse as the Very Coarse case. We are optimistic that future embellishments, such as a more complex reaction mechanism and more realistic initial fuel distributions, will increase the utility of the LEM simulations.

PLIF Measurements

In collaboration with Sandia's HCCI engine program, Ron Hanson's group at Stanford University is developing in-cylinder temperature diagnostics. Both TDL absorption and LIF techniques have produced useful measurements in Sandia engines–this report highlights the successes of Stanford's two-laser PLIF diagnostic capable of simultaneous temperature and composition measurements. Excitation wavelengths of 277 and 308 nm (from two excimer lasers, with the output of one laser shifted in an H_2 Raman cell) were selected from seven candidate wavelengths to optimize temperature sensitivity when using the tracer 3-pentanone. A fast dual-frame camera records the fluorescence signal from each laser in rapid succession, and the ratio of the signals provides a 2-D image of in-cylinder temperature. Following temperature determination, simultaneous composition can be quantified using either of the fluorescence signals.

During this reporting period, we extensively tested the LIF diagnostic in the automotive HCCI optical engine. We began the tests with a homogeneous charge (both temperature and composition), measuring in-cylinder temperature in the core region of the engine during the compression stroke. Figure 4 compares these measurements with predictions based on isentropic compression and predictions from our GT-Power 1-D cycle simulation code. The LIF measurements are uniformly higher than the predictions, but remain within ±5% of those values over the entire range. Examination of the uniform temperature data allow us to estimate a sensitivity better than 10 K (one standard deviation).

Figure 5 presents measurements from a test in which a cool, unseeded nitrogen jet was injected into one intake port while hot, seeded air entered the other. This motored test simulates the addition of EGR in an engine, and the results in Figure 5 demonstrate the diagnostic's ability to capture simultaneous temperature and composition distributions. The simulated EGR is clearly concentrated on one side of the cylinder in Figure 5a, and Figure 5b shows a less distinct but complementary distribution of higher temperatures on the other side.

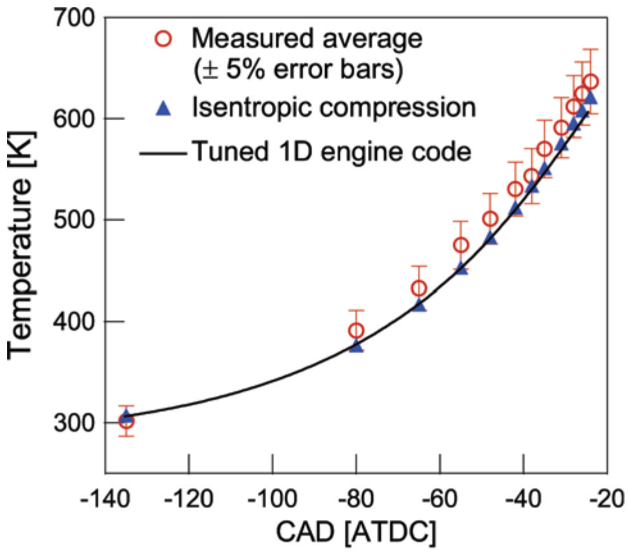

FIGURE 4. PLIF measurements of in-cylinder mean temperature during homogeneous motored operation. Red circles with error bars = PLIF measurements; blue triangles = predictions based on isentropic compression; line = predictions from 1-D cycle-simulation code.

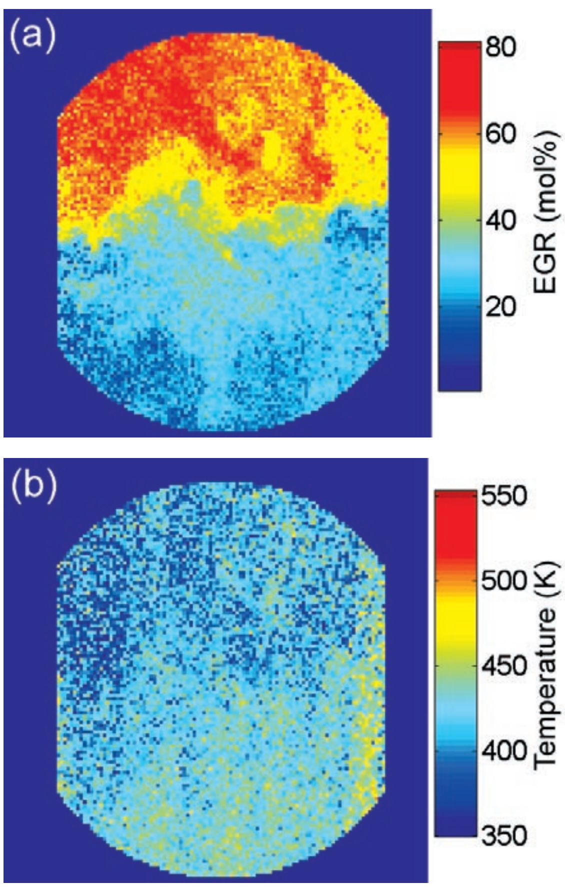

FIGURE 5. Single-cycle simultaneous composition/temperature images captured during motored operation with simulated EGR and temperature stratification. 5a: EGR mole fraction; 5b: temperature.

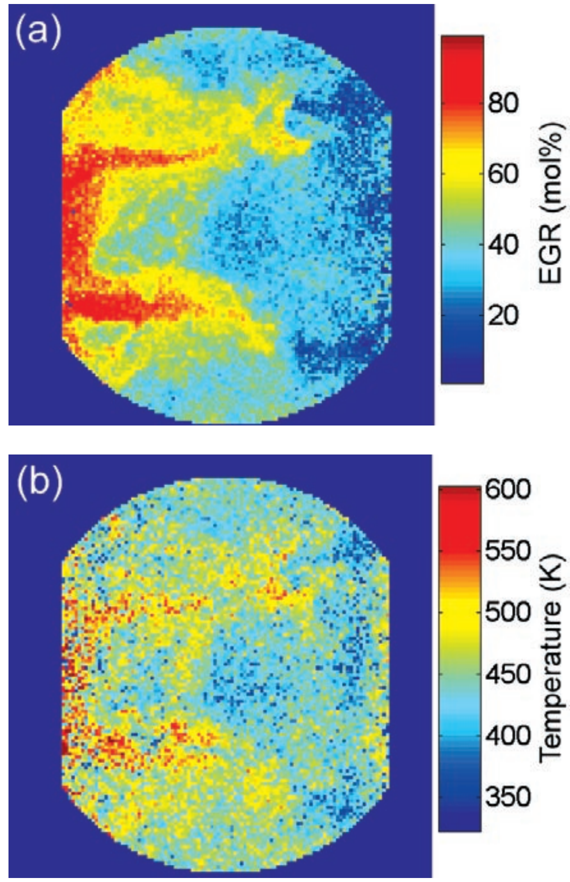

FIGURE 6. Single-cycle simultaneous composition/temperature images captured during fired operation with natural stratification. 6a: EGR mole fraction; 6b: temperature.

From these tests, we progressed to fired experiments, as illustrated in Figure 6. Figure 6a displays the distribution of retained residuals pushed to the exhaust (left) side of the cylinder soon after the opening of the intake valves (located on the right). The corresponding temperature distribution in Figure 6b shows that regions of high EGR concentration are hotter, as expected.

Conclusions

- New NVO cams installed in our optical HCCI engine enable fired operation with high-octane, automotive fuels.
- The LEM/KIVA modeling tool provides useful predictions relating mixture preparation to combustion performance. Simulation results predict that when the turbulence integral length scale matches the fuel-distribution length scale, turbulent mixing is most efficient and can influence phasing and heat-release rates during HCCI combustion. In such cases, cycle-to-cycle variation estimates (a unique feature of the LEM simulations) are predicted to be significant.

- Motored engine tests using Stanford's 2-laser LIF diagnostic indicate excellent temperature-measurement accuracy (±5%) and sensitivity (10 K). Further tests demonstrated an ability to characterize stratified-charge conditions (simultaneous temperature and composition) during fired operation. By seeding both the intake air and liquid fuel with 3-pentanone tracer, the technique successfully quantified in-cylinder residual-gas concentrations.

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8. Steeper, R. R., "Improving the NO_X-CO_2 Trade-Off of an HCCI Engine Using a Multi-Hole Injector," SAE World Congress, Detroit, April 2007.

9. Steeper, R. R., "Sandia Automotive HCCI Engine Project," DOE Advanced Combustion Engine Program Review, Washington, D.C., June 2007.

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

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

II.A.10 Spark-Assisted HCCI Combustion

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Objectives

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

Accomplishments

- Established Cooperative Research and Development Agreement (CRADA) with Delphi Automotive Systems on "Control Strategies for HCCI Mixed-Mode Combustion."
- Developed data-based method to estimate global kinetic parameters from combustion measurements and form the basis of a low-order dynamic model to be used for prediction and control.
- Developed Wiebe-based combustion metric to be used for feedback control as well as improving model estimates of global kinetic parameters.

Future Directions

- Baseline and map SI-HCCI regions of operation on a multi-cylinder engine located at Delphi Automotive Systems.
- Perform detailed kinetics simulations of SI-HCCI transition to improved physical understanding of multiple combustion modes and inter-mode switching. Simulations will be performed in-house as well as in collaboration with Lawrence Livermore National Laboratory.
- Improve low-order combustion model for use in the development of fast diagnostics and control strategies.

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Introduction

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

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

Approach

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

A single-cylinder research engine is being used for a fundamental investigation of SI-HCCI combustion dynamics. The engine used in this study is a 0.5-L single-cylinder AVL research engine with an 11.34:1 compression ratio. The engine has two intake valves and one exhaust valve and is equipped with a full-authority hydraulic variable valve actuation system. Only a single intake valve was used in this study to promote swirl and mixing. The transition from SI to HCCI is achieved in this engine with high levels of exhaust gas retained in the cylinder through manipulation of the intake and exhaust valve events. All experiments were performed at stoichiometric fueling conditions and a range of speeds and loads.

A multi-cylinder research engine is being developed by Delphi Automotive Systems for use in this activity and is expected to be complete in early FY 2008. Specific tasks for this agreement include:

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

Results

One of the most widely used methods for achieving the preheat conditions required to initiate HCCI is retention of high levels of exhaust gas in the cylinder from one cycle to the next through manipulation of the intake and exhaust valve events. While effective, this internal exhaust gas recirculation (EGR) creates a strong coupling between successive cycles, and small variations in the thermal and chemical composition of the retained exhaust gas can lead to large variations in the combustion process. Recent results from our research have shown that, due to this highly variable combustion, the SI-HCCI mode transition is very unstable, with high torque variations, high unburned hydrocarbon emissions, and potential engine stall. Figure 1 illustrates the trend in engine stability and engine-out NOx emissions as internal EGR is increased to transition from SI to HCCI. The results reported here focus on observations from the transition region where combustion instability is highest but NOx emission levels are near HCCI levels. This interest is motivated by the recognition that it may be possible to limit variability in the transition region by applying the appropriate type of feedback control. The potential benefits would be to smooth the SI-HCCI transition and extend the window of steady-state operation with HCCI-like NOx emission levels.

A conceptual model of the SI-HCCI transition and intermediate mixed-mode combustion events has been developed based on experimental observations. Spark ignition combustion is dominant for low levels of EGR. As EGR is increased further, the inlet fuel-air mixture is diluted with exhaust and the SI flame speed decreases. In the transition region, combustion typically begins when the spark creates a reaction front that expands and propagates through the premixed charge. Energy is transferred from the reaction front to the unburned mixture which, if conditions are right, results in an

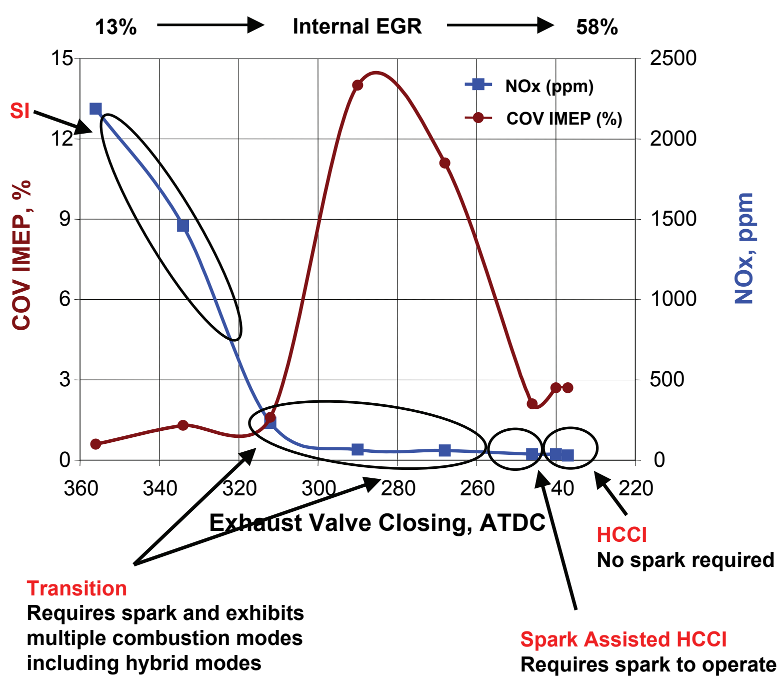

FIGURE 1. General combustion trends observed in the SI-HCCI transition experiments for 1,600 RPM, 3.4 BMEP. Internal EGR referenced in the figure was estimated using a full engine simulation code.

instantaneous, volumetric reaction over all (or some portion) of the remaining unburned charge. Thus, in the transition region, combustion occurs as a hybrid or mixed-mode event consisting of both propagating-flame and HCCI combustion during the same cycle (see Figure 2).

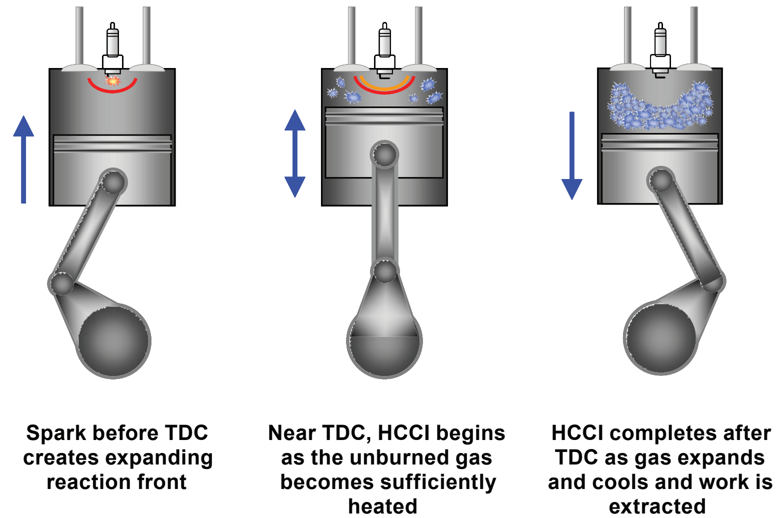

FIGURE 2. Illustration of the Possible Role of the Initial SI flame in SI-HCCI

Analysis of experimental data indicates that the large combustion instabilities typical of the transition region arise from variations in the timing and relative strength of the secondary HCCI combustion process. These observations were used to develop a data-based combustion model for estimating global kinetic rate constants and ultimately a low-order empirical model of the combustion process. The global kinetic rate constants estimated from experimental data suggest that the HCCI combustion is actually switching between two different modes (or mechanisms) with different propensities to auto ignite. We hypothesize that the mode of combustion that occurs on a given cycle is determined by the presence or absence of sufficient concentration of partially oxidized fuel species that act as an enabler for HCCI combustion and accumulate in the cylinder through exhaust recirculation. As EGR is increased further, EGR heat becomes sufficient to stimulate HCCI, which preempts flame initiation (transition to HCCI is complete).

Characteristic post-top dead center (TDC) burn times (from estimates of global kinetic rate parameters) are shown in Figure 3 as a function of the unburned gas temperature at TDC. This figure clearly illustrates the distinct modes of HCCI combustion as was discussed previously. Of particular interest is the negative temperature effect (*i.e.*, where the burn rate decreases with increasing temperature) exhibited by both forms of HCCI. One of the observed HCCI modes appears to have a strong similarity to the predictions of fundamental kinetic mechanisms for HCCI such as the Pitsch mechanism for n-heptane shown in Figure 4. The similarity between the experimental results and the Pitsch mechanism suggests that at least part of the cycle-to-cycle combustion variations for our engine in the SI-HCCI transition involved n-heptane-like kinetics. Interestingly, we have not seen the level of negative temperature effect behavior observed in these experiments reported for indolene in other studies.

The experimental observations discussed above were used to develop a model of the hybrid combustion events, where combustion is divided into the initial propagating-flame event and the subsequent HCCI event. The strength and timing of the HCCI event is determined by the initial charge conditions and the

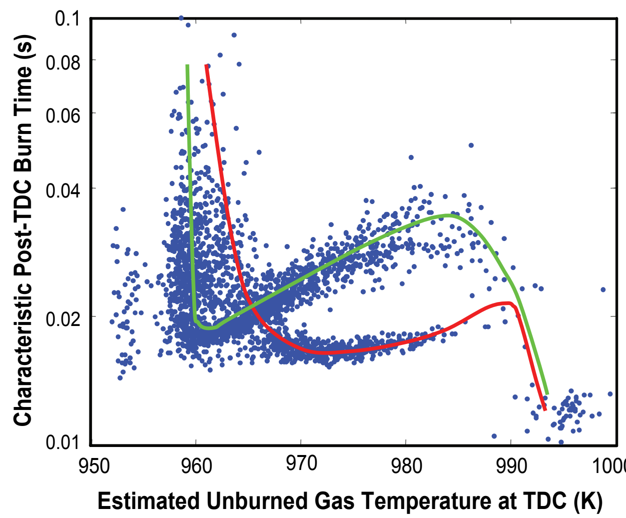

FIGURE 3. Characteristic Post-TDC Burn Time for SI-HCCI for $\phi = 1$ and EGR = 46%

amount of energy released during the initial reaction. An empirically derived switching rule is added to determine when combustion switches between the two modes. As shown in Figure 5, early attempts show promise in reproducing the dynamic behavior observed experimentally. The low-order model is able to predict the basic dynamic behavior observed in the experimental data and is expected to form a basis for future real-time control models and more detailed models for evaluating control algorithms.

A technique has also been developed that uses multiple Wiebe relations to estimate the timing and relative strengths of the two portions of the hybrid combustion event from experimental data. This

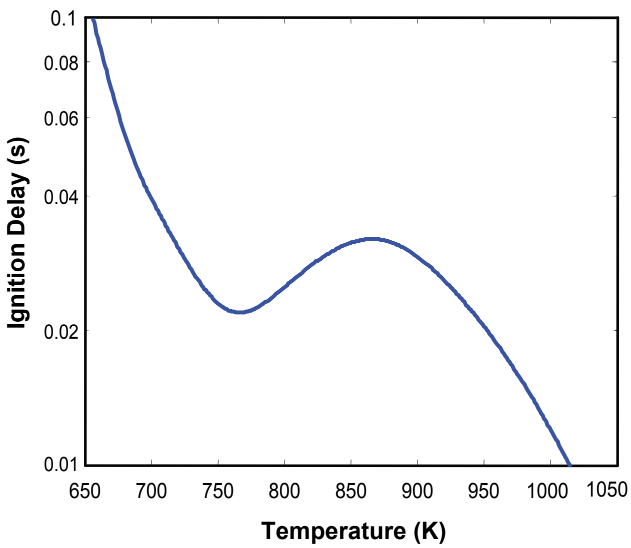

FIGURE 4. Ignition Delay for n-Heptane from Pitsch Mechanisms with $\phi = 0.4$, P = 8.2 atm, and intert/O_2 = 5

information will be useful in further refining our model and potentially as a combustion metric for feedback control. An example of the multiple-Wiebe analysis is shown in Figure 6. In this example, pure SI and pure HCCI combustion modes are best represented by a single Wiebe functions while the hybrid modes require two Wiebe functions for a reasonable fit. The selection of one or two Wiebe functions and correspondingly quality of the fit is based on a comparison of the sum of mean squared errors.

Conclusions

The results of this study indicate that global kinetic parameters may be estimated from sequential unstable cycle-resolved combustion measurements in the SI-HCCI transition. This information was then used to develop an empirical model capable of simulating the complex dynamics observed experimentally on a single-cylinder engine, providing new insight into the physics and chemistry of the transition dynamics. The next phase of this activity involves adapting these concepts to a multi-cylinder engine for the development and implementation of adaptive control strategies.

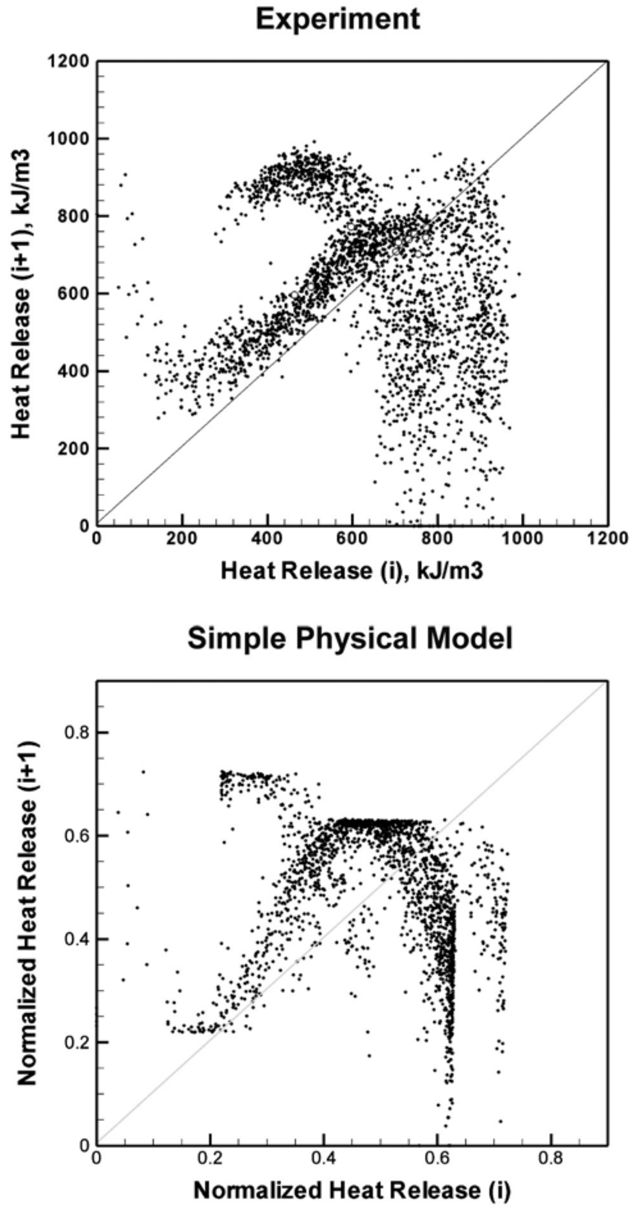

FIGURE 5. Comparison of Simple Physical Model and Experimental Observations of SI-HCCI

FY 2007 Publications/Presentations

1. R. M. Wagner, C. S. Daw, K. D. Edwards, J. B. Green Jr., "Global kinetics model for spark assisted HCCI," SAE HCCI Symposium 2007 (Lund, Sweden; September 2007). *Invited*.

2. K. D. Edwards, R. M. Wagner, C. S. Daw, J. B. Green Jr., "Ignition control for HCCI by spark augmentation and advanced controls", 2007 DOE National Laboratory Merit Review & Peer Evaluation (Washington, D.C.; June 2007).

3. K. D. Edwards, R. M. Wagner, C. S. Daw, J. B. Green Jr., "Hybrid SI-HCCI combustion modes and the potential for control", Proceedings of the 5th U.S. National Combustion Meeting (San Diego, CA USA; March 2007).

4. C. S. Daw, K. D. Edwards, R. M. Wagner, J. B. Green Jr., "Modeling cyclic variability during the transition between SI combustion and HCCI", Proceedings of the 5th U.S. National Combustion Meeting (San Diego, CA USA; March 2007).

5. R. M. Wagner, K. D. Edwards, C. S. Daw, J. B. Green Jr., "Understanding the dynamic instability of the SI-HCCI transition and the potential for control", SAE HCCI Symposium (San Ramon, CA; September 2006). *Invited*.

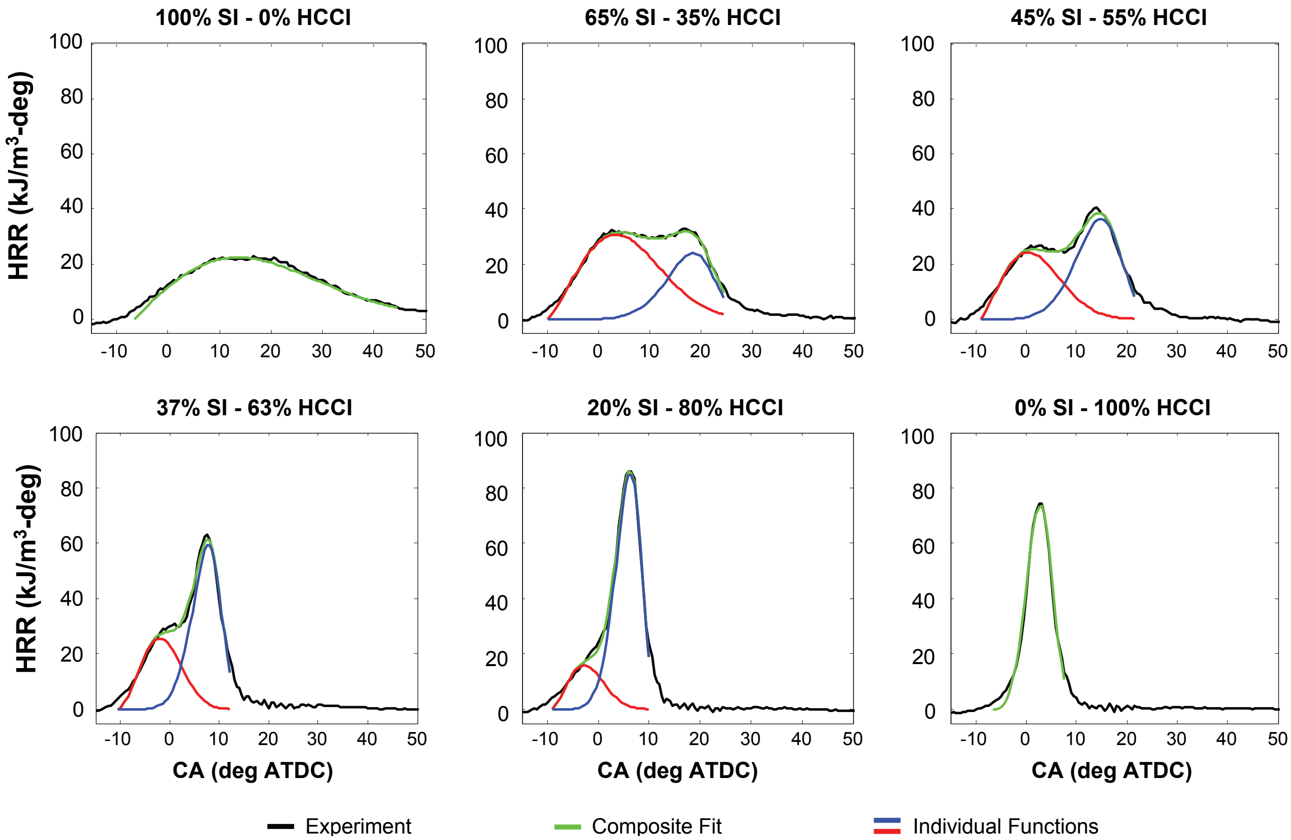

FIGURE 6. Examples of experimental heat release rate profiles and Wiebe function approximations for combustion cycles with various degrees of SI and HCCI as determined by a double Wiebe algorithm.

Special Recognitions & Awards/Patents Issued

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

2. Activity was recognized as a 2007 Science & Technology highlight for the Energy & Engineering Sciences directorate at ORNL.

II.A.11 KIVA-4 Development

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Objectives

- Validate parallelization of KIVA-4 in realistic geometries
- Develop a parallel collocated version of KIVA-4
- Implement advanced combustion models in KIVA-4
- Develop converters to KIVA-4 from established mesh generation software
- Develop remapping capability in KIVA-4
- Reduce spray dependence on grid

Accomplishments

- The parallelization of KIVA-4 was tested in realistic geometries including 4-valve pentroof and 3-valve engine geometries.
- The collocated version of KIVA-4 was parallelized and run in parallel in a vertical valve engine geometry.
- The University of Wisconsin's chemistry and spray submodels were implemented in KIVA-4 and tested in a 2-D sector geometry.
- Reaction Design's chemistry package was interfaced with KIVA-4.
- Mesh converters to KIVA-4 format were developed for the TrueGrid and ICEM software programs.
- Remapping capability was demonstrated in a cylindrical tetrahedral mesh.
- Reduced spray dependence was achieved by using the grid overset method in KIVA-4.

Future Directions

- Continue validation of KIVA-4 in unstructured geometries and in parallel simulations of realistic engine geometries.
- Implement Lawrence Livermore's multi-zone combustion model [1] into KIVA-4.
- Develop the capability to perform turbulent calculations with the large eddy simulation (LES) turbulence model in KIVA-4.

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Introduction

We have focused our efforts on parallelizing realistic geometries, developing a collocated version of KIVA-4, incorporating improved combustion and spray models, building interfaces with mesh generation software packages, developing remapping capability for KIVA-4 and reducing the spray dependence on the grid.

We previously had worked with relatively simple geometries in our parallel version of KIVA-4. In our recent work, we simulated two realistic engine geometries in parallel. These geometries include a 4-valve pentroof geometry and a 3-valve engine which has been studied experimentally by Dick Steeper at Sandia National Laboratory, Livermore.

We also developed a collocated version of KIVA-4 where the velocity is located at the cell-center along with the other field variables (pressure, temperature and density). This version is more appropriate for unstructured meshes that use a large percentage of tetrahedra or prisms. This version also has opened the door to more advanced meshes which include the grid overset technique in which two different meshes can be combined to model engine phenomena.

KIVA-4 inherited the combustion models of KIVA-3V which are Arrhenius type chemistry controlled combustion models. The University of Wisconsin Engine Research Center has had many years of experience with combustion models including mixing controlled models and ignition models which previous versions of KIVA-3V had not incorporated. We implemented the University of Wisconsin's combustion models into KIVA-4 to enhance the code and its applicability.

KIVA traditionally has accommodated large mesh movements with its snapper algorithm, where layers of cells become activated or deactivated during piston or valve movement. We have complemented KIVA's snapper routines with the capability of remapping fields to an entirely different mesh and continuing the engine simulation on the second mesh.

KIVA uses a grid generation program called K3PREP to construct its engine meshes. However, K3PREP can only generate structured meshes while KIVA-4 can accommodate unstructured meshes as well as structured meshes. Mesh generation is a complex field in itself and we felt the best use of time would be spent developing interfaces from existing grid generation software. We have developed interfaces for ICEM (via its CHAD output format). Robert Rainsberger at TrueGrid developed a mesh output format for KIVA-4 with assistance from LANL. We have also run a simple mesh generated with the Cubit mesh generator with KIVA-4.

KIVA uses a set of Lagrangian particles that move through the computational mesh to model the liquid fuel spray. The computational mesh is used to model the gaseous phase. The Lagrangian particles experience a drag during their motion and momentum is transferred from the particles to the grid. The Lagrangian particles also collide and evaporate. Each of these processes is dependent on the resolution of the underlying grid. We have implemented the grid overset method in KIVA-4 which allows one to resolve the region around the spray without resolving the entire engine geometry, thus allowing one to calibrate sprays with a fine resolution.

Approach

We have focused our efforts on continued development of KIVA-4. Our approach is to develop KIVA-4 in areas that are most essential and will have the greatest impact. We believe that KIVA-4 would be adopted more readily and have more applicability if it could be complemented with a grid generator, could perform calculations of realistic geometries in parallel and could access advanced combustion and spray models.

Results

We present the results of parallel computations in a 4-valve engine shown in Figure 1. Table 1 shows the speed-up achieved with varying amounts of processors. One can see that four processors are being used effectively. Beyond four processors, the speed-up diminishes. The parallel performance tends to plateau for two reasons. First, the grid is relatively small using 38,392 cells. For comparison, we have achieved a speed-up of 10.21 in a cylinder with 430,000 cells with 14 processors in KIVA-4. Second, the mesh partitioning could be improved considering the fact that cells become deactivated when the piston moves up. Partitioning refers to how the mesh is subdivided among processors (or equivalently the way the computational load is divided among processors). We have implemented a means of repartitioning a mesh during the course of a simulation, thus providing a means of improving the parallel performance with larger amounts of processors. Figure 2 shows the 3-valve engine run in parallel. We were able to achieve a speed-up of 1.71 with 2 processors and 2.62 with 4 processors. In the 3-valve engine parallel computation, entire ports become deactivated during the course of the simulation which makes an effective single partitioning even more difficult.

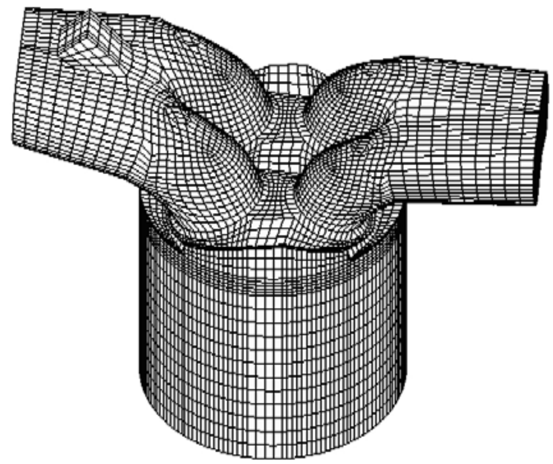

FIGURE 1. 4-Valve Pentroof Geometry Simulated in Parallel with KIVA-4

TABLE 1. Parallel Speed-Up with 4-Valve Engine

Number of Processors	Time (hours)	Speed-up
1	9.6	1.0
2	5.24	1.83
4	3.0	3.2
8	2.76	3.48
16	2.36	4.1

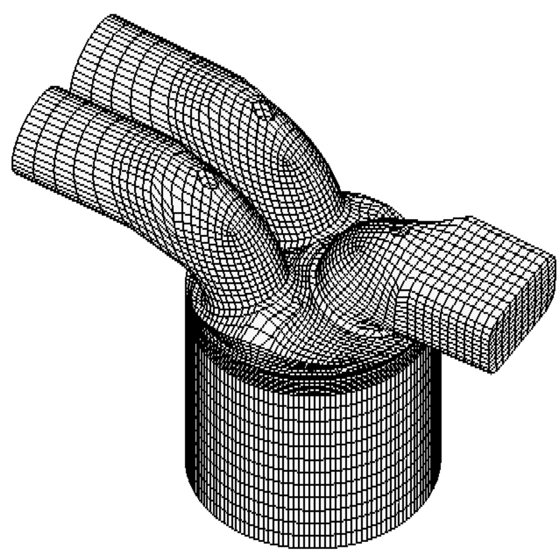

FIGURE 2. 3-Valve Geometry Run in Parallel with KIVA-4

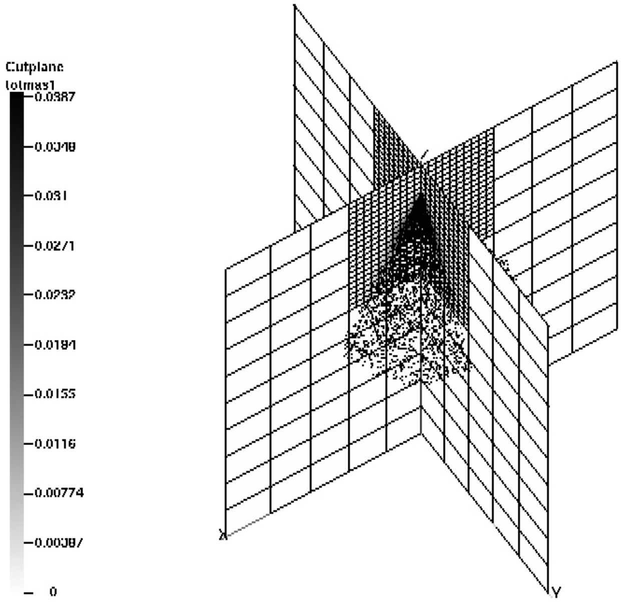

FIGURE 3. Use of Grid Overset Method to Resolve Spray

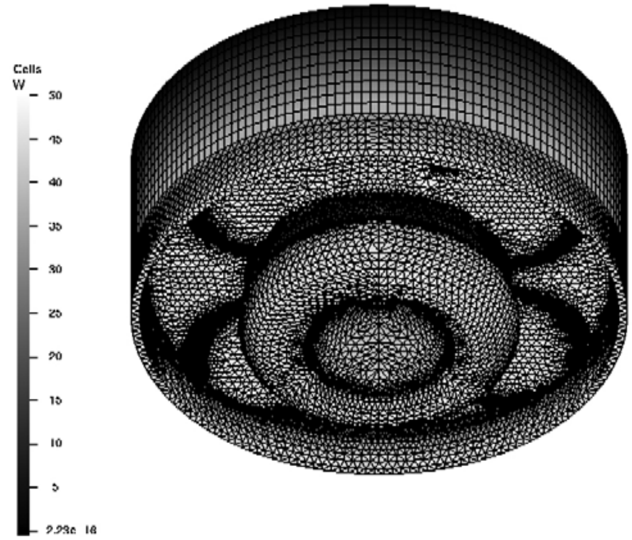

FIGURE 4. Vertical Velocity in Tetrahedral and Prism Mesh

Our repartitioning algorithm should prove effective in improving the 3-valve parallel efficiency.

Figure 3 shows a computation in a cylinder with the overset grid method where two grids are simultaneously used – one specifically for the spray and another for the engine geometry. Finer resolutions will improve the accuracy of the spray dynamics up to a point. We also hope to incorporate the collision improvements of Abani, et al. (2006) in the future to further decouple the spray dynamics from the underlying grid.

Figure 4 shows a mesh with tetrahedra and prisms that was simulated with KIVA-4. This mesh was created by Valmor de Almeida at Oak Ridge National Laboratory. We expect to use this strategy of using tetrahedra in the bowl and head region and prisms in the squish region for future simulations of engine meshes.

Conclusions

KIVA-4 has simulated realistic geometries in parallel. Advanced combustion models have been tested in KIVA-4. Grid converters have been developed to convert meshes to KIVA-4 format. Restart capability has been developed to remap fields from one mesh to another mesh and continue the KIVA-4 simulation on the second mesh. The grid overset method has been developed in KIVA-4 to reduce the dependence of the spray on the grid.

We would also like to acknowledge the help and suggestions of Qingluan Xue, Yuanhong Li and Song-Charng Kong of Iowa State University, Zheng Xu at Ford Motor Corporation and Valmor de Almeida at Oak Ridge National Laboratory.

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2. N. Abani, A. Munnannur and R. Reitz, Reduction of Numerical Parameter Dependencies in Diesel Spray Models, ILASS Americas, 19th Annual Conference of Liquid Atomization and Spray Systems, 2006.

FY 2007 Publications

1. D. J. Torres, Collocated KIVA-4, International Multidimensional Engine Modeling User's Group Meeting Proceedings at SAE Congress, April 2007.

2. Q. Xue, S.C. Kong, D.J. Torres, Z. Xu and J. Yi, DISI Spray Modeling using Local Mesh Refinement, submitted to Society of Automotive Engineers.

3. M. Fife, P. Miles, M. Bergin, R. Reitz and D.J. Torres, The Impact of a Non-Linear Turbulent Stress Relationship on Simulations of Flow and Combustion in an HSDI Diesel Engine, submitted to Society of Automotive Engineers.

FY 2007 Presentations

1. D. J. Torres, "KIVA-4 Development", Advanced Engine Combustion Working Group Meeting, Detroit, October 2007.

2. D. J. Torres, "KIVA Modeling to Support Diesel Combustion Research", DOE National Laboratory Advanced Combustion Engine R&D, Merit Review, Washington, D.C., June 2007.

3. D.J. Torres, "Collocated KIVA-4", International Multidimensional Engine Modeling User's Group Meeting, April 2007.

4. D.J. Torres, "KIVA-4 Development", Advanced Engine Combustion Working Group Meeting, Livermore, February 2007.

II.A.12 Chemical Kinetic Modeling of Combustion of Automotive Fuels

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Objectives

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

Accomplishments

- Developed a chemical kinetic model for n-hexadecane, a primary reference fuel for diesel fuel, and a realistic representation of n-alkanes in diesel fuels.
- Developed understanding of the chemical kinetics that control HCCI combustion under boosted conditions using LLNL surrogate fuel models and Sandia HCCI engine data.
- Developed a chemical kinetic model for methyl decanoate, a realistic component to represent methyl esters contained in biodiesel.

Future Directions

- Extend model capabilities to additional new classes of fuel components, including hepta-methyl-nonane which is a primary reference fuel for diesel fuel and represents iso-alkanes in diesel fuel.
- Further validate chemical kinetic model for n-hexadecane.
- Continue development of increasingly complex surrogate fuel mixtures to represent fuels for HCCI and diesel engines.
- Increase collaborations with programs outside LLNL dealing with automotive and heavy-duty truck fuel issues.

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Introduction

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

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

Approach

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

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

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

Results

During the last year we completed chemical mechanisms for important components to include in surrogate models for diesel and bio-derived fuels. These components are n-hexadecane and methyl-decanoate (Figure 1). First, an n-hexadecane mechanism was developed to represent n-alkanes in diesel fuel. n-Hexadecane is a primary reference fuel for diesel fuel and is an important component to include in a diesel surrogate fuel model as recommended by the diesel research community [1]. Assembling a mechanism for n-hexadecane is very ambitious since it requires the inclusion of thousands of chemical species and reactions. The thermodynamic properties of each species and the rate constant of each reaction must be estimated. These estimations are performed by group additivity for the thermodynamic parameters and by established rules for the reaction rates [2]. The reaction mechanism addresses low temperature chemistry that is essential for simulation of low-temperature combustion in diesel engines. Low-temperature combustion strategies can lead to low soot and NOx emissions in diesel engines. The mechanism includes the reactions to address the oxidation and pyrolysis of n-alkanes from n-propane to n-hexadecane. It is built in a modular fashion so that users can easily pare down the mechanism from the full mechanism of 2,116 species and 8,130 reactions for n-hexadecane to a smaller mechanism of 940 species and 3,878 reactions for n-decane. Comparisons of computed results for n-decane and experimental data are shown in Figures 2 and 3. Figure 2 shows ignition delay times for n-decane and n-heptane from the chemical kinetics model and measured in a shock tube. The initial conditions for the ignition delay times are stoichiometric fuel/air mixtures, 13.5 bar and 670 K-1,350 K, conditions that are highly relevant to diesel and HCCI engines. The n-decane and n-heptane chemical kinetic models are able to reproduce the measured behavior over the entire temperature range including the critical region (700-800 K) important for low-temperature combustion. In Figure 3, results of the model are compared to measurements in a jet-stirred reactor [3]. These experiments were performed for stoichiometric mixtures of n-decane in O_2/N_2 at 10 atm and 750-1,100 K which are also conditions that are highly relevant to those in diesel and HCCI engines. The n-decane chemical kinetic model performed quite well, mimicking the experimental behavior for

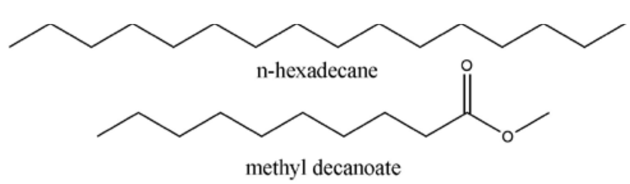

FIGURE 1. Molecular Structure of n-Hexadecane and Methyl-Decanoate

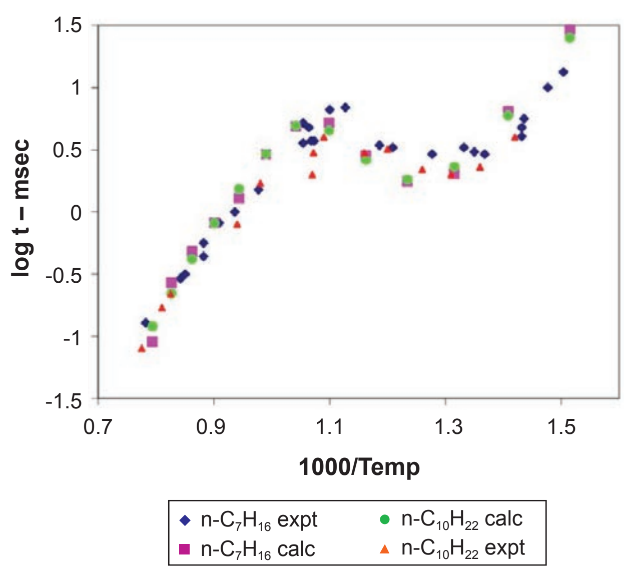

FIGURE 2. Shock tube ignition delay times for n-heptane and n-decane, all at 13.5 bar pressure and stoichiometric fuel/air. Experiments are from Ciezki and Adomeit [9] and Pfahl et al. [10]. n-Heptane computed results from ref [2].

the intermediate species concentrations as a function of reactor temperature. These results show that the evolution of species as the reaction proceeds from fuel/O_2/N_2 to products is being properly reproduced by the model at engine-like conditions. This chemical kinetic model is now available to the DOE supported Advanced Engine Combustion and HCCI University Working Groups for use in modeling engine combustion.

The second new fuel that was added as a surrogate fuel model was methyl decanoate (Figure 1). It is a large molecular weight methyl ester species to represent biodiesel fuel. Again, mapping out the reaction paths, estimating the thermodynamic properties for the needed species, and estimating the reaction rates was a very ambitious project. The thermodynamic property of each species needs to be estimated by group additivity and the reaction rate constants acquired from reaction rate rules. The reaction mechanism consists of 3,034 species and 8,580 reactions. The chemical kinetic model was validated by comparison to high pressure experiments in a jet stirred reactor at 800-1,040 K and 10 atm (Figure 4). These conditions are relevant to diesel and HCCI engine conditions. The agreement between the biodiesel surrogate (methyl decanoate) and the rapeseed derived methyl esters is very good. The biodiesel surrogate correctly simulates the early formation of CO_2 that is observed in the oxidation of esters. This early formation of CO_2 "wastes" some of the oxygen in the fuel that would otherwise help to reduce soot under diesel conditions [4]. Next the methyldecanoate model was used to simulate experiments in a single-cylinder engine [5] (Figure 5). The model was able to simulate the early formation of CO_2 in the engine and the evolution of intermediate products (CO and aldehydes). This chemical kinetic model represents a new capability to model biodiesel combustion in engines.

Finally, we investigated the behavior of an HCCI engine with increasing boost pressure and its effect on combustion phasing. Increasing the boost pressure is an important way to increase the load range for a HCCI engine. As boost pressure is increased and the intake temperature decreased, the combustion phasing is uniquely affected due to the onset of low temperature chemistry [6,7]. For reactive fuels such as gasoline, PRF80, and methylcyclohexane, the intake temperature must be reduced significantly to maintain combustion phasing at top dead center (TDC) as the intake pressure is increased [6]. This is due to the increased reactivity from the onset of low temperature chemistry at high intake pressure and low intake temperature.

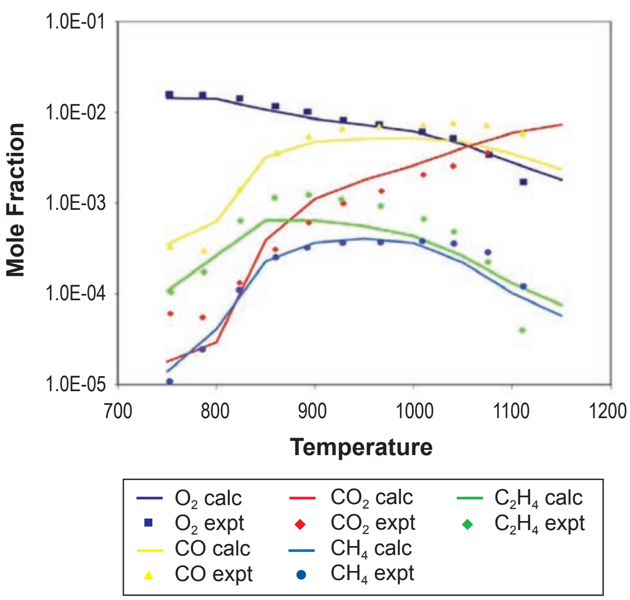

FIGURE 3. Chemical species concentrations in a jet stirred reactor for stoichiometric n-decane/O_2/N_2 mixtures at 10 atm and a residence time of 0.5 sec. n-Decane inlet mole fraction is 1,000 PPM. Lines represent computed values, symbols are experimental results [3].

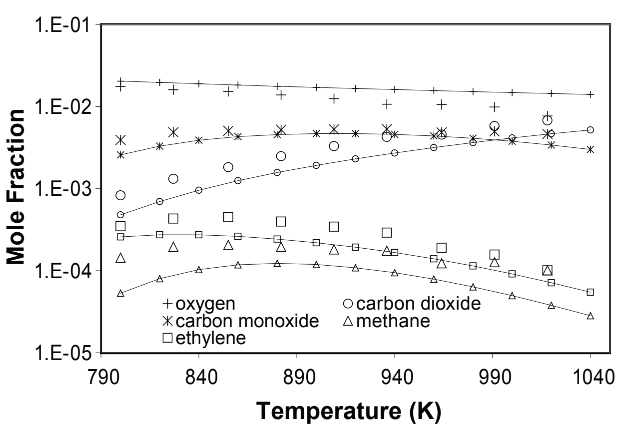

FIGURE 4. Comparison of the methyl decanoate model with rapeseed oil methyl ester experiments in a jet stirred reactor (P = 10 atm, equivalence ratio = 0.5, residence time = 1 s) [11].

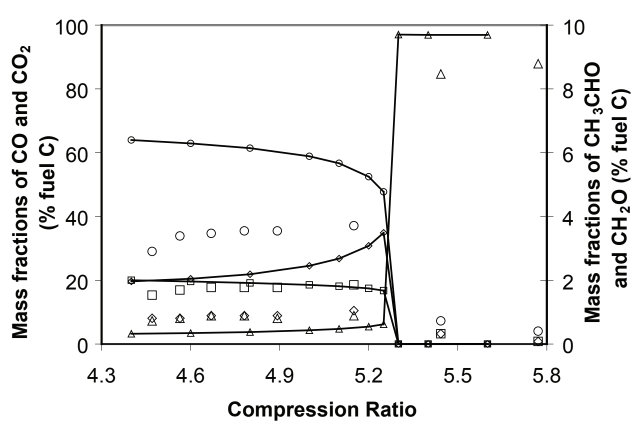

FIGURE 5. Comparison of methyl decanoate simulations in a CFR engine with experiments. Mass fractions of CO (◊), CO_2 (∆), CH_2O (O) and CH_3CHO (□) at an equivalence ratio of 0.25. Open symbols correspond to experiments [5] and lines to simulations.

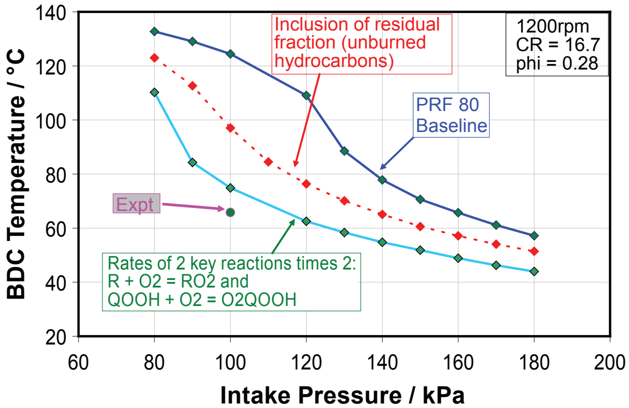

FIGURE 6. Bottom-dead-center (BDC) temperature required to maintain top-dead-center phasing in an HCCI engine. The model used is the LLNL primary reference fuel (PRF) model for gasoline. The fuel is PRF80 and the equivalence ratio is 0.28. The blue curve is for the baseline simulation. The red curve is when residuals left over from the previous cycle are included. The turquoise curve is when the rate constants of two key reaction rates are increased. The pink point is an experimental point take in an HCCI engine at Sandia National Laboratories [8].

In our recently submitted paper [7], we tested the ability of LLNL chemical kinetics models for gasoline, cyclohexane and PRF80 to simulate this behavior with increased boost pressure. We found that the inclusion of residual fractions from the previous cycle was critically important in these calculations because it sensitizes the next cycle so that reaction begins at an earlier time. We also found that the behavior was highly sensitive to two key reactions that lead to low temperature reactions,

$$R + O_2 = RO_2$$

$$QOOH + O_2 = O_2QOOH$$

(where R is a fuel molecule with one H atom removed and Q is a hydrocarbon structure representing the fuel with two H-atoms removed). Figure 6 shows the bottom dead center (BDC) temperature required to maintain TDC combustion phasing as the intake pressure is increased. The figure shows a baseline calculation with the LLNL chemical kinetic model for PRF80 and then the effect of including residual fraction in these calculations. The one experimental point available from Sjöberg and Dec's HCCI engine at Sandia [8] is also shown. The inclusion of residual fraction results in a better comparison to the experiment. Additionally, increasing the rate constants of the key reactions above improves the agreement with experiment and shows the importance of these reactions in controlling HCCI behavior with increased boost pressure.

Conclusions

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

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1. Westbrook, C. K., Pitz, W. J., Herbinet, O., Silke, E. J. and Curran, H. J., "A Detailed Chemical Kinetic Reaction Mechanism for n-Alkane Hydrocarbons from n-Octane to n-Hexadecane," Fall Meeting Western States Section of the Combustion Institute, Livermore, CA, 2007.

2. Silke, E. J., Pitz, W. J. Westbrook, C. K., Sjöberg, M., Dec, J. E., "Understanding the Chemical Effects of Increased Boost Pressure under HCCI Conditions", 2008 SAE World Congress, Detroit, MI, submitted, 2007.

3. Herbinet, O., Pitz, W. J. and Westbrook, C. K., "Detailed Chemical Kinetic Oxidation Mechanism for a Biodiesel Surrogate," Fall Meeting of the Western States Section of the Combustion Institute, Livermore, CA, 2007.

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1. Westbrook, C. K., Pitz, W. J., Herbinet, O., Silke, E. J. and Curran, H. J., "A Detailed Chemical Kinetic Reaction Mechanism for n-Alkane Hydrocarbons from n-Octane to n-Hexadecane," Fall Meeting Western States Section of the Combustion Institute, Livermore, CA, 2007.

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3. C. K. Westbrook, W. J. Pitz, O. Herbinet, and E. Silke, "Chemical Kinetics Modeling of Large n-Alkanes up to n-Hexadecane", Advanced Engine Combustion Working Group Meeting, Southfield, MI, October, 2007.

4. O. Herbinet, "Chemical Kinetics Modeling of a Biodiesel Surrogate", Advanced Engine Combustion Working Group Meeting, Southfield, MI, October, 2007.

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

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Objectives

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

Accomplishments

- Achieved and demonstrated 2007 FreedomCAR goal of 42% peak BTE on two light-duty diesel engines.
- Completed installation of modern engine platform donated to ORNL by General Motors (GM).
- Developed thermodynamic analysis methods for use with engine simulation codes as well as experimental data to evaluate potential opportunities for waste heat recovery (WHR).
- Demonstrated potential of advanced combustion operation for achieving Tier 2 Bin 5 emissions regulations.
- Improved interactions with other national laboratories, universities, and industry through the Advanced Engine Combustion (AEC) working group, Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) working group, and other forums.

Future Directions

- Characterize thermodynamic availability of engine system components (*e.g.*, exhaust gas recirculation [EGR] system, exhaust system, etc.) over the speed-load range of the engine.
- Evaluate potential efficiency benefits of bottoming cycle for WHR from the EGR system, exhaust system, etc.
- Investigate low-temperature combustion (LTC) approaches on the GM 1.9-L engine for reducing aftertreatment needs and improving overall system efficiency.
- Develop model of the GM 1.9-L and auxiliary systems for evaluating potential efficiency benefits of advanced technologies including variable valve actuation.

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Introduction

Modern light-duty diesel engines have peak BTEs in the range 38-40% for high-load operation and considerably lower efficiencies for part-load operation. The FreedomCAR roadmap has established several goals over the next several years with a 45% peak efficiency being demonstrated in 2010, while meeting the Tier 2, Bin 5 emissions levels. The objective of this project is not to develop all the necessary technology to meet the efficiency and emissions goals but to serve as a focus for the integration of technologies into a multi-cylinder engine platform and to provide a means of identifying pathways for improved engine efficiency.

Approach

This activity makes use of knowledge discovery from internal ORNL activities, other national laboratories, universities, and industry. Internal activities include those focused on advanced combustion operation, aftertreatment, fuels, and novel or unconventional approaches to stretch efficiency. Significant external contributions occur through regular interactions with the AEC working group administered by Sandia National Laboratories and the CLEERS working group administered by ORNL.

Significant improvements in efficiency require new insight into understanding loss mechanisms as well as identifying efficiency opportunities. A Second Law of Thermodynamics perspective is being used toward this purpose and to provide guidance on developing and evaluating a path for meeting 2010 as well as intermediate milestones.

The following methodology will be used in this activity:

1. Establish baseline for modern light-duty diesel engine.
2. Acquire and/or develop models to characterize loss mechanisms.
3. Conceive methods to mitigate losses.

4. Evaluate methods (paths) with system models.
5. Integrate technologies and methods into engine experiments to characterize effects on BTE and emissions.

Technologies for improving efficiency and emissions in light-duty diesel engines are being investigated at ORNL on a highly modified Mercedes-Benz (MB) 1.7-L common rail four-cylinder diesel engine and a GM 1.9-L common rail four-cylinder diesel engine. These engines are equipped with microprocessor-based dSpace control systems which permit unconstrained access to engine hardware including the integration of custom control algorithms. The GM engine also has an electronic control unit donated by GM which allows for the monitoring and manipulation of the base engine calibration.

Results

A peak brake thermal efficiency of 42% was demonstrated on a GM 1.9-L engine satisfying a Joule milestone in Vehicle Technologies. The engine was donated by GM and is equipped with state-of-the-art features including a versatile microprocessor-based control system, variable geometry turbocharging, and common-rail fuel injection capable of multiple injections. Integrated control of the turbocharger and fuel injection phasing were critical to reaching this level of engine efficiency. This efficiency milestone was also achieved intermittently on a modified 1999 MB 1.7-L diesel engine. Efficiency results are shown in Figure 1 with comparisons to measured original equipment manufacturer (OEM) peak BTE.

A 1.9-L GM engine was commissioned at ORNL in FY 2007 and will eventually be the primary engine platform for this activity. A preliminary mapping of the performance and emissions characteristics of the engine at 36 speed-load combinations was performed to satisfy an interim FY 2007 milestone. BTE as a function of speed and load is shown in Figure 2. A peak BTE of approximately 40% was initially observed on this engine, which was considerably lower than the 42% expected based on the open literature and discussions with GM. The reduced peak BTE is most likely due to a non-optimized calibration for lower cetane U.S. diesel fuel and/or the engine not being sufficiently broken-in. A more detailed map (~120 speed-load combinations) is scheduled to be performed in FY 2008. The more detailed map will be used for calibrating a full engine model as well as for estimating thermodynamic availability and the potential of WHR across the speed-load range.

Meeting 2010 and interim BTE milestones will require some form of energy recovery from the engine system. Potential sources of recoverable energy are summarized in Figure 3. WHR in light-duty diesel engines has not been significantly explored due to the light-load operation common to this engine platform where engine temperatures are low. With LTC (or high dilution) combustion modes being implemented more and more to reduce emissions, a significant amount of heat rejection is necessary in the EGR system. This increased heat rejection is an opportunity for low-load WHR where pre-turbo exhaust/EGR temperatures are high. The implementation of WHR with modern advanced engines will require the consideration of numerous issues:

- Source, quality, and recovery method of energy.
- Integration with other technologies such as LTC operation, turbo-compounding, variable valve actuation, aftertreatment, etc.

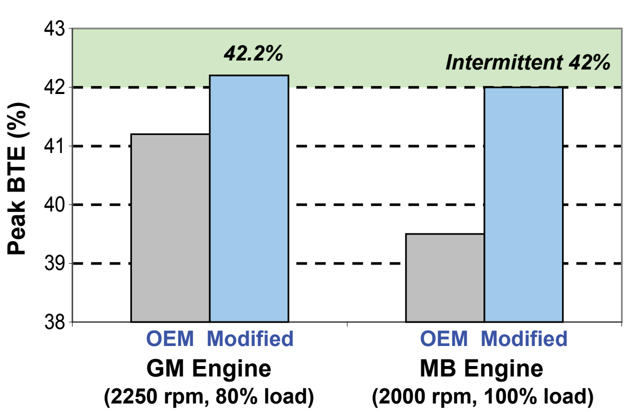

FIGURE 1. Maximum BTE Achieved on GM and MB Light-Duty Diesel Engines (Also shown for reference is the peak BTE of the OEM calibrations.)

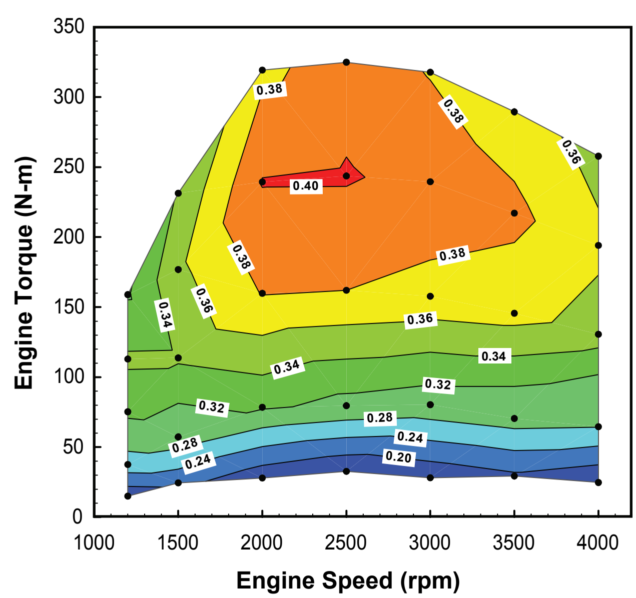

FIGURE 2. Preliminary Performance Mapping of GM 1.9-L Light-Duty Diesel Engine with 2007 Ultra-Low Sulfur Diesel Fuel

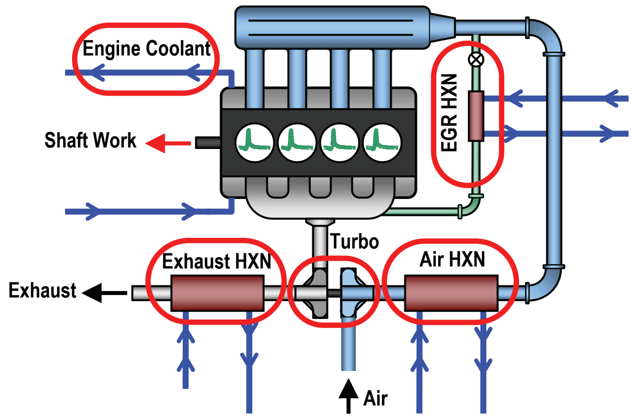

FIGURE 3. Schematic of Engine System with Potential Sources for Recovery of Waste Energy

- Potential benefits across the speed-load range of engine.
- Reintroduction of recovered energy to engine system.

A thermodynamic Second Law perspective is important for managing these issues as well as evaluating efficiency opportunities and providing guidance on developing and evaluating a plan for meeting 2010 as well as intermediate milestones. Analysis routines have been developed for use with WAVE™ and GT Power™ engine simulation codes for identifying availability and loss mechanisms for individual components. An example of a Second Law characterization of the MB engine simulation at 2,000 rpm, 100% load is shown in Figure 4 (a) with no insulation on exhaust manifold and (b) with insulation on exhaust manifold. This analysis is useful for evaluating the potential of different strategies (experiment and simulation) on the availability of unused energy from engine system components. For example in Figure 4, adding insulation from to the exhaust manifold results in an increase from 10% to 14% availability in the exhaust stream. As mentioned above, this perspective will also be critical in the thermal management of complicated engine-systems, which may include a combination of technologies competing for the same thermal resources.

Advanced combustion strategies were used as the primary method of achieving reduced emissions and were focused on the MB 1.7-L for FY 2007. Four speed-load conditions and weighting factors were used to estimate the magnitude of drive cycle emissions for advanced combustion operation. ORNL is working with the Advanced Combustion & Emissions Controls Technical Team to re-evaluate these modal conditions for estimating drive-cycle emissions and to suggest a new set of conditions if appropriate. The composite emissions estimates for high-efficiency, clean combustion (HECC) operation are shown in Figure 5 and compared to U.S.

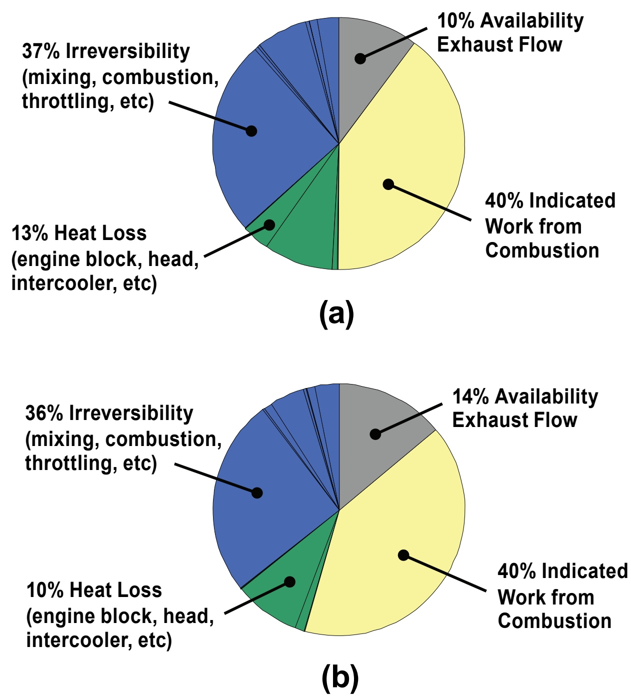

FIGURE 4. Example of Second Law Characterization of Fuel Energy for MB Engine Simulation at 2,000 RPM and 100% Load with (a) No Insulation on Exhaust Manifold and (b) Insulation on Exhaust Manifold

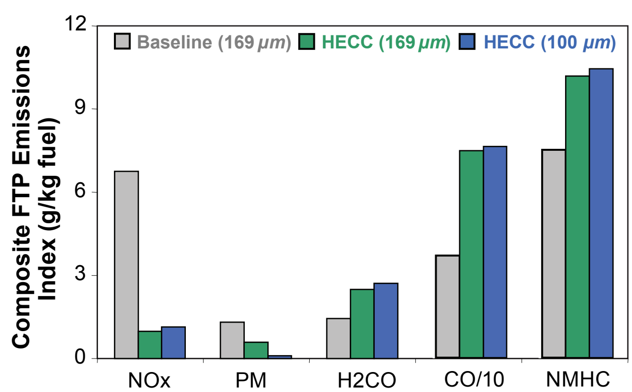

FIGURE 5. Composite Emissions Indices Based on Steady-State Modal Conditions Representative of the FTP Drive-Cycle

Tier 2 Bin 5 regulatory standards in Table 1. Recall that these emissions estimates are based on steady-state data from a fully warm engine and do not include important effects associated with cold-start and transient load-speed operation. Examination of Table 1 indicates some form of aftertreatment will most likely still be required for the form of HECC used in this activity. While significant in-cylinder NOx reduction was achieved and dramatically reduces the NOx aftertreatment requirement, HC and CO emissions were increased in the process, resulting in the need for increased aftertreatment oxidation as compared to conventional operation. Also note that a diesel particulate filter was used in the low-pressure EGR system and is necessary to meet the engine-out HECC emissions values shown in Table 1. In the future, simultaneous improvements in efficiency and emissions will most likely involve a combination of advanced combustion operation working synergistically with the appropriate aftertreatment technologies. The reader is encouraged to reference the publications/presentations list for more information.

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

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

A long range path is being developed at ORNL through thermodynamic analysis as described above and experiments/modeling in LTC, waste heat utilization, and thermal management. A summary of technologies and status are summarized below:

- **Advanced Combustion.** Continued leveraging with existing ORNL activity on light-duty diesel HECC as well as other DOE sponsored activities at national laboratories, universities, and industry.
- **Waste Heat Recovery.** Continued development and implementation of WHR systems for recovering energy from the EGR cooler, air charge cooler, and post-turbocharger exhaust system.
- **Turbo-Compounding.** In discussion with Woodward and BorgWarner to evaluate hydraulically or mechanically coupled turbo-compounding concept for light-duty diesel engines.
- **Variable Valve Actuation.** Potential of this approach for improved efficiency is being evaluated with simulation models. Implementation would most likely be cam phase system developed by Delphi.
- **Friction Reducers.** Multiple projects recently proposed at ORNL and elsewhere to evaluate coatings for advanced combustion and novel lubricants including ionic fluids.

Conclusions

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

- The 2007 FreedomCAR goal of 42% peak BTE was demonstrated on a 2005 GM 1.9-L and a modified 1999 MB 1.7-L light-duty diesel engines. Enablers for meeting this milestone on both engines included variable geometry turbochargers, revised fuel injection parameters, and control of air temperature.
- A GM 1.9-L engine with flexible control systems was commissioned at ORNL. This engine geometry is being used at Sandia National Laboratories (optical single-cylinder engine), Lawrence Livermore National Laboratory (modeling), and the University of Wisconsin (metal single-cylinder and multi-cylinder engines) and has resulted in improved collaboration in DOE funded activities in support of meeting FreedcomCAR efficiency and emissions milestones.
- Improved thermodynamic analysis methods were developed for use with engine simulation codes as well as experimental data.
- The potential of advanced combustion strategies for achieving Tier 2 Bin 5 emission levels was investigated on the MB 1.7-L engine.

FY 2007 Publications/Presentations

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

2. K. D. Edwards et al., "Identification of Potential Efficiency Opportunities in Internal Combustion Engines Using a Detailed Thermodynamic Analysis of Engine Simulation Results", 2007 AEC Working Group Meeting at USCAR (Southfield, MI; September 2007).

3. K. D. Edwards et al., "Identification of Potential Efficiency Opportunities in Internal Combustion Engines Using a Detailed Thermodynamic Analysis of Engine Simulation Results", Diesel Cross-Cut Team meeting (Southfield, MI; July 2007).

4. R. M. Wagner et al., "Modeling and Experiments to Achieve High-Efficiency Clean Combustion (HECC) in LD Diesel Engines", Advanced Combustion & Emissions Control Technical Team meeting (Southfield, MI; July 2007).

5. K. D. Edwards, R. M. Wagner, S. P. Huff, R. L. Graves, "A Thermodynamic Analysis of WAVE Engine Models for Identifying Potential Opportunities for Improving Efficiency in Internal Combustion Engines", 2007 Ricardo Software North American Users Conference (Plymouth, MI; June 2007). *Invited.*

6. R. M. Wagner et al., "Modeling and Experiments to Achieve High-Efficiency Clean Combustion (HECC) in LD Diesel Engines", 2007 Department of Energy (DOE) Advanced Combustion Engines Merit Review (Washington, D.C.; June 2007).

7. C. Scott Sluder, R. M. Wagner, "An Estimate of Diesel High-Efficiency Clean Combustion Impacts on FTP-75 After-treatment Needs", 2006 Powertrain & Fluid Systems Conference (Toronto, Ontario Canada; October 2006).

Special Recognitions & Awards/Patents Issued

1. DOE EERE Weekly Report.

2. ACEC Technical Team summary to USCAR Board of Directors.

3. ACEC Technical Team highlight.

4. FreedomCAR Technical Highlight in 2007.

II.A.14 Hydrogen Free Piston Engine

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Objectives

- Optimize and quantify the efficiency of the linear alternator and associated control circuitry when utilized in a plug-in hybrid battery charger application.
- Design opposed piston research experiment.
- In collaboration with General Motors (GM) and the University of Michigan, assess the performance of a free piston generator as the auxiliary power unit (APU) in a series hybrid vehicle.
- Improve the efficiency of small output (30 kW) reciprocating generators by at least 20%, along with reduced emissions.

Approach

- Utilize Flux2D (electromagnetic analysis software), Mathematica-based model, and MATLAB/Simulink to optimize the Sandia-designed linear alternator for a battery charging application.
- Use PSpice to analyze and understand the voltage/current relationships.
- Recruit Ph.D. student and post-doc to replace moving-on students.
- Design the research experiment utilizing SolidWorks/COSMOS and experience base available from Sandia's Combustion Research Facility.
- Utilize homogeneous charge compression ignition combustion of lean mixtures to achieve the 20% efficiency improvement and emissions reductions via low-temperature combustion.

Accomplishments

- Developed linear alternator/multi-level converter configuration calculated to exceed 30 kW power output charging a battery at greater than 95% conversion efficiency.
- Hired Nan Jiang as a post-doc (University of Minnesota) and Jerry Fuschetto as a Ph.D. student (University of Michigan).
- Determined with collaborators that the opposed piston concept is preferred for hybrid vehicle applications due to its capability to operate independently of other units (due to self balance).
- Developed opposed piston research experiment design.

Future Directions

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

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Introduction

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

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

Approach

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

This year, our research activities concentrated on utilizing and optimizing numerical codes and waveform aids, modeling the linear alternator/electrical power management system for a battery charging application (plug-in hybrid), and designing the opposed piston experiment intended to quantify the indicated efficiency of a hydrogen-fueled APU. Our collaborators (GM and the University of Michigan) have concentrated on a ground-up hybrid vehicle model to optimize the size and configuration of the free piston APU.

Results

The most important result of the past year is the modeling result of the battery charging application required for hybrid vehicle optimization (particularly plug-in hybrid). Figure 2 shows the output energy per coil per cycle as a function of battery state of charge. The plot shows that the linear alternator is able to operate at full output power and charge the battery at this rate over a broad range of battery state of charge, essentially from fully discharged to fully charged.

The electrical configuration utilized is a multi-level converter approach. In this implementation each alternator coil (21 coils in our design) is matched to a single battery unit optimized in size to match the coil output. Figure 3 displays an individual coil/battery circuit. The solid state switches in the center (rectifier) are controlled to rectify the alternating, variable frequency output of the linear alternator, charging the battery shown in the center of the circuit. The solid state switches on the right (converter) side are controlled to assemble a sinusoidal output approximation, where each of seven batteries is added to form a single phase of a three phase output (there are three each of seven

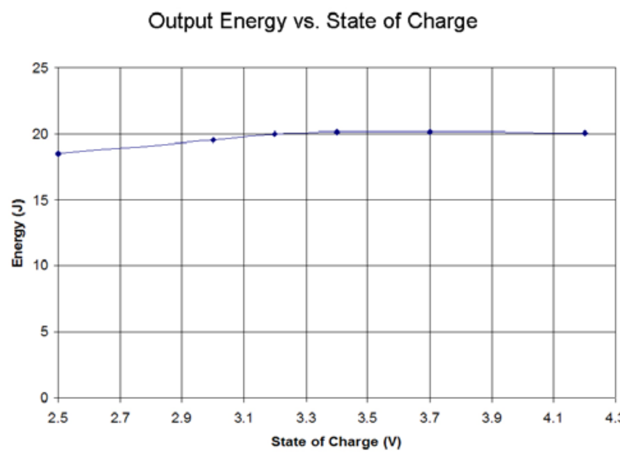

FIGURE 2. Output Energy per Coil per Cycle as a Function of Battery Cell State of Charge

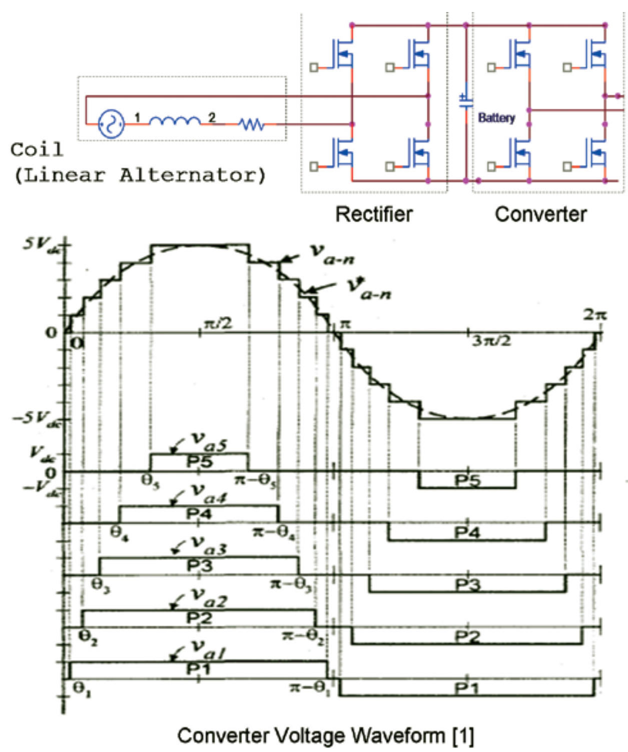

FIGURE 3. Electrical Circuit of Individual Coil/Rectifier/Battery/Converter and Converter Output Voltage Waveform

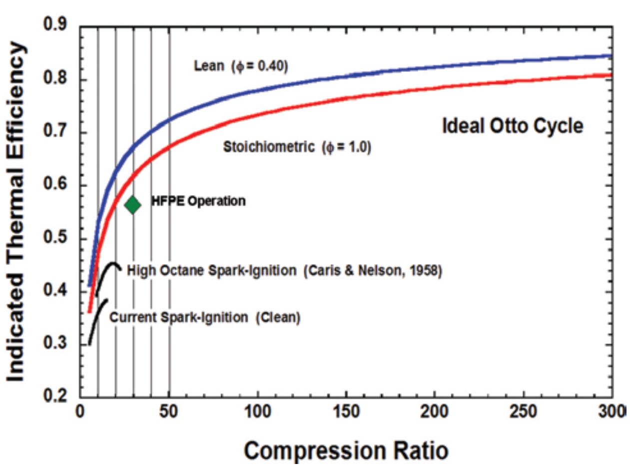

FIGURE 1. Indicated Efficiency as a Function of Compression Ratio – Ideal and Actual

battery phases). This output waveform construction is shown at the bottom of Figure 3.

This configuration has three significant attributes. First, the charging operation is independent of the motor driving application, yet all batteries can be maintained at the desired state of charge by varying how much of each individual battery output is utilized in constructing the approximate sine wave motor driving waveform. Second, the controlled switches have losses of less than 1% of the output power, far less than diodes. Third, individual battery voltage can be maintained in the 50 V range, not posing any significant personnel hazard in a maintenance or accident scenario. Tolbert et al [1] has more details on multi-level converters.

Another significant effort involved modifying the Sandia-designed linear alternator for higher efficiency. Figure 4 shows the linear alternator mechanical-to-electrical output efficiency as a function of stator weight. Note that a rather small increase in weight results in a significant efficiency increase, with 95% achievable at small cost.

The final electrical optimization is shown in Figure 5. Power output per coil per stroke is shown for four various switching/capacitance combinations. The synchronous rectifier scheme controls the switches to behave like diodes and is the starting point. It can be seen that modifying the switching parameters can improve the power out by 15%, but adding a snubber/switch/capacitor can increase the output by 70%. Ron Moses, our former Los Alamos National Laboratory collaborator now retired, has developed the snubber concept.

Figure 6 shows the SolidWorks model of the opposed piston experiment. We will soon begin procuring the parts to assemble the device. We are working closely with C. Lee Cook Corporation, a builder of high pressure compressors and the supplier of piston rings for the optical engines in Sandia's Combustion Research Facility. We plan on using Cook as the prime supplier of the cylinders and pistons.

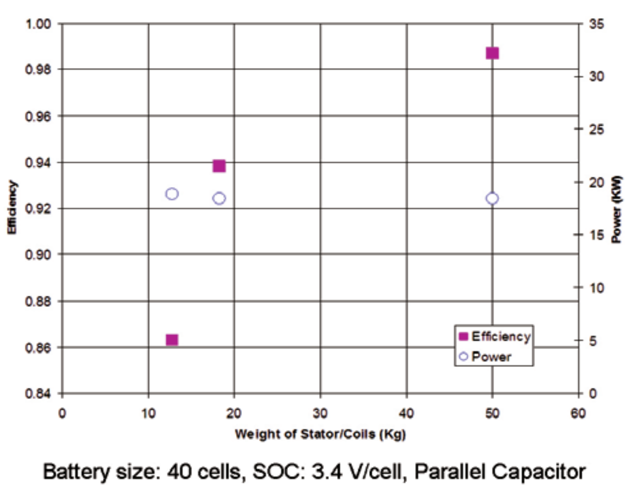

FIGURE 4. Power Output and Conversion Efficiency as a Function of Stator Weight

Conclusions

- The free piston/linear alternator generator is capable of charging a battery in a series/plug-in hybrid powertrain configuration at high efficiency (95%) and over a wide state of battery charge.
- Power output from the linear alternator can be significantly increased (70%) by application of snubber capacitors and computer controlled switches.
- Opposed piston design continues to have attractive features for prototype and for hybrid vehicles where low power output is often required.
- Prototype fabrication and characterization are on track to begin this fiscal year.

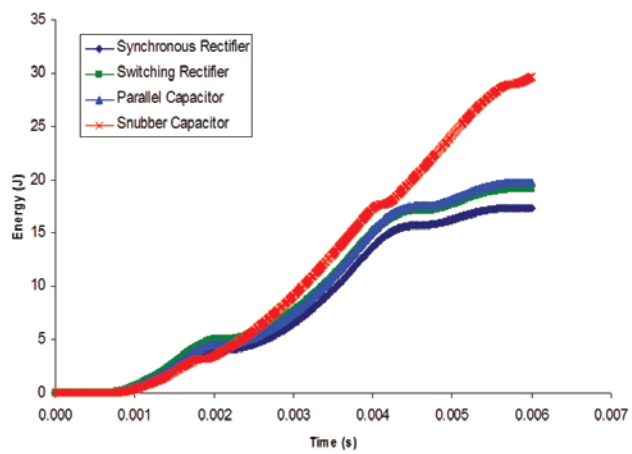

FIGURE 5. Energy Output per Coil per Cycle for Various Rectification Approaches

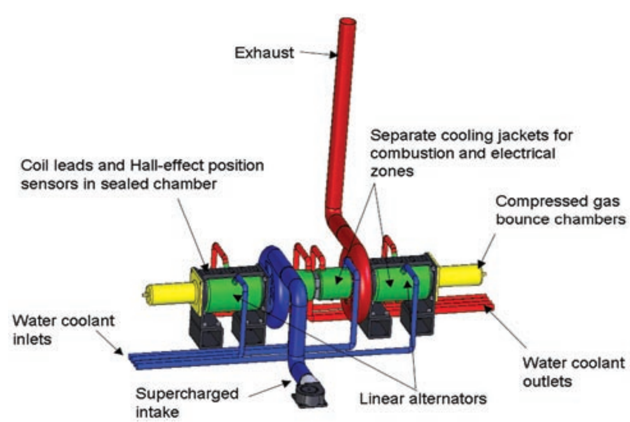

FIGURE 6. Solid Model of Opposed Piston Experiment

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

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Objectives

- Quantify the efficiency and emissions behavior of a hydrogen-powered combustion engine with particular focus on direct injection operation.
- Optimize the hydrogen combustion engine through improved injection strategies, multiple injection and injector nozzle designs.
- Demonstrate the potential of advanced diagnostic tools (endoscope imaging and spectroscopy) for optimization of hydrogen engine operation.

Accomplishments

- Characterized the influence of injection timing on engine efficiency and emissions in direct injection operation.
- Determined that nozzle design significantly influences brake thermal efficiency and emissions (2% increase in brake thermal efficiency and 47% decrease in nitrogen oxide [NOx] emissions at low engine load with changed nozzle design).
- Captured images of a multiple injection strategy.
- Performed and refined spectroscopic gas temperature measurements.
- Installed new cylinder head with central and side injector locations – specific injector nozzles designed and manufactured for either location.
- Expanded existing collaboration with Ford, BMW and the European HyICE consortium.

Future Directions

- Expand engine testing to include central direct injection in addition to current side injection location (new cylinder head provided by Ford Motor Company).
- Evaluate newly designed injector nozzles for performance and emissions benefits.
- Analyze the potential of water injection.
- Conduct test runs at higher engine speed conditions to evaluate the high-flow performance of the improved injectors.
- Evaluate hydrogen direct injection in a multi-cylinder engine (separate project proposal for FY 2008).

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Introduction

In order to achieve the targets for hydrogen engines set by the U.S. Department of Energy (DOE) – a brake thermal efficiency of 45% and NOx emissions below 0.07 g/mi – while maintaining the same power density as comparable gasoline engines, researchers need to investigate advanced mixture formation and combustion strategies for hydrogen internal combustion engines. Hydrogen direct injection is a very promising approach to meeting DOE targets; however, there are several challenges to be overcome in order to establish this technology as a viable pathway toward a sustainable hydrogen infrastructure.

Approach

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

This report describes the use of endoscopic imaging as a diagnostic tool that allows further insight into the processes that occur during hydrogen combustion. It also addresses recent progress in the development of advanced direct-injected hydrogen internal combustion engine concepts.

The hydrogen combustion behavior in a single-cylinder research engine is characterized and an analysis of the results of hydrogen direct-injection operation is performed. In addition to conventional combustion analysis, which employs pressure traces and derived information (e.g., rate of heat release) as well as emissions measurement, the combustion characterization is performed by using an ultraviolet (UV)-transmitting endoscope in combination with an intensified charge-coupled device (ICCD) camera. By using this technique, we were able to obtain a two-dimensional optical signature of hydrogen combustion, even at high engine speeds and loads. Analysis of the optical information allowed us to draw conclusions about the mixture homogeneity and possible stratification effects for different injection strategies.

Results

For the results shown, the injector was located on the intake side of the combustion chamber between the intake valves. Because of the 4-valve configuration with split intake ports, there is sufficient space available to accommodate the injector, as well as the hydrogen supply to the injector.

Influence of Injection Timing on Mixture Distribution and Emissions Behavior

Injection timing during hydrogen direct-injection operation has a crucial influence on the mixture distribution and, therefore, on the combustion characteristics. With early injection (shortly after intake valve closing) the injected fuel has sufficient time to mix with the air inside the combustion chamber and form an almost-homogenous mixture. With late injection, only limited time for mixing is available, resulting in a stratified charge at spark timing. This basic trend has also been shown by three-dimensional computational fluid dynamics (CFD) simulation tools [1].

The impact of this trend on NOx emissions is highly dependent on the engine load i.e. overall fuel/air equivalence ratio (Figure 1). At low engine loads (low ϕ) and unthrottled operation, early injection results in extremely low NO_x emissions because the mixture at ignition timing is very likely to be homogeneous. Thus, the lean homogeneous mixture burns without forming NOx emissions. Late injection at low loads, on the other hand, results in a stratified mixture with hydrogen-rich zones, as well as zones with very lean mixtures – or even pure air. Although the overall mixture is still lean, the combustion of rich zones causes a significant increase in NOx emissions. At high engine loads (high ϕ), this trend appears to be inverted. Early injection results in homogeneous mixtures that approach stoichiometry and produce high NOx emissions. Late injection is expected to result in stratification, with zones that are even richer than stoichiometric, along with lean zones. This kind of stratification avoids the NOx critical air/fuel ratio regime of ϕ~0.75 and thereby reduces overall NO_x emissions.

The above-described trends can be seen in analyzing the cylinder pressure and rate of heat release (ROHR) traces shown in Figure 2. The black lines represent early injection (start of injection [SOI] = 120° crank angle before top dead center [CA BTDC])and the grey lines represent late injection (SOI = 60°CA BTDC) at medium engine load (wide-open throttle, fuel/air equivalence ratio of ϕ~0.47, indicated mean effective pressure (IMEP) of ~6 bar. The rather homogenous mixture resulting from early injection (black line) requires an earlier spark timing (11°CA BTDC) than the late injection (6°CA BTDC) to achieve optimal combustion phasing. The overall lean and homogenous mixture with early injection also results in distinctively longer combustion duration (~35°CA) than the stratified case with late injection (~25°CA). Although the rate of pressure increase is higher with the stratified mixture than in the homogenous case, the peak pressures are almost identical, due to the earlier spark timing with early injection.

Influence of Injector Nozzle Geometry on Mixture Distribution, Emissions Behavior and Efficiency

The lean-burn capabilities of hydrogen are superior to those of any other fuel. The theoretical flammability limits of hydrogen in air are in a range of $0.09 < \phi < 2.0$ (gasoline: $0.7 < \phi < 2.5$) [2]. Although these wide flammability limits allow for homogenous unthrottled

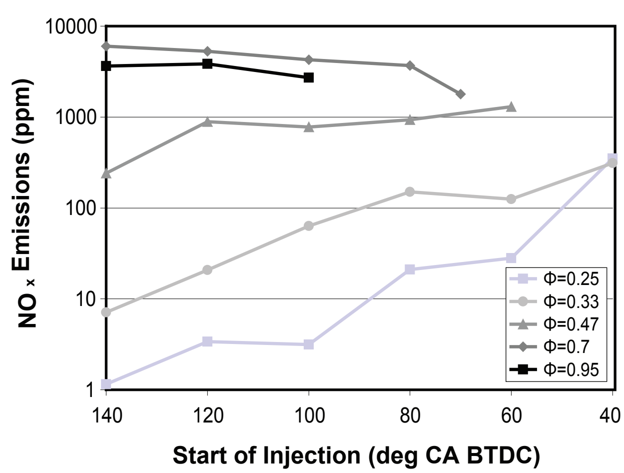

FIGURE 1. Influence of Injection Timing And Engine Load (Fuel/Air Equivalence Ratio) on NOx Emissions

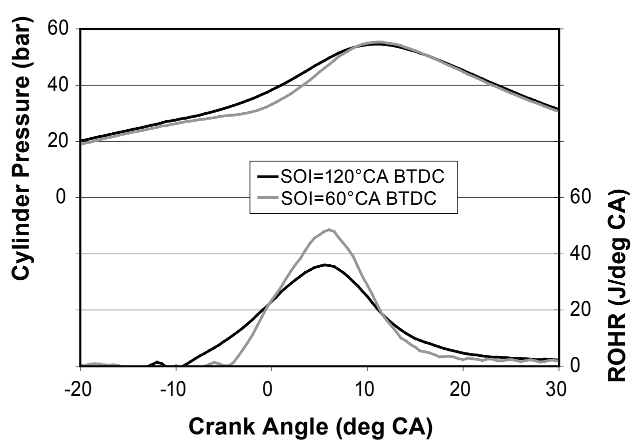

FIGURE 2. Comparison of Pressure Traces and Heat Release Rate with Variation of SOI at Medium Load

operation even under idling conditions, in many cases, more efficient engine operation can be realized with stratification.

Two different injector configurations were tested in an attempt to evaluate the influence of nozzle configuration on mixture stratification (Figure 3). The baseline nozzle was a 13-hole nozzle with one central hole and 12 surrounding holes staggered at an angle of 60°. The included injection angle was also 60°. With a hole diameter of ~0.38 mm, the total injector hole area was 1.5 mm^2. The second nozzle was a 5-hole nozzle with central hole and four surrounding holes. The included injection angle was 100°. The total injector hole area was held constant (1.5 mm^2), resulting in an individual hole diameter of ~0.62 mm. Because of the constant total injector hole area, the injection durations for the different nozzles at the same load are comparable. The larger hole diameter of the 5-hole nozzle theoretically results in a higher penetration depth of the individual jets [3] – the larger cone angle on the other hand is supposed to reduce the penetration depth as a result of increased wall interactions.

Different nozzle designs in hydrogen direct injection influence this stratification and, therefore, the engine performance at low engine load (IMEP~2 bar), as shown in Figure 4. The engine was operated at 2,000 RPM at wide-open throttle with an overall air/fuel ratio of ϕ~0.25. The start of injection was set to 40°CA BTDC with spark timing at 5°CA BTDC. The resulting torque is about 3 Nm. Although the amount of unburned hydrogen is significantly higher with the 5-hole nozzle (more than 4,000 ppm versus 1,000 ppm with the 13-hole nozzle), the brake thermal efficiency with the 5-hole nozzle is significantly better.

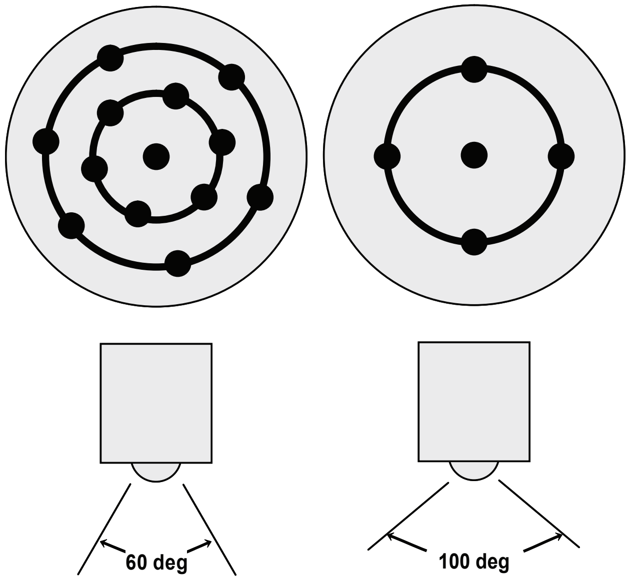

FIGURE 3. Schematics of Direct-Injection Nozzle Configurations

The low absolute levels of brake thermal efficiency are attributable to the low engine load and the high friction losses of the single-cylinder research engine. In addition to the efficiency advantage, the 5-hole nozzle also offers a significant reduction in NOx emissions.

To correlate the trends shown in Figure 4 to the stratification effects caused by the different nozzles, we measured the OH* chemiluminescence intensity during combustion. Figure 5 shows the OH* intensity for low engine load at a speed of 2,000 RPM. Figure 5a shows the results for the 13-hole nozzle with an injection angle of 100°; Figure 5b shows the intensity distribution for the 5-hole nozzle with a 60° injection angle. Injection and ignition parameters are identical to those in Figure 4 – a start of injection of 40°CA BTDC and a spark timing of 5°CA BTDC.

The first two frames for the 13-hole injector show the spark discharge; the third frame (top dead center) already shows a slight increase in the size of the area with high OH* intensities, which indicates the beginning of combustion. The area of high intensities increases in size within the next few frames. At 8°CA ATDC, an almost-symmetrical zone of high intensities close to the top of the combustion chamber has developed. This zone further expands in size in the subsequent frames, whereas the peak intensities already begin to decrease. Although the fuel/air equivalence ratio is very lean (ϕ~0.25) OH* chemiluminescence intensity signals can be detected during combustion. This is only possible because of the mixture stratification caused by the late injection. Early injection, resulting in an almost homogeneous mixture distribution, would result in very low (almost undetectable) OH* intensities.

Figure 5b shows the OH* intensities for the 5-hole nozzle with a much wider injection angle. Unlike for the 13-hole nozzle, there are no detectable OH* intensities besides the spark discharge with the 5-hole nozzle during the first six frames (the high intensity

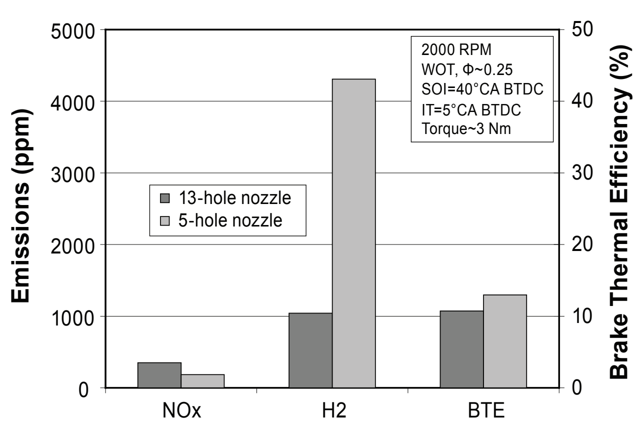

FIGURE 4. Influence of Nozzle Design on Efficiency and Emissions at Low Engine Load

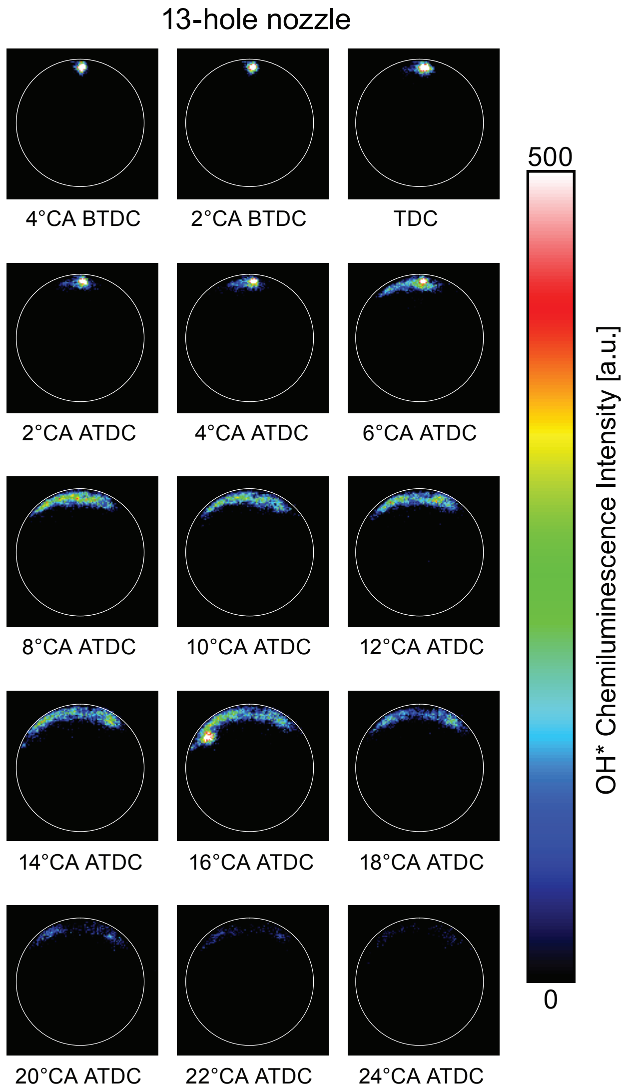

FIGURE 5A. Influence of Nozzle Geometry on Local Combustion Intensity at Low Engine Load – 13-Hole Nozzle

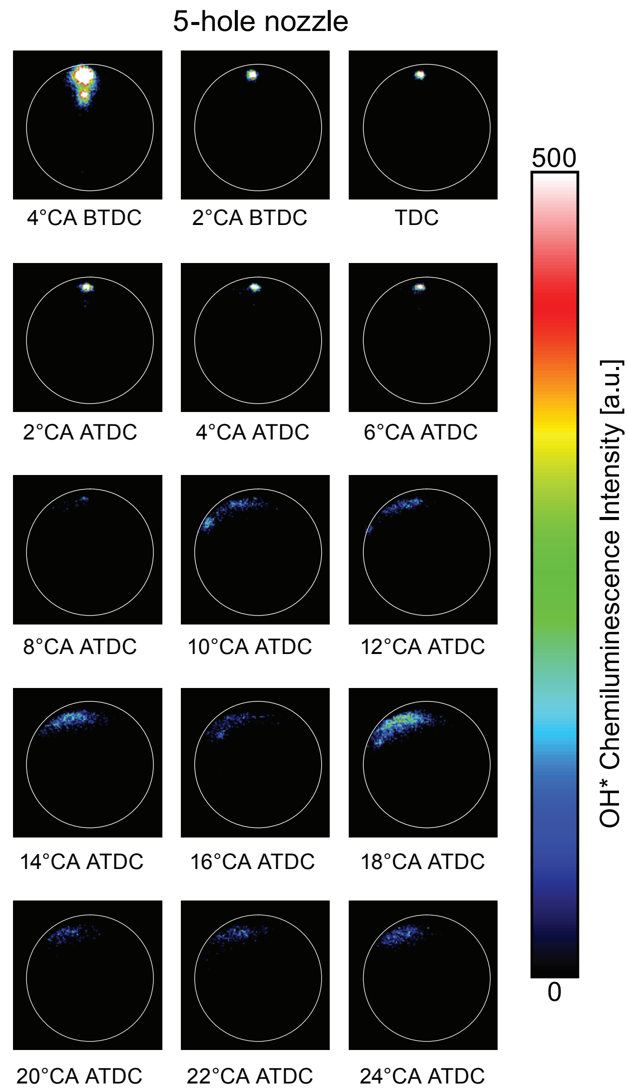

FIGURE 5B. Influence of Nozzle Geometry on Local Combustion Intensity at Low Engine Load – 5-Hole Nozzle

in frame 1 is a reflection of the spark discharge on the piston). Starting from frame 7 (8°CA ATDC), a zone of low (but detectable) OH* intensities start to form at the intake side of the combustion chamber (right side in the chemiluminescence results). The peak intensities occur at 18°CA ATDC, but the maximum intensities are significantly lower than with the 13-hole nozzle.

The intensity distribution for the 5-hole nozzle with high OH* intensities on the intake side (close to the fuel injector) is very likely attributable to the fact that the wider injection angle (100°) causes the injection jet to hit the combustion chamber walls and piston. In the case of the 13-hole nozzle with the 60° injection angle, the hydrogen jets are more likely to penetrate the combustion chamber.

The lower peak intensities also correspond with the lower NOx emissions, as shown in Figure 4. The lower intensities indicate leaner hydrogen air mixtures, which result in a lower local combustion temperature and thus in lower NOx emissions. The opposite can be said about the hydrogen emissions. Flame speed is highly dependent on local fuel/air equivalence ratio with high combustion velocities in rich zones [4]. An overall lean mixture with local rich zones is more likely to cause less unburned hydrogen than an overall lean homogenous mixture. Thus, the significant increase in unburned hydrogen with the 5-hole nozzle seen in Figure 4 is caused by the reduced stratification.

Overall, the general trends observed in the global emission results agree with the mixture distribution derived from the OH* chemiluminescence images.

Conclusions

- Injection parameters, such as injection timing and injector nozzle design, have a significant influence on the performance of a direct-injected hydrogen internal combustion engine.
- Imaging by using endoscopic access to the combustion chamber is a helpful tool to understanding the processes and mechanisms that influence emissions and efficiency behavior.
- By changing the nozzle design from a 13-hole nozzle with a 60° injection angle to a 5-hole nozzle with a 100° injection angle, we can significantly reduce NOx formation with late injection, while maintaining high brake thermal efficiency.
- Advanced nozzle designs as well as changes in injector location will be crucial steps toward reaching the challenging goals for hydrogen engines set by DOE.

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II.A.16 Quantitative Measurements of Mixture Formation in a Direct-Injection Hydrogen ICE

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Objectives

The H_2ICE (hydrogen internal combustion engine) project aims to provide the science base for the development of high-efficiency hydrogen-fueled vehicle engines. The technical focus is on direct-injection strategies, using laser-based in-cylinder measurements closely tied to advanced numerical simulations (performed by J. Oefelein at Sandia, see "Large Eddy Simulation Applied to Low-Temperature and Hydrogen Engine Combustion Research"). Specifically, at this point the goals of the project are to:

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

Accomplishments

- Quantitative, instantaneous two-dimensional images of equivalence ratio and corresponding high-quality velocity measurements were made during the compression stroke with and without direct hydrogen injection.
- Analysis of the velocity field revealed that the observed substantial fuel stratification for late injection is favored by a relatively stable counter-flow situation created by jet-wall interaction.
- Velocity and fuel distribution measurements are initial building blocks of a database for the validation of companion large-eddy simulations by J. Oefelein at Sandia.

Future Directions

- Measure velocity field in the vertical (axial) plane during the intake stroke to validate pre-injection accuracy of the companion simulation.
- Implement *simultaneous* two-dimensional measurements of velocity/equivalence ratio.
- Install new engine head, supplied by Ford R&D, featuring central injection and central ignition. Engine geometry will then be identical to that of collaborating labs at Ford and ANL.
- Install emissions bench (already purchased, NOx and O_2).
- Use OH-planar laser-induced fluorescence (PLIF) to quantitatively investigate the influence of mixture formation on combustion.

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Introduction

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

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

Approach

In the optically accessible DI-H_2ICE, separate two-dimensional, quantitative measurements of equivalence ratio and velocity were made. Different post-IVC injection timings and a case corresponding to port fuelling were investigated at a global equivalence ratio of $\phi = 0.55$, intake pressure = 0.5 bar, an engine speed of 1,200 RPM, and an injector pressure of 25 bar. Equivalence ratio was measured using PLIF of acetone seeded in small amounts into the hydrogen fuel. Velocity was measured using particle image velocimetry (PIV) while seeding silicon oxide particles into the intake plenum. Both sets of experiments were performed with non-fired engine operation, since the pre-combustion charge movement and air/fuel mixing were of primary interest here. Results shown are for image acquisition at 32° crank-angle before top dead center (TDC), the latest position in the compression stroke for which both high-quality PLIF and PIV results could be obtained. The imaging plane is parallel to the flat top of the piston, as shown in the experimental schematic of Figure 1. Three different injection timings were investigated: "early" injection (starting just after IVC), "late" injection (with the injection extending just past the crank-angle at which imaging was performed), and "intermediate" (starting well after IVC, ending well before data acquisition). For reference, a near-homogeneous mixture was created by injecting during the intake stroke.

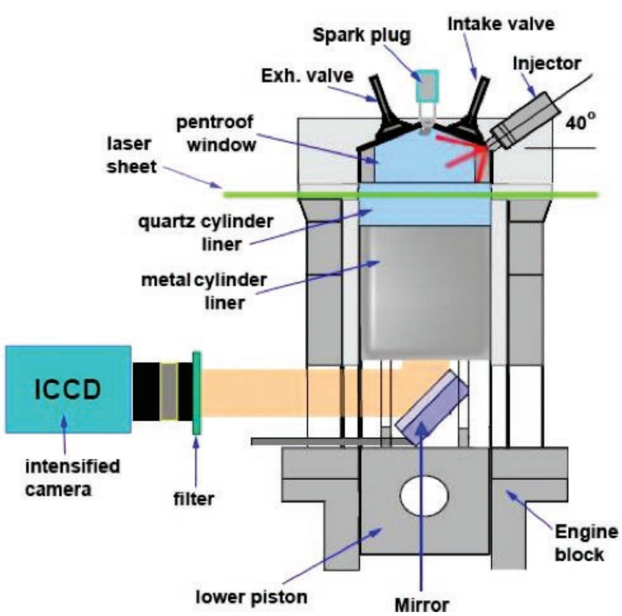

FIGURE 1. Optical Engine Experimental Set-Up

Results

PLIF measurements were reduced to equivalence-ratio images through a combination of calibration measurements with a homogenous mixture and a local temperature correction based on adiabatic mixing [2,3]. Currently, the PLIF-measurement precision is limited by the amount of acetone (the fluorescent tracer) that can be added to the high-pressure hydrogen in the gas cylinder supplying our laboratory with hydrogen. Because the vapor pressure of acetone is low compared to the cylinder pressure (200 bar), only about 0.5 % (by volume) can used before condensation occurs. To overcome this problem, a heated high-pressure compatible seeder has been built. The slightly increased temperature and the seeder's location in the lower-pressure part of the fuel supply system (at injector pressure, 25–100 bar) should allow us to achieve any practically useful acetone concentration. The new system is being tested now.

PIV measurements in engines are challenging because the necessary seed tends to accumulate on the optical surfaces (cylinder liner, piston window) and interfere with the measurement. Careful selection of seed particles, seeding system, and operating procedures enabled us to measure the instantaneous velocity field with high resolution. This will be important for a quantitative comparison with LES results. As opposed to KIVA-type simulations, LES can provide detailed, instantaneous realizations of the turbulent flow-field, demanding an at least equal level of detail from validation experiments. Although the bulk of the initial investigations this fiscal year involved non-fired, pre-combustion conditions, we did verify that high-quality velocity measurements could also be taken during and after combustion. Many previous flow studies have used oil droplets for seeding, thereby limiting the applicability to the low-temperature part of the engine cycle. The ability to measure two-dimensional velocity distributions throughout the entire cycle will be the basis of some of the future work (see above), including validation of the corresponding simulation during the expansion stroke.

Figure 2 shows the results of fuel and velocity measurements in a plane parallel to the piston, covering the central 65 mm of the 92 mm bore. Early injection (SOI/end of injection at -112°/-62° CA) results in a nearly homogenous fuel distribution. However, comparing the corresponding velocity field to that of the non-fuelled case we can see that the charge motion has been altered drastically by the injection event. The velocity magnitudes have greatly increased. The plots show that well-defined large-scale flow structures (i.e., turbulent vortices) are a common occurrence. At this crank angle, early injection timing in the mean yields a central, counter-rotating vortex pair that transports fluid from near the cylinder wall to the central region of the

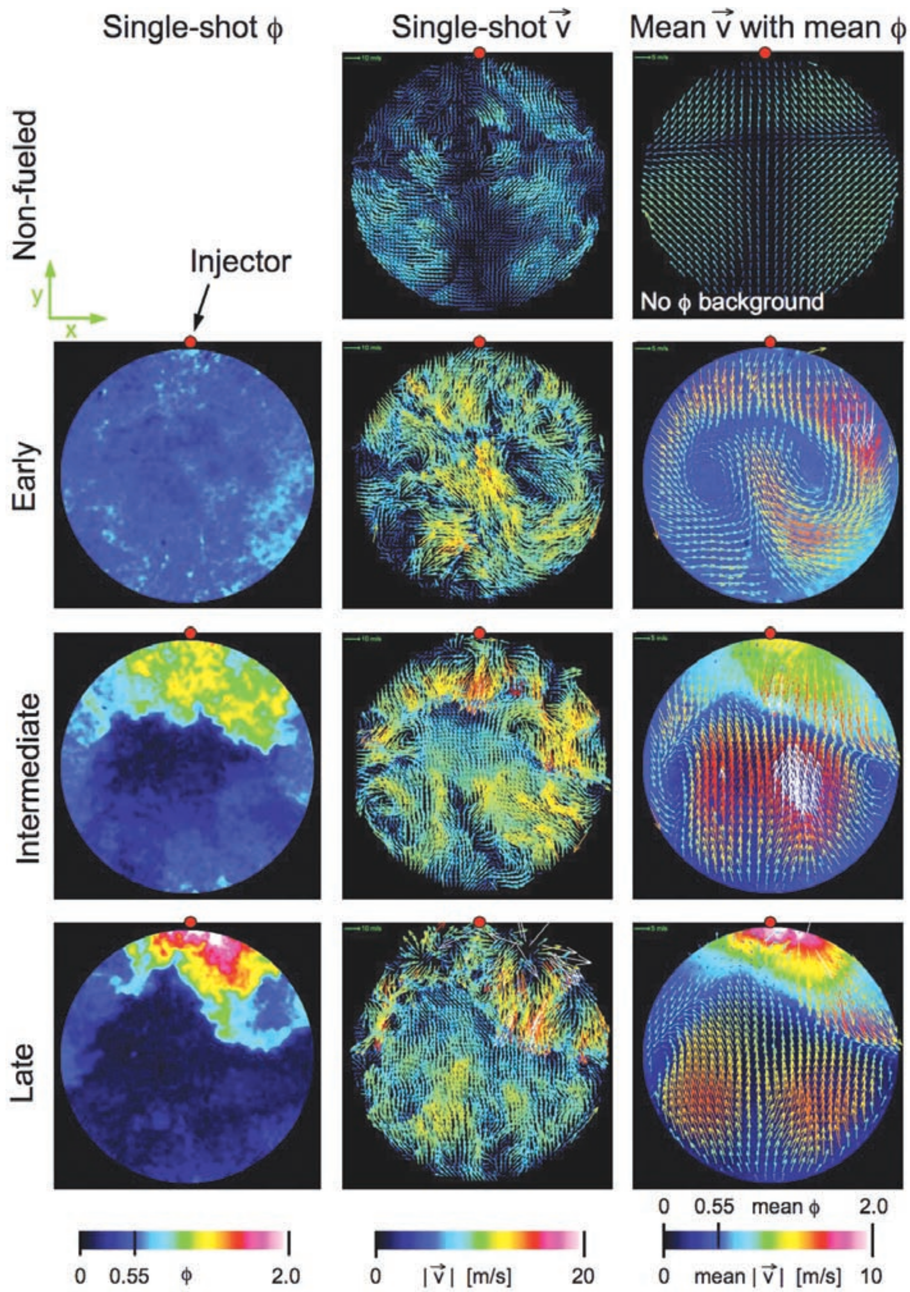

FIGURE 2. Equivalence ratio and velocity for different injection timings: a single instantaneous equivalence-ratio field (left column), a single instantaneous velocity field (center column), and the mean velocity field with the mean equivalence ratio as background (right column). Note that the vector color scale for the mean velocity is different from that for the single shots. For the non-fueled condition ($\phi = 0$), the background of the mean velocity vector plot is chosen uniformly black.

measurement plane. The PLIF images for early injection indicate that the flow is effective in mixing the hydrogen with air.

The fuel-distribution images show that intermediate and late injection produce progressively more inhomogeneous mixtures. This is to be expected due to the shorter time for mixing, but the velocity plots reveal one mechanism which in particular could be responsible for preventing effective mixing until late in the compression stroke: in the measurement plane, the injection has created a counter-flow situation, with a stable, strong bulk flow towards the injector separated by a sharp front from the turbulent, fuel-rich flow originating from the injector. The overlay of the PIV and PLIF means (right column) shows that on average the two regions and the dividing "turbulent front" are spatially exactly collocated in vector and scalar field.

Motivated by this strong correlation, it is conjectured that the observed flow fields for both the intermediate and late injection timings result from jet and wall interactions that redirect the flow from those jets that are directed along the pent roof vertically back down towards the injector. In the y-z plane, the schematic sketch in Figure 3 shows this idea. Additionally, the injector geometry and the "inverted V" shape of the turbulent front suggest that those jets that issue to the sides, i.e., towards the cylinder liner, could supply additional momentum to the "upward" (positive y direction) flow after wrapping around the cylinder. As a result, the flow in the visible part of the measurement plane is effectively a counter flow that inhibits further jet penetration. The net result of these two effects would be high hydrogen concentration near the injector, consistent with the PLIF images. This scenario, although tentative at this point, suggests that the injector tip geometry, injector location, and injection timing are critical parameters with respect to in-cylinder mixing. Correspondingly, engine simulations would have to accurately capture the injection-induced flow to be able to make valid predictions for the ensuing combustion. Clearly, in this context the measurements presented here can only be considered preliminary and will have to be expanded for the purpose of understanding mixture preparation and in order to provide meaningful simulation validation.

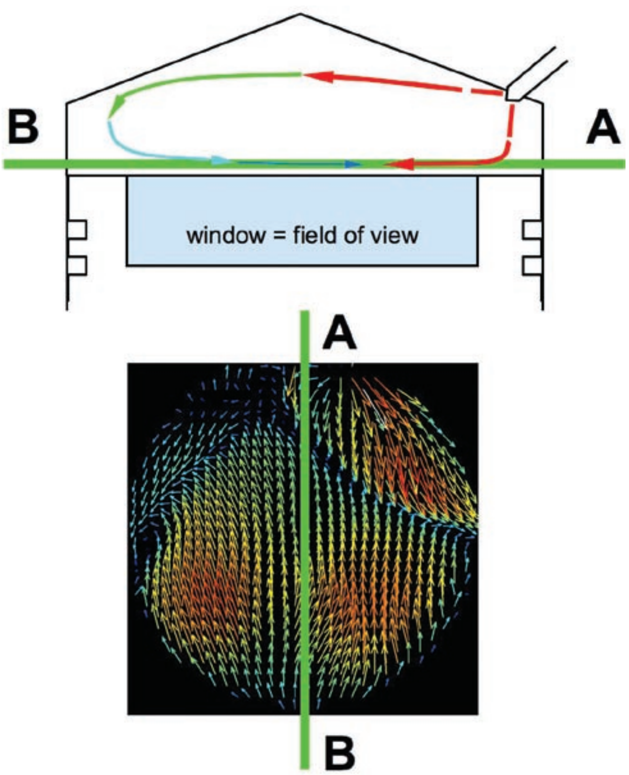

FIGURE 3. Conceptual Sketch of the Opposed-Flow Situation Created by the Wall/Jet Geometry

FY 2007 Publication 1 expands on the above observations and quantifies the global fuel distribution in form of probability density functions. Line-of-sight measurements of chemiluminescence from the excited hydroxyl radical (OH*) for the same series of injection timings, but after ignition, are reported in Publication 2. These qualitative measurements, which indicate the local equivalence ratio during the early burn, are in agreement with the non-fired fuel-imaging data described above. Additional velocity measurements investigating the flow-field throughout the compression cycle with and without injection have been made. A detailed evaluation is in progress and will be the basis for extensive validation of the hydrogen-jet sub-model being developed within the corresponding numerical effort.

Conclusions

- In the optically accessible DI-H_2ICE, high-quality measurements of the velocity field were possible for motored and fired conditions.
- In the same plane, quantitative images of equivalence ratio could be obtained. Accuracy and precision were reasonable and are being improved further.
- Direct hydrogen injection fundamentally alters the in-cylinder flow field.
- For the given side-injecting six-hole injector, three different post-IVC injection timings were investigated. At a point in the compression stroke shortly before the time of ignition, early injection produced a nearly homogeneous mixture, while intermediate and late injection resulted in significant stratification.
- Analysis of the velocity plots showed that the injection event creates a counter-flow situation, which inhibits mixing until breaking up into a vortex pair later in the cycle.
- Although the current injector geometry and location are not ideal for late-injection strategies from an engine-development point of view, the scalar and velocity data will be very useful for the validation of numerical simulations.

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II.A.17 Enabling High Efficiency Clean Combustion in Diesel Engines

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Subcontractors:
- Oak Ridge National Laboratory
- BP Global Fuels Technology

Objectives

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

Accomplishments

- U.S. EPA 2010 steady-state oxides of nitrogen (NOx) emissions compliance achieved on the 15L ISX engine without NOx aftertreatment and 7% improvement in brake thermal efficiency against the 10% project objective.
- A 0.4 g/bh-hr NOx emissions level has been demonstrated on the 15L ISX for the U.S. EPA transient Federal Test Procedure (FTP) cycle with an improvement of 7% in brake thermal efficiency against the 10% project objective.
- U.S. EPA 2010 steady-state and transient NOx emissions compliance has been achieved without NOx aftertreatment for the 6.7L ISB engine while exceeding the 10% improvement in brake thermal efficiency project target.
- Analysis and design of additional subsystem technology for the 15L ISX have been completed to enable full U.S. EPA NOx emissions without NOx aftertreatment while achieving the target 10% improvement in brake thermal efficiency.
- Analysis and design of additional subsystem technology for the 6.7L ISB have been completed to enable additional 5% improvement in brake thermal efficiency.
- The design and procurement of a new generation of Cummins XPI high pressure common rail fuel system has been completed.
- Advanced turbomachinery has been designed and procured to provide fast transient response that is expected to allow engine-out transient NOx emissions compliance with acceptable particulate matter for the 15L ISX engine.
- A new exhaust gas recirculation (EGR) cooling system has been designed and tested that provides 3% to 4% fuel economy improvement on the 15L ISX and 6.7L ISB engines.
- A new analysis tool was created that can be used to simulate the engine system (air handling, EGR system, combustion, etc.), aftertreatment (diesel oxidation catalyst and diesel particulate filter), sensors, and controls algorithms over transient duty cycles.
- New model-based air handling and combustion control algorithms have been created for the 15L and 6.7L engine applications.
- HECC engine technology developed as part of this project has been shown to be robust for fuel economy and emissions with variations in diesel fuel properties representative of commercially available fuels in the marketplace. However, fuel sensing technology is required to maximize the fuel economy benefit for the HECC technology enabling changes in the engine controls strategy.
- The fuel economy benefits associated with the HECC engine technology developed can not be maintained when using biofuels at constant NOx emissions. However, a reduction of 20% to 40% in particulate matter can be achieved with the use of biofuels.
- The impact of biodiesel blends on NOx emissions have been explored extensively for a wide variety of engine technology and engine duty cycles.

Future Directions

- Multi-cylinder engine testing of advanced turbomachinery (electronic boosting, 2-stage turbocharging, and supercharging).
- Multi-cylinder engine testing of advanced EGR cooling system (EGR pump, 2-stage cooling, variable displacement pumps, etc.).
- Evaluation of variable valve actuation (VVA) including cylinder deactivation.
- Evaluation of piezo, common rail, fuel systems at high injection pressures.
- Development of combustion control using cylinder pressure sensor and VVA.
- Completion of calibration development of the 15L ISX and 6.7L ISB engines with advanced subsystem technology identified during the exploratory development phase of the program.
- Fuel economy and emissions robustness evaluation of HECC engine architectures operating on a wide variety of biofuels (soy, rapeseed, palm, mustard, and coconut).
- Evaluation of real and virtual fuel sensing technology for HECC engine architectures.
- The impact of biofuels on diesel particulate filters will be explored.
- Development of on-board diagnostics associated with the implementation of the new HECC subsystem technology to function properly during in-use.

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Introduction

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

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

Approach

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

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

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

Results

During FY 2007, all Phase 2 milestone and deliverables have been met for the Cummins HECC project with the successful close-out of the Phase 2 work. The Phase 2 portion of the project focused on exploratory development of subsystems and related component technologies as depicted in Figure 1.

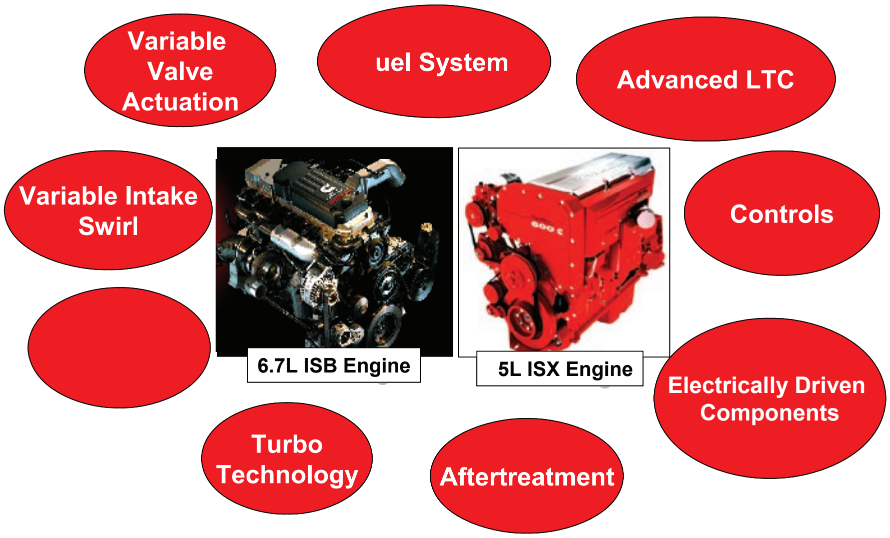

FIGURE 1. Cummins Component Business Technologies for High Efficiency, Clean Combustion

- A considerable amount of effort was concentrated on demonstrating significant fuel economy improvement on the 6.7L ISB engine used in light-duty engine applications in addition to the 15L ISX heavy-duty engine. The combustion strategy employed to achieve high efficiency is illustrated in Figure 2. The mixed mode combustion strategy relies on extending the early premixed charge, compression ignition (PCCI) combustion mode to encompass as much of the engine operating range as possible while implementing lifted flame diffusion controlled combustion for the remainder of the higher load operating range.

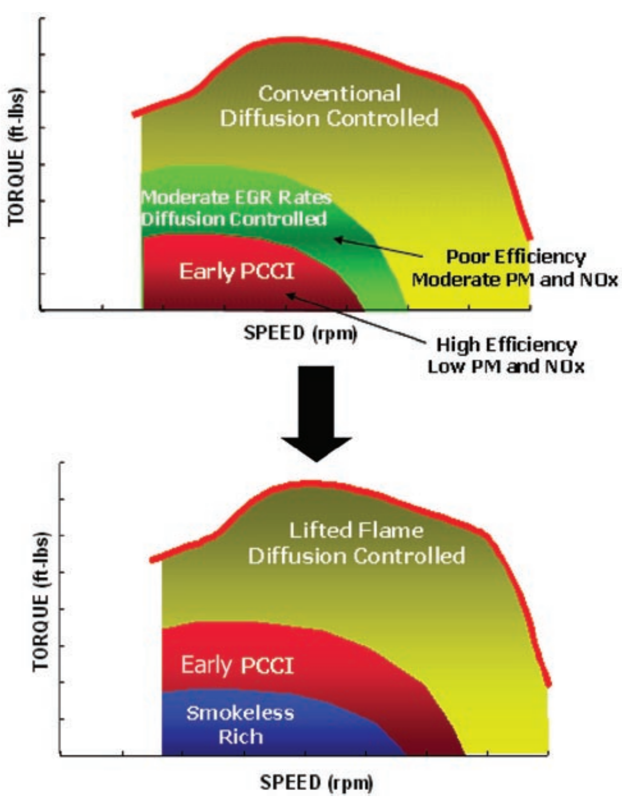

FIGURE 2. Mixed Mode Combustion Strategy for High Efficiency, Clean Combustion

- The fuel economy improvement targets have been exceeded for the ISB engine with low temperature, PCCI combustion technology that has demonstrated 2010 emissions capability (see Figure 3). An average of 12% fuel economy improvement has been realized. This is a significant accomplishment for the project. Additional engine technology has been explored during Phase 2 that is expected to provide an additional 5% fuel economy improvement that will be demonstrated in Phase 3 Multi-Cylinder System Integration portion of the project.
- Important fuel economy improvements have been achieved for the 15L ISX heavy-duty engine. The majority of the collaborative effort during Phase 2 has been concentrated on realizing high pressure injection, mixed-mode combustion. The specific engine technology explored in Phase 2 has demonstrated the ability to achieve steady-state emissions targets for 2010 assuming the availability of particulate filter aftertreatment. Transient emission results have been demonstrated, but are still above the target (approximately 0.4 g/bhp-hr NOx). Equivalent fuel economy improvement to baseline is 7% relative to a 10% project goal (including aftertreatment fuel penalty) as shown in Figure 4. It is anticipated that full engine-out transient emission targets will be difficult to achieve and further technology development will be necessary. Additional technology development in Phase 2 has been focused on advanced air handling systems to provide air on demand during transient engine

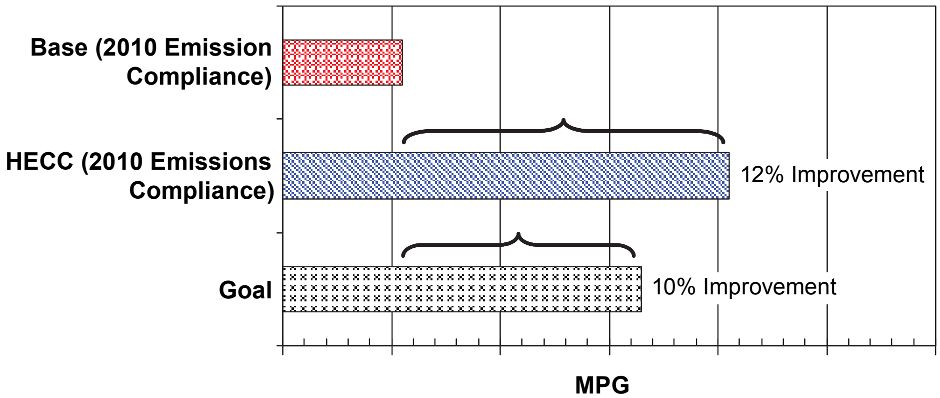

FIGURE 3. Fuel Economy Improvement of the HECC Engine Architecture for the 6.7L ISB Engine for Light-Duty Applications

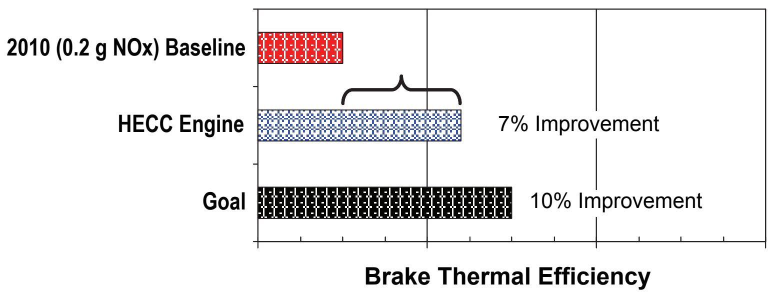

FIGURE 4. Thermal Efficiency Improvement for the 15L ISX Engine

operation. The advanced air handling systems include 2-stage turbocharging, electronic turbo, and supercharging. Other technology development explored in Phase 2 includes VVA, high frequency fuel injection, and EGR pumps. These technologies will enable full transient emissions compliance while meeting the project fuel economy target.

- The collaborative fuels study by Oak Ridge National Laboratory, Cummins and BP remained on plan during Phase 2 with the completion of the diesel fuels portion of the project. The fuel parameters selected for initial evaluation include cetane, aromatics, T10, and T90 distillation temperatures. Analysis of the ISB single-cylinder engine data collected at Cummins for the diesel fuels has been completed. The following conclusions have been formulated:
- Engine calibration parameters have the most significant impact on PCCI combustion compared to fuel properties.
- Lower cetane number fuels provided the best emissions and fuel economy results for PCCI combustion.
- Expected issues with PCCI combustion robustness at off-nominal engine operation such as cold ambient conditions with the expected variation in commercially viable ultra-low sulfur diesel fuel:
  - Unburned hydrocarbon and carbon monoxide emissions.
  - Diesel oxidation catalyst can be used to make PCCI emissions robustness possible.
  - Fuel economy deterioration expected.
  - Closed-loop combustion control is needed to offset fuel economy impact.

Conclusions

- During FY 2007, all Phase 2 milestone and deliverables have been met for the Cummins HECC project with the successful close-out of the Phase 2 work. Accomplishments include:
- U.S. EPA 2010 steady-state NOx emissions compliance achieved on the 15L ISX engine without NOx aftertreatment and 7% improvement in brake thermal efficiency against the 10% project objective.
- A 0.4 g/bh-hr NOx emissions level has been demonstrated on the 15L ISX for the U.S. EPA FTP cycle with an improvement of 7% in brake thermal efficiency against the 10% project objective.
- U.S. EPA 2010 steady-state and transient NOx emissions compliance has been achieved without NOx aftertreatment for the 6.7L ISB engine while exceeding the 10% improvement in brake thermal efficiency project target.

- Analysis and design of additional subsystem technology for the 15L ISX have been completed to enable full U.S. EPA NOx emissions without NOx aftertreatment while achieving the target 10% improvement in brake thermal efficiency.
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- Advanced turbomachinery has been designed and procured to provide fast transient response that is expected to allow engine-out transient NOx emissions compliance with acceptable particulate matter for the 15L ISX engine.
- A new EGR cooling system has been designed and tested that provides 3% to 4% fuel economy improvement on the 15L ISX and 6.7L ISB engines.
- A new analysis tool was created that can be used to simulate the engine system (air handling, EGR system, combustion, etc.), aftertreatment (diesel oxidation catalyst and diesel particulate filter), sensors, and controls algorithms over transient duty cycles.
- New model-based air handling and combustion control algorithms have been created for the 15L and 6.7L engine applications.
- HECC engine technology developed as part of this project has been shown to be robust for fuel economy and emissions with variations in diesel fuel properties representative of commercially available fuels in the marketplace. However, fuel sensing technology is required to maximize the fuel economy benefit for the HECC technology enabling changes in the engine controls strategy.
- The fuel economy benefits associated with the HECC engine technology developed can not be maintained when using biofuels at constant NOx emissions. However, a reduction of 20% to 40% in particulate matter can be achieved with the use of biofuels.
- The impact of biodiesel blends on NOx emissions have been explored extensively for a wide variety of engine technology and engine duty cycles.

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

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- Sandia National Laboratories, Livermore, CA
- IAV Automotive, Detroit, MI
- eServ, Peoria, IL

Objectives

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

Sandia Optical Experiments: Utilize state-of-the-art optical diagnostics at Sandia National Laboratories to image the HCCI combustion process to gain a fundamental understanding of the mixing and combustion process.

Advanced Fuel System Concept Identification and Selection: Develop state-of-the-art fuel injection technologies to enhance the mixing and combustion process for HCCI.

Fuel Property Effects: Collaborate with ExxonMobil to understand the effects of fuel property changes on fuel/air mixing, combustion, emissions and thermal efficiency in HCCI engines.

Cooling System and Heat Rejection Analysis: Develop technologies to mitigate the air and water heat rejection increases associated with HCCI.

Advanced Controls Algorithm Development: Develop required sensors and advanced controls techniques to successfully achieve transient operation on multi-cylinder HCCI engines.

Combustion CFD Model Development Activities: Develop and validate combustion computational fluid dynamics (CFD) modeling tools so they are fully predictive and can be used to provide fundamental understanding of the mixing and combustion processes, design hardware and limit the required testing.

Combustion Development for Advanced Multi-cylinder HCCI Engines: Develop and demonstrate the advanced multi-cylinder engine technologies necessary to achieve the overall project objective.

Accomplishments

- Phase 2 optical diagnostic experiments complete.
- Single-cylinder engine fuels testing on low-cetane diesel boiling-range fuels completed.
- Prototype fuel injection system developed and tested on single-cylinder engine demonstrating ultra-low NOx and smoke emissions.
- Advanced multi-cylinder engine with compression ratio flexibility developed and tested demonstrating benefits for emissions, efficiency and controls.

Future Directions

- Continue optical engine tests to further develop fundamental understanding of low-temperature combustion.
- Improvements to further advanced fuel system capability and demonstration of benefits.
- Additional fuels effects testing to discern fuel property effects.
- Refine and validate improved CFD sub-models.
- Refinement of control strategies and implement on advanced multi-cylinder engines.
- Investigation of mixed mode combustion to utilize part-load HCCI with other low-temperature combustion for higher operating modes.

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Introduction

Maintaining and improving fuel efficiency while meeting future emissions levels in the diesel on-road and off-road environments is an extremely difficult challenge but is necessary to maintain the level of customer value demanded by the end-users of compression ignition engines. Caterpillar® is currently engaged with several partners to address this challenge using advanced low-temperature combustion. This project provides a fundamental understanding of the in-cylinder fuel/air mixing and combustion process through advanced optical diagnostics and CFD. We are also actively developing new fuel injection, controls, heat rejection reduction and engine technologies to enable this clean, efficient combustion. We are exploring the impact of different fuel types to understand the robustness of this combustion process to fuel variability. Successful completion of this project will provide Caterpillar and DOE with a clear understanding of the technology hurdles that must be overcome to increase the thermal efficiency and reduce emissions on future compression ignition engines.

Approach

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

A research prototype fuel injection system was developed and validated on a fuel systems bench in Task 2. This piezo-based research common rail fuel system is capable of multiple fuel injections and >250 MPa injection pressure.

Applied research in the area of fuels effects is the subject of Task 3. This work builds upon the collaboration between Caterpillar and ExxonMobil to better understand fuel property effects on HCCI combustion. Prior to shipment of any fuels, standard fuel property tests and detailed chemical characterization of each fuel were performed by ExxonMobil. These fuels were evaluated for performance in Caterpillar metal engines.

The cooling requirements for the HCCI engine are higher than normal combustion, and the heat rejection from such a system is a significant challenge to deal with in "real world" applications. Task 4 included a comprehensive modeling effort that was initiated to understand and identify alternatives to mitigate this risk. Conventional and alternative heat exchanger designs for combustion gas intercoolers and charge air inter/after coolers were evaluated including gas-to-coolant, gas-to-air, separate circuit and primary surface heat exchangers.

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

Task 6 involved model development activities to enhance current predictive capabilities in cycle simulation and 3D combustion simulation tools. This task included the development and validation of reduced kinetic mechanisms for use in these combustion simulation calculations to model ignition, combustion, and pollutant formation. The optical diagnostic results from Task 1 were to be used to validate and tune the models of the combustion process to enable future HCCI combustion development in a virtual environment. The goal is to accurately simulate all of the important processes in HCCI combustion. In particular, the goal is to represent the spray droplet size and spatial distribution, the fuel vapor distribution, wall film thickness and location, combustion, and emissions formation accurately as they occur in a diesel engine. With a more complete model of the HCCI process, modeling activities then focused on refinement of piston bowl and spray geometries to minimize hardware procurement.

An advanced multi-cylinder HCCI engine was also developed and tested in Task 7. This engine has full variable compression ratio flexibility as well as variable valve timing flexibility. It has been used to demonstrate the performance, emissions and controls benefits such an engine can potentially offer.

Results

Task 1- Sandia Optical Engine Experiments: Many upgrades to the laboratory were completed in the first full year of the project. During this year, the SCORE head utilized in the HECC work was fitted with sealed valve guides to reduce the amount of lube oil entering the cylinder in order to bring the SCORE smoke levels closer in line with those observed in the single-cylinder test engine (3401 single-cylinder test engine) at Caterpillar. Cycle-integrated natural luminosity (CINL) imaging at 1,200 rpm, 300 kPa, 400 kPa, and 500 kPa conditions was completed to verify the sealed valve guide design. These images were collected and compared to the images in last year's report. The CINL images do not show the bright spots indicative of lube oil combustion as previously noted.

Shortly after work on this project commenced, it became evident that a peak cylinder pressure (PCP) capability of 20 MPa would be necessary to study high-load operating conditions of interest. This amounts to nearly doubling the PCP capability of the optical engine. Thus, all the combustion chamber components require re-evaluation for safe operation at 20 MPa PCP. Work continues on this task.

A new set of nozzles was delivered to Sandia in May 2007. This set of nozzles was matched to the flow rate of the nozzle used in the first two years of the HECC collaboration. Emissions and performance data as well as high-speed camera spray visualization, and natural luminosity images were collected with diesel fuel in the SCORE. Sweeps of load, injection timing, injection pressure, EGR level, boost and equivalence ratio were collected. Apparent heat release rate, spatially-integrated natural luminosity, and emissions data were collected. In-cylinder natural luminosity movies were collected using a Phantom V7.3, 14-bit, high-speed camera. Two camera views were utilized to provide the best possible spatial information about the bright soot luminosity. The first camera view is in through a cylinder-wall window. The second view is up through the piston window utilizing the Bowditch piston extension of the SCORE engine.

Figure 1 shows the injection spray visualizations with diesel fuel. From the image, fuel interaction with the piston bowl can be observed in the second and third rows of images. Figure 2 shows selected frames from the cylinder window view high-speed natural-luminosity movie. From Figure 2 it is clear that the soot luminosity begins with many small dots spread throughout the height of the piston bowl near top-dead-center (TDC), and then rapidly shifts to the bottom surface of the piston bowl where the intensity greatly increases. These results along with the spray visualizations substantiate the claim of diesel fuel jets impinging on the surface of the piston bowl are a significant factor in soot emissions.

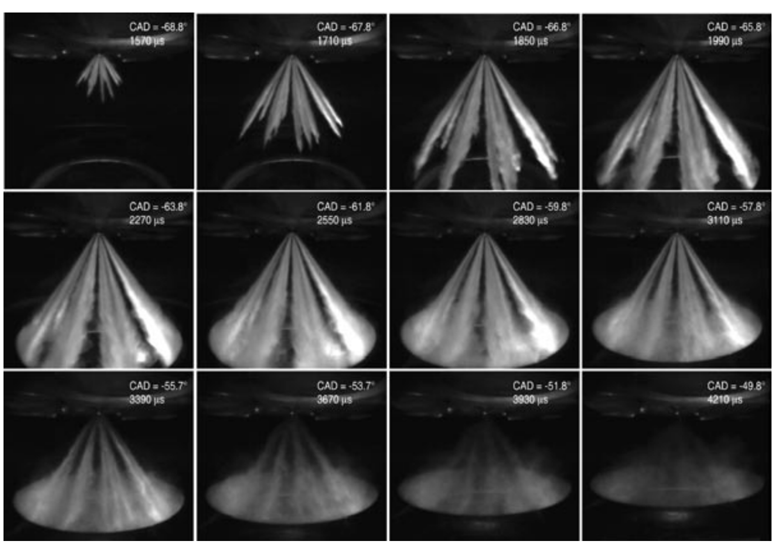

FIGURE 1. Injection spray visualization images acquired illustrating liquid fuel interaction with the piston bowl.

Task 2 - Advanced Fuel System Concept Identification and Selection: An advanced common rail fuel system was developed to enable low emissions and high efficiency combustion. The first version (Phase 1) features the ability to perform pilot injections of less than 5 mm^3 at rail pressures greater than 250 MPa with dwell between injections of less than 200 microseconds. The Phase 1, piezo-actuated injector has been fully characterized on the single-cylinder test engine. Several discrete tests have been successfully completed, which have demonstrated the benefits of the high injection pressure, and the multiple injection strategies, facilitated by this advanced injector. During this year, the work focused on HCCI combustion development utilizing the injection pressure and multiple injection capabilities of the advanced piezo injector design. As a baseline, single-shot HCCI combustion was studied over a range of injection pressures and timings while holding phasing, intake manifold pressure, intake temperature, and load constant. This baseline data provides insight into the fundamental injection parameters that affect HCCI combustion. The second set of experiments focused on multiple injection strategies to reduce the amount of EGR required for phasing and heat release of HCCI by increasing the mixture homogeneity through earlier injection timings. The results are shown in Figures 3 and 4 and indicate the effectiveness of advanced injection strategies. In addition, some simple spray modeling and spray visualization was performed to provide insight into the engine out emissions.

Task 3 - Fuel Property Effects on Emissions and Combustion Phasing: Significant progress was made towards understanding the effects of fuel properties on the operability and emissions of a heavy-duty engine performing under HCCI conditions. Five fuels in the diesel boiling range were prepared covering a wide range of fuel ignition quality and hydrocarbon composition. These fuels were developed using blend recipes with available fuels and fuel components. Fuel additives were included in each blend to ensure sufficient lubricity of engine components and fuel stability. After blending, all test fuels were subjected to a thorough analytical characterization, with particular emphasis on ignition quality, distillation/volatility, elemental composition (*e.g.,* sulfur content), and hydrocarbon composition, especially aromatics content. The ignition quality of the fuels was determined by both the cetane number, measured using ASTM method D613, and the derived cetane number (DCN), measured by the ignition quality tester using ASTM method D6890. The blended fuels covered a range of ignition quality from a DCN of 24.2 to 45.2.

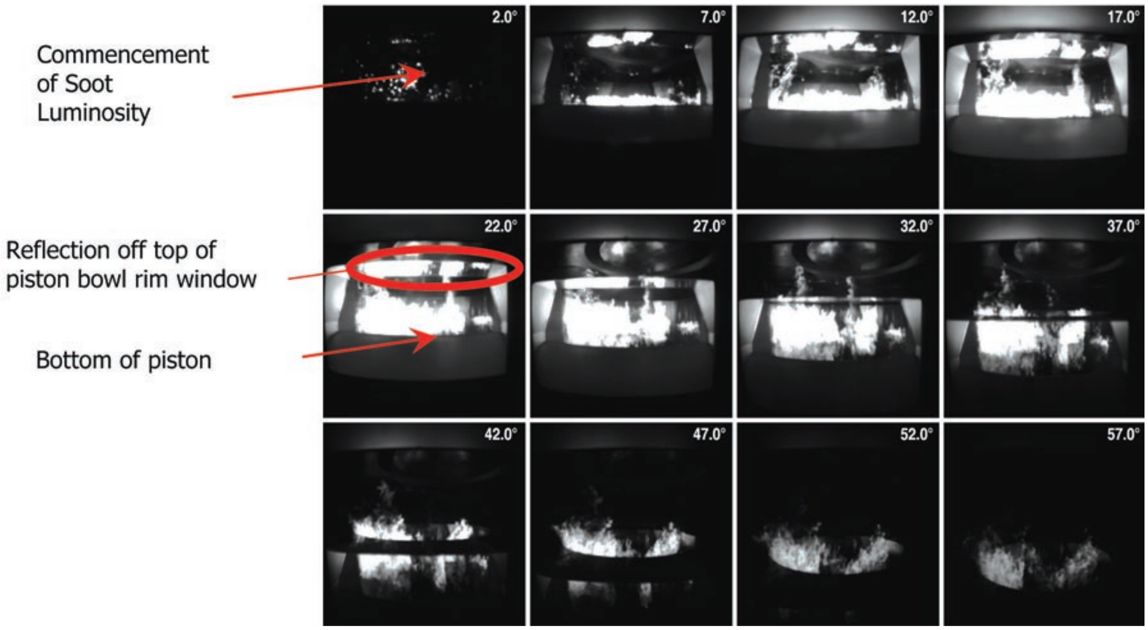

FIGURE 2. Natural luminosity images acquired illustrating liquid fuel impingement on the piston bowl as a significant factor for soot emissions.

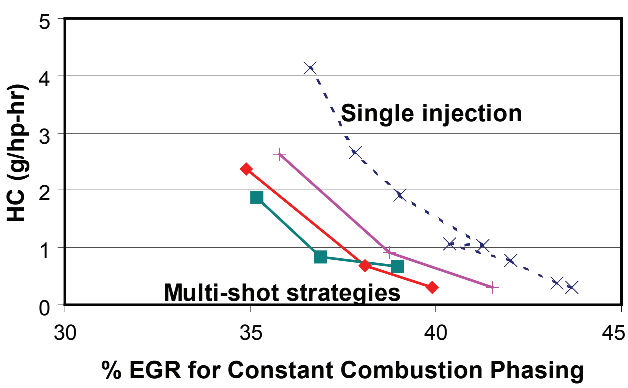

FIGURE 3. Multi-shot strategies using a Phase 1 advanced injector resulted in lower unburned hydrocarbon emissions.

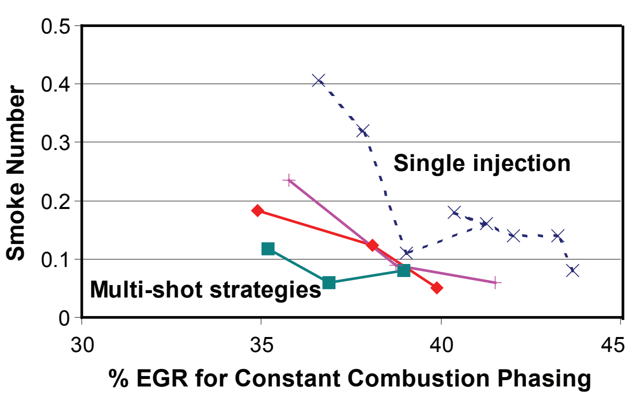

FIGURE 4. Multi-shot strategies using a Phase 1 advanced injector resulted in lower smoke emissions.

All five diesel boiling-range fuels were engine-tested in the Caterpillar 3401E single-cylinder oil test engine under HCCI conditions using a compression ratio of 14:1. This engine is rated at 62 kW at 1,800 rpm, and is equipped with a flexible air handling system, which includes intake boost temperature and pressure along with exhaust backpressure. The fuel injector is a Caterpillar hydraulically actuated electronically controlled unit injector, which allows for injection pressures up to 150 MPa.

In determining the minimum and maximum loads which could be achieved with each test fuel, several experimental limits were imposed based on the mechanical limitations of the engine, future emissions regulations, and heat rejection/packaging constraints. Figure 5 shows the operability results, which were attained as a function of the ignition quality of the fuel at an engine speed of 1,200 rpm. For the diesel fuel with a DCN of 45.2 (ignition quality representative of typical U.S. diesel fuel), a maximum load of nearly 1,000 kPa was achieved. However, the maximum load which could be attained generally increased as the ignition quality of the fuel decreased. The highest load was achieved for the fuel with the lowest DCN (24.2), which corresponds to an ignition quality well below that of conventional diesel fuel.

Differences in the hydrocarbon composition of the fuel were observed to have no significant effect on HCCI operability for the five fuels tested. The only fuel property, which was found to have a significant effect on operability, was the ignition quality of the fuel. In terms of emissions, fuel properties did not influence oxides of

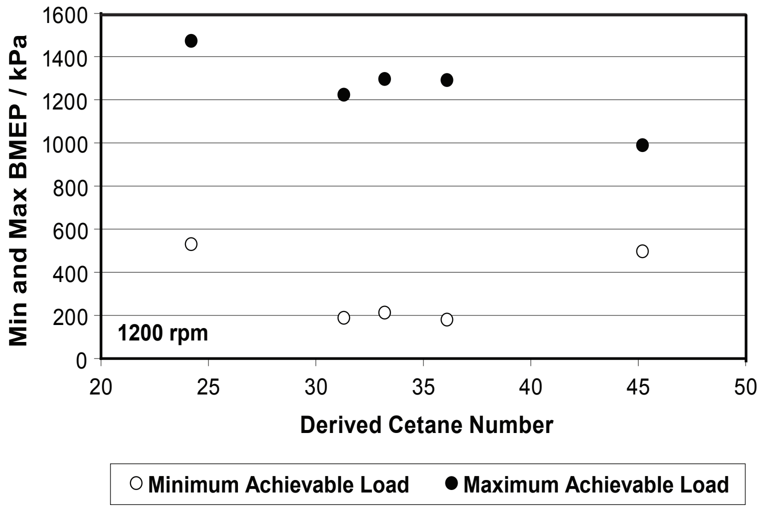

FIGURE 5. Engine Operating Range vs Derived Cetane Number (CR=14)

nitrogen (NOx), hydrocarbon (HC), or carbon monoxide emissions; however, a fuel with a lower aromatics content did show some modest benefit in reducing particulate matter emissions at high loads, compared to a fuel with a substantially higher aromatics content.

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

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

Task 5 - Advanced Controls Algorithm Development: A rapid prototyping system was developed for controls development using Matlab/Simulink software for model building and code generation. The rapid-prototyping hardware consists of an xPC™ target box equipped with CAN™ cards and a Caterpillar-designed programmable field programmable gate array (FPGA) card enabling processing of speed-timing pulses from the crank/cam targets and generation of the output pulses needed for the various engine sub-systems such as fuel injection. In order to implement the control models into this real time engine controller, a fast and reliable data acquisition system that can capture crank angle based in-cylinder pressure values for combustion-timing feedback is required. The first device used to accomplish high-speed sampling of in-cylinder pressure sensors was based on FPGA chips. The former data acquisition system had robustness issues resulting in an occasional dropped data point or a corrupted crank angle measurement. Moreover, it was limited in its functionality. Its only purpose was to transfer the pressure measurements to the xPC™, which then performed all of the required calculations for desirable parameters (maximum pressure, crank-angle for maximum pressure, maximum pressure rise rate, and crank-angle for maximum pressure rise rate). In the new, microcontroller-based data acquisition (DAQ) system, all such calculations are performed within and only the desired parameters are passed to the real-time controller (xPC™) ensuring significant reduction in overhead on the real-time controller.

Experimental results for in-cylinder pressure are obtained from a single-cylinder engine running in HCCI combustion mode at different engine speeds. The new DAQ system results are benchmarked against the AVL™ Indimeter results obtained simultaneously. The microcontroller results show excellent match with the AVL™ results. Performing statistical analysis on the 100 cycles averaged maximum pressure rise rate values, as acquired by both AVL™ and the microcontroller-based

DAQ system, it is observed that the microcontroller-based DAQ has significantly less errors. Hence it is concluded that the microcontroller-based DAQ system is sophisticated enough to perform fast and robust pressure data sample and at the same time perform calculations on the acquired pressure data to determine parameters of interest (maximum rate of pressure rise and its crank angle).

The DAQ system is then coupled with the xPC™-based feedback controller to control combustion phasing at a desired crank angle while other control factors (like injection timing, etc.) are varied. One such experimental result is shown in Figure 6. Excellent control of combustion phasing is obtained at the desired combustion-phasing angle of 1 crank angle degree before TDC while the fuel injection timing is varied. In the next phase development of a similar DAQ system for a multi-cylinder (up to six cylinders) engine is planned. Initial hardware layout and communication protocols are selected. Software development efforts are underway. Once the software development is complete, validation using engine test data is planned.

Demonstration of transient operation of an HCCI engine has been completed. Five different control inputs are identified that can affect the transient operation of the HCCI engine. These are compression ratio (CR), intake valve actuation (IVA, for the purpose of this report it is the crank angle at which intake valve is closed), EGR, fuel injection pressure and end of injection angle. All of these parameters can be controlled in real time using our existing control architecture.

In order to best model the system, models must be developed that account for multiple inputs and non-linear behavior. Artificial neural networks have been chosen as one option to provide the level of accuracy and computational efficiency required. A neural networks-based approach requires collecting a diverse set of output data (emissions and performance) for a widely varying range of input parameters. Hence, a map-based approach is followed to accommodate different sets of input maps for a widely varying range of input parameters. A key requirement in successfully capturing the system response in a data-driven approach (like neural network based modeling) is to collect output data for almost all possible input parameters combinations. Since it is not realistically possible to exploit all possible input combinations, a large number of maps were generated to accommodate sufficient combinations of input parameters. Transient operations of a multi-cylinder HCCI engine within two points in the engine operation, with different control maps, are realized. These transients provide understanding of the effects of different control parameters on performance parameters during transients. This understanding helped in developing better maps for control parameters, which allowed improving engine performance during transients. The input-output data recorded during these transients are also utilized to develop the neural network based model for the engine. This model is used to perform multi-variable optimization on different input parameters and can be instrumental in developing optimum transient control strategies for HCCI engines.

Task 6 - Combustion CFD Model Development Activities: Significant improvements in the areas of liquid to gas momentum exchange, wall film treatment, and chemical kinetics have been made to the in-house CFD-code, CAT3D. This has made it possible to apply the tool to gain a deeper understanding of the physical processes underlying HCCI combustion. Simulations of the Caterpillar metal and Sandia optical engines have provided valuable insights into the mixing and combustion processes. The CFD tool has been used to design combustion systems (piston bowls and spray angles) for the single and multi-cylinder engines.

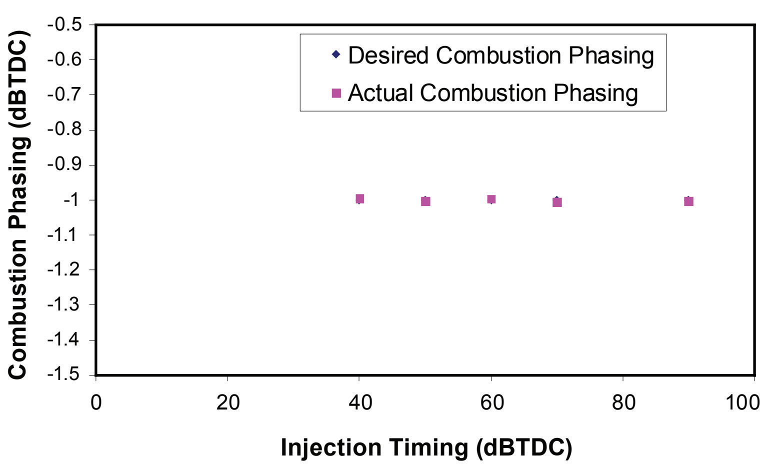

FIGURE 6. Utilizing the microcontroller-based DAQ system and real time engine controller, the combustion phasing is controlled at desired combustion phasing while injection timing is varied.

Task 7 – Combustion Development for Advanced Multi-cylinder HCCI Engines: A new variable compression ratio (VCR) engine was built and tested. The operational limits of the VCR HCCI engine were examined at two different engine loads. Specifically, the engine was run at numerous combinations of compression ratio, EGR fraction and IVA that yielded a combustion phasing of 2 degrees after TDC. Intake temperature and fuel injection timing, which are the other two parameters that can affect combustion phasing in this particular engine, were held constant for those tests. Tests were conducted at operating conditions as seen in Figure 7. In general,

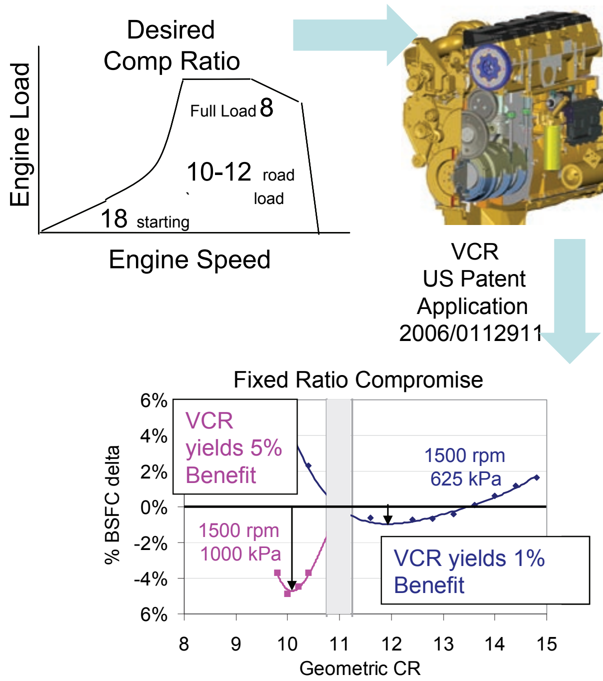

FIGURE 7. Utilizing the VCR engine, the compression ratio for each operating point can be optimized.

the range of IVA, EGR and CR settings over which the engine could run with a near-TDC combustion phasing was limited by either pressure rise rates, combustion retard, air-fuel ratio, NOx emissions or VCR mechanism limitations. The first sweeps were for three different combustion phasings from a baseline operation of fixed compression ratio, EGR fraction and IVA setting, which represented the best fuel consumption point at B25. The first sweep of combustion phasing was obtained by varying IVA from its baseline value while holding compression ratio and EGR constant. The second sweep was obtained by varying the compression ratio from its nominal setting while holding IVA and EGR constant, while the third sweep was obtained by varying EGR from its nominal setting while holding IVA and compression ratio constant. This set of data explored the effects of combustion phasing and highlighted the differences between the various methods by which the desired combustion phasing can be achieved. The second set of data consists of several EGR sweeps, each at a different combustion phasing value. This new data set illustrated how the limits of engine operation change for different values of combustion phasing. An understanding of this is required to get the complete picture of the interaction between CR, EGR, IVA and combustion phasing. To further support increased understanding of these fundamental trade-offs, the same approach was used on additional single-cylinder test engine work.

Conclusions

Significant progress was demonstrated on all tasks. See Accomplishments:

- Phase 2 optical diagnostic experiments complete.
- Single-cylinder engine fuels testing on low-cetane diesel boiling-range fuels completed.
- Prototype fuel injection system developed and tested on single-cylinder engine demonstrating ultra-low NOx and smoke emissions.
- Advanced multi-cylinder engine with compression ratio flexibility developed and tested demonstrating benefits for emissions, efficiency and controls.

FY 2007 Publications/Presentations

1. Q1, Q2, Q3, Q4 Quarterly reports
2. Presentation at 2007 DOE Merit Review
3. Presentation at 2007 DOE DEER Conference

Special Recognitions & Awards/Patents Issued

1. Ignition Timing Control with Fast and Slow Control Loops (IVP and EGR).
2. Mixed High and Low Pressure EGR in HCCI Engine.
3. Strategy for Extending the HCCI Operation Range using Low Cetane Number Diesel Fuel and Cylinder Deactivation.
4. Recipe for High Load HCCI Operation.
5. Caterpillar, Power Balancing Cylinders in HCCI Engine.

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

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Subcontractors:
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- ConocoPhillips, Portland, OR
- University of California, Berkeley, CA
- FEV, Auburn Hills, MI

Objectives

- Demonstrate engine performance with conventional power density (12.6 bar brake mean effective pressure [BMEP].
- Demonstrate ability of engine operation over transient emission cycles.
- Attain compatibility with exhaust aftertreatment devices.
- Achieve U.S. 2010 engine-out emissions without aftertreatment.
- Achieve competitive efficiency over conventional combustion.

Accomplishments

The present Phase III of the demonstrator project involves steady-state testing of a redesigned International 6.4L V8 engine with technology to support low-temperature combustion (LTC). Phase I consisted of a design phase involving combustion and engine cycle simulations to select the necessary hardware to run LTC to the power density of 12.6 bar BMEP. Phase II consisted of exploratory development of LTC with the base hardware while the hardware designed in Phase II was being procured. The fuel used is standard diesel fuel.

The key technologies implemented and function tested on the engine to date consists of:

- A custom charge air cooler (CAC) and intake heater bypass system,
- Multi-hole multi-row injector nozzles for better atomization and mixture,
- A range of compression ratio pistons,
- Improved flow cylinder head,
- Two-stage, dual-variable nozzle turbine (VNT) turbocharger system,
- Two parallel exhaust gas recirculation (EGR) coolers,
- Stand alone processor, programmed to schedule multiple injection pulses, control the EGR, VNT and CAC/bypass, with crank-angle-based data acquisition for cylinder pressure, and
- Combustion diagnostics and feedback control over start of combustion and torque on each cylinder.

Technologies being procured for future engine builds include:

- A variable valve actuation (VVA) system.
- A variable compression ratio (VCR) system.

Engine testing results include:

- Demonstrated LTC combustion up to 1,500 RPM and 6 bar BMEP, with plans to extend to the full range in the remaining portion of Phase III. Oxides of nitrogen (NOx) levels are limited to below 0.2 g/bhp-hr with soot levels below 2 mg/mm^3. Fuel efficiencies are comparable to 'conventional' operation.
- Critical to operating at LTC conditions are the integration of injection timing with high EGR levels and sufficient air-to-fuel ratios (AFRs). The engine controller plays a decisive role to maintain combustion phasing and avoiding misfire.

Future Directions

- Complete the engine builds and benchmark the attributes of the VCR and VVA prototypes.
- Conduct KIVA3V combustion simulation to further optimize combustion hardware.
- Continue to conduct steady-state testing to optimize combustion hardware for U.S. 2010 HD emission regulations. Special emphasis will be in fuel economy.
- Develop a prototype engine control unit to handle in-cylinder combustion diagnostics and feedback.

Introduction

LTC offers a new method of diesel combustion with the potential to reduce engine-out NOx and particulate matter (PM) emissions to levels that will meet the 2010 limits without the use of aftertreatment devices [1]. The benefits of LTC have been documented in the literature [2,3,4]: the capability to lower NOx emissions due to low combustion temperatures and improved fuel economy and lower soot emissions due to lean mixtures.

A challenge to LTC is the increased unburned hydrocarbon (HC) emissions from long mixing times due to local equivalence ratios (ϕ) below the lean combustion limit [5], from locally rich regions due to over fueling or injector dribble, and from decreasing in-cylinder temperatures as the piston moves away from top-dead-center. A second challenge for the application of LTC is the controllability of the ignition timing [6]. This is particularly challenging as a diesel mixture tends to ignite at relatively low temperatures and too abruptly.

Extending the operating region to high loads may require the introduction of VVA to adjust the effective compression ratio or preferably by VCR to adjust the geometric ratio.

Approach

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

- Phase I (completed) consisted of applied research, determining engine boundary conditions, combustion system design and simulation.
- Phase II (completed) consisted of exploratory development, engine hardware procurement, engine subsystem prove out, control system hardware procurement, controls software development.
- Phase III (in progress) consists of advanced development, steady-state testing of engine, combustion hardware development, fueling strategy development, and further controls system development.
- Phase IV consists of transient testing and production engine control unit development.

Results

The engine is designed to run LTC combustion with equivalence ratios 0.3 to 0.4 with 50% EGR. The engine will allow a maximum torque of 670 Nm (12.6 bar BMEP) at 2,000 RPM. Figure 1 shows the engine schematic.

Unique to this project are injector drivers capable to tune current slope (mA/µs) and opening and closing voltage supplied to the piezo stack. A variety of multi-hole, multi-row nozzles were bench tested and classified for their potential merits. Also unique, is that the controller optimizes the relative contribution of each turbocharger stage and coordinates the activity of the EGR valves. The rapid prototype system features cylinder pressure feedback control. Parts for the VVA system are being procured and are illustrated in Figure 2. Phase 3 of the project will yield two multicylinder V8 VCR prototype engines.

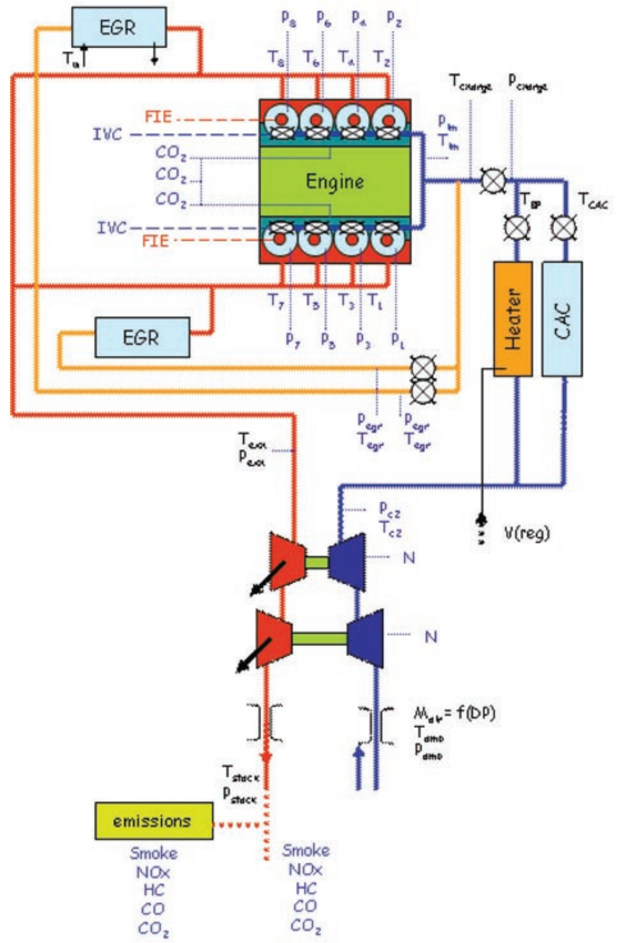

FIGURE 1. Test Engine Schematic

Test results to date have demonstrated LTC at 50% load or 6 bar BMEP. Operating at LTC involves flowing high EGR ratios, where combustion robustness depends on delivering sufficient AFR. Here the engine controller plays a decisive role to maintain combustion phasing and avoid misfire.

Figure 3 and 4 illustrate two LTC conditions at 1,500 RPM, 6 bar BMEP. The EGR rates are same, at 50%. In both cases, the controller is highly responsible for adjusting the injection timing to maintain the CA50 at 5° after top dead center. Despite good control over CA50, Figure 3 shows the combustion system at the edge of stability. The instability appears in cylinders 1 and 2, noticeably different from cylinder 3 through 8.

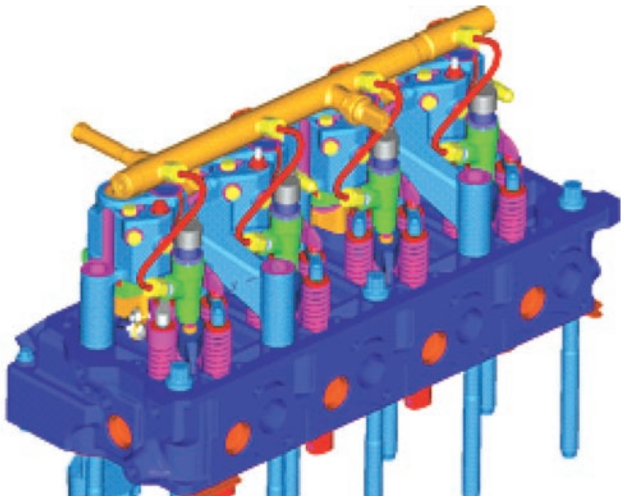

FIGURE 2. VVA Set-Up

Cylinders 1 and 2 display heat release traces (and dP/dtheta) characteristic of low oxygen concentrations (or higher EGR) with a stronger onset of a cool flame reaction. Figure 4 shows these cylinders becoming stable with increasing the boost and AFR. This issue illustrates the challenges of providing adequate EGR distribution in a real production-like application and the compensation techniques that may be implemented.

Figure 5 shows the performance and emissions corresponding to the speed and load above for varying engine configurations. Each subsequent hardware upgrade is capable of providing higher EGR rates. For the third configuration, corresponding to the above figures, demonstrates LTC conditions with 0.17 gNOx/bhp and 0.01 g/bhp-hr.

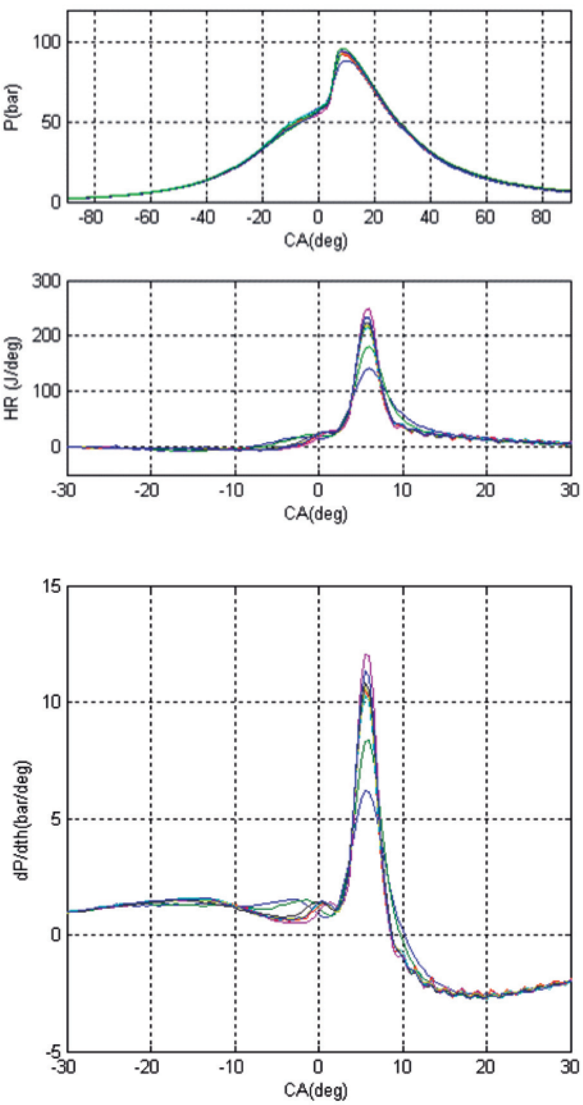

FIGURE 3. LTC at 1,500 RPM, 6 bar BMEP

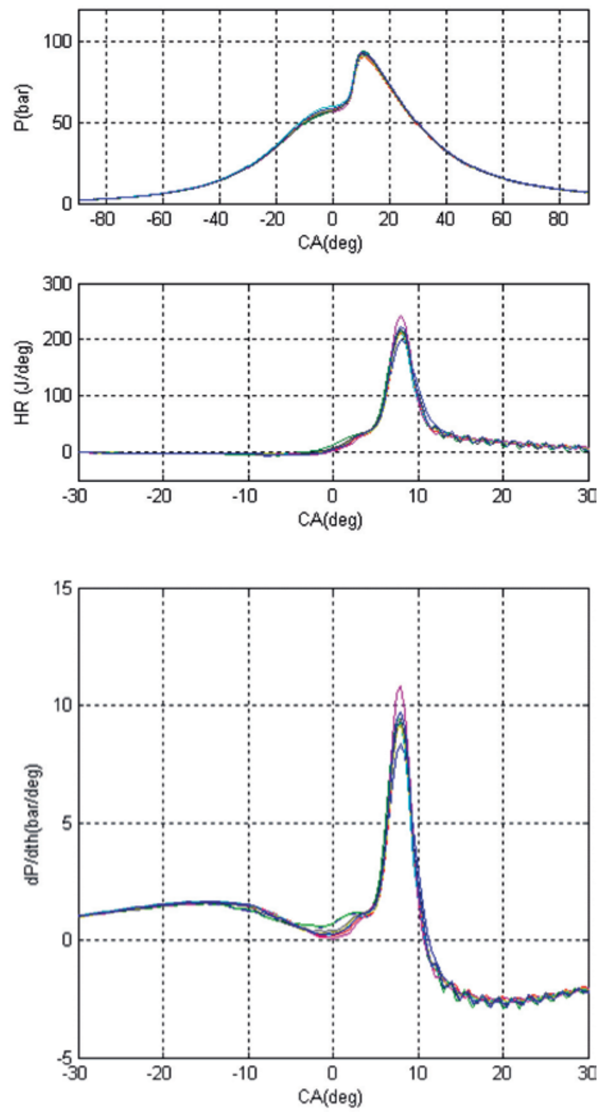

FIGURE 4. LTC at 1,500 RPM, 6 bar BMEP with AFR Adjustment

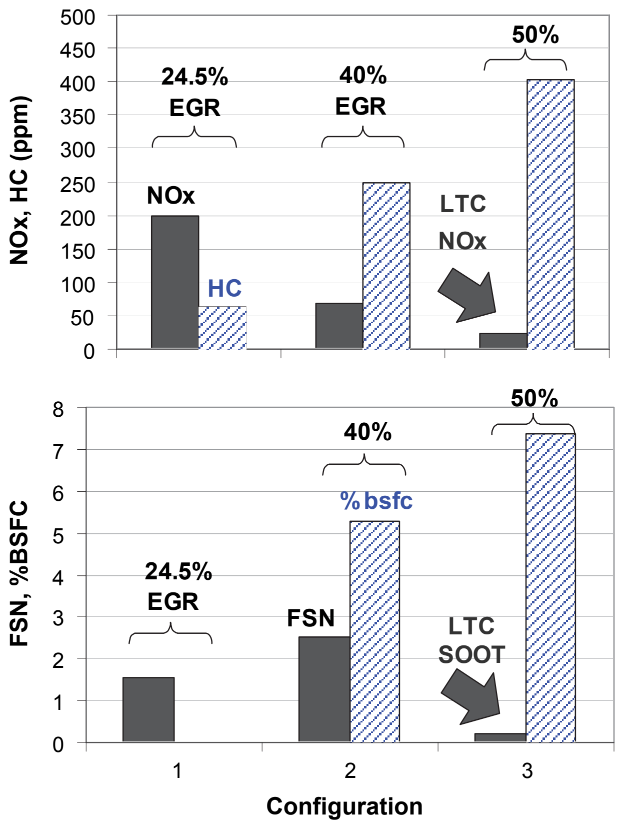

FIGURE 5. LTC NOx, Soot and Impact to BSFC (% Penalty), HC at 1,500 RPM, 6 bar BMEP

Conclusions

- To date, LTC-like emissions results were obtained up to 1,500 RPM and 6 bar BMEP, with plans to extend in the near future to 12.6 bar. NOx and soot levels were limited to 0.2 g/bhp-hr and 2 mg/mm^3, respectively.
- Integration of injection timing control with AFR is decisive to maintain combustion phasing and avoid misfire. Future work on either to detect or foresee misfire, and subsequent corrective action, will be critical to maintain combustion robustness.
- The present capability is owed to an optimum matching of engine hardware. The complete the engine build is still underway, however, with the design and procurement of the VCR and VVA prototypes.

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2. de Ojeda, W., Zoldak, P., Espinosa, R., Kumar, R., Cornelius, D., "Multicylinder Diesel Engine Design for HCCI operation", Diesel Engine Development, DEER 2006, August 20-24, Detroit, Michigan.

II.A.20 21st Century Locomotive Technology 2007 Annual Report: Advanced Fuel Injection

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Objective

Develop and demonstrate an advanced fuel injection system to minimize fuel consumption, while meeting Tier 2 emissions levels.

Approach

- Use General Electric (GE) Global Research's locomotive single-cylinder engine as the experimental test facility.
- Determine baseline engine performance using current production unit pump system.
- Optimize engine performance with advanced high-pressure common rail (HPCR) fuel injection system.
- Investigate the hardware space (injector parameters, nozzle geometry, bowl shape) and fuel injection command sequence to determine most advantageous fuel injection strategy.
- Develop transfer functions and models, which guide and allow down-selecting the combinations of hardware and injection commands for various engine loads.

Accomplishments

- Installed new diagnostics tools. These include an opacity meter and an engine exhaust particle sizer (EEPS) for particulate matter (PM). In addition, an in-cylinder combustion visualization spray and flame characterization system was installed.
- Completed study to examine the effect of the following parameters on engine performance:
  - total nozzle flow,
  - number of nozzles holes,
  - spray cone angle,
  - needle seat diameter,
  - injector needle lift and fall rate,
  - piston crown geometry (two geometries studied), and
  - fuel sulfur level.
- Engine performance is evaluated by specific fuel consumption (SFC), nitrogen oxides (NOx) emissions, and PM emissions.
- Explored pilot injection experimental space (dwell and duration) at both medium and high load conditions for selected rail pressures and documented effect on engine performance.
- Quantify PM benefits for post injections and their effect on SFC-NOx tradeoff.

Future Directions

- Continue to optimize the performance by leveraging the obtained knowledge on hardware change trade-offs and injection command sequences.
- Validate the combination of down-selected hardware and injection sequences.
- Expand validation efforts to include all load conditions, allowing for a duty cycle entitlement estimation.
- Further optimize our multiple injection strategy. This includes combinations of pilot and post injections and multiple pilot and multiple post injections.

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Introduction

GE's 21st Century Locomotive Program has the objective to develop freight locomotive engine technology and locomotive system technologies, which maximize the fuel efficiency while meeting Tier 2 freight locomotive emissions. The Tier 2 regulations have been in effect since 2005 in the U.S. GE's response to the Tier 2 emission regulations was to develop a completely new locomotive. In order to achieve future regulations like Tier 3 and Tier 4, GE is looking ahead, and developing new technologies and engine concepts. Existing technologies allow to a certain degree for reduction of emissions at a cost of increased fuel consumption. Compliance with tighter NOx and PM regulations while achieving a fuel consumption benefit requires new technologies; this is the objective of GE's project.

The following report summarizes GE's efforts over the past year, October 2006 to September 2007. During that time, GE focused on the development of an advanced fuel injection system and demonstrated and quantified the benefits of this system over the existing technology currently used.

Objective and Approach

The objective is to develop and demonstrate an advanced fuel injection system to minimize fuel consumption, while meeting Tier 2 emissions levels.

Fuel injection has a significant impact on a diesel engines' performance as it governs key parameters as atomization, penetration, fuel rate and ultimately mixing. A HPCR injection system was used to achieve performance and emissions improvements over the production unit pump system (UPS). The maximum injection pressure of the HPCR is above 1,800 bar. Multiple post and pilot injection commands allow for a flexible injection rate over the combustion cycle. The experimental facility being used for the studies is the locomotive single cylinder engine at the GE Global Research Center.

In a first step, geometrical fuel injector parameters such as number of holes, nozzle flow cone angle, have been studied over a wide range. This study resulted in a down-selected set of nozzle geometries to be tested with multiple injection strategies. While the focus in those studies was on part-load (Notch 4) and full-load (Notch 8), a wide range of injection pressures was covered. In a second step, designed experiments have been executed in order to explore and optimize the multiple injection strategy. In order to validate and quantify the benefits of the HPCR system, a baseline was established on the single-cylinder engine using the UPS system.

Accomplishments and Results

In the following section the main accomplishments are described in more detail. They are organized in five groups: a) diagnostics, b) nozzle geometry and injector configuration, c) multiple injections, and d) fuel type.

Diagnostics

An optically accessible engine head was installed on the single-cylinder engine test bed at the end of 2006. This allowed for combustion event visualization via a high-speed camera. The engine head also allows for illumination of the cylinder and studies on fuel spray and mixing. The modified engine head is also equipped with thermocouples to record the metal temperatures at eight locations, including the hottest regions of the combustion chamber. The metal temperatures were used to monitor bulk gas temperature due to various fuel injection strategies and changes. Furthermore, an EEPS was purchased and installed. The EEPS system allows for real-time analysis of particle size distribution.

Nozzle Geometry and Injector Configuration

The following key parameters defining the nozzle geometry have been studied: total nozzle flow, number of holes, spray cone angle, needle seat diameter and sac volume. Furthermore, by using various orifice plates the injector configuration was changed. Combinations of nozzle geometry and needle lift profiles were systematically studied and their impact on engine performance evaluated.

The nozzle flow area was changed over a range of approximately 20% of the baseline flow rate. The rates of needle velocity in the opening and closing where unchanged. Other parameters, including number of holes and spray angle, were held constant in the first set of designed experiments, in order to isolate the effect of total flow. To understand possible interaction between nozzle parameters, in later experiments, multiple parameters have been changed simultaneously. The study was carried out for a range of injection pressures. While the results indicated a fairly monotonic trend of PM as a function of nozzle flow area, the effect on fuel consumption was found to be more complex.

Nozzle flow, number of holes and hole diameter are dependent variables, from which only two can be chosen independently. In our nozzle geometry study we changed flow and number of holes independently. The number of nozzle holes was varied by up to four. The PM emissions level was strongly dependent on the number of holes. The effect of number of holes was notably stronger than the effect of injection pressure in the range tested. The SFC seemed to be less affected by the number of holes and more a function of the fuel injection pressure. The dependence of PM emissions on fuel injection pressure was found to be fundamentally different for different number of holes.

In order to explore the effect of spray cone angle on engine performance study the cone angle changed over a range of approximately 4% of the baseline nozzle. In the range studied, the trends for PM and SFC were found to be opposite. Changing the cone angle monotonically led to a benefit in fuel consumption while the PM emissions increased and vice versa.

Needle seat diameter and orifice plate flow have a strong effect on the needle lift profile. The needle seat diameter was increased by up to 12.5% compared to the baseline nozzle while the orifice plate flow was changed by up to a factor of two. A study was performed to investigate four different combinations of seat diameter and orifice plate flow. The choices were made to achieve four distinct needle lift and fall rates for the test matrix. The choice of seat diameter seems to affect the

PM emissions only for low injection pressures. The fuel consumption is affected for all injection pressures, even though the effect is minor compared to the other nozzle parameters studied. For certain needle lift profiles fuel consumption benefits have been observed. The effects were stronger at part-load than at full-load.

We demonstrated that specific nozzle geometries (hole number and angle) could offer fuel consumption benefits at NOx-parity over our baseline nozzle with a very minor increase in PM emissions. The nozzle geometry study was based on single injection performance. The optimum nozzle selection process was based on the observed SFC benefits at Tier 2 NOx-emissions levels while meeting PM regulations. Among the geometries tested, the most favorable nozzle geometry at part-load was found to be different to the most favorable one at full-load. Also, performance results where strongly dependent on rail pressure. Therefore, the overall optimum nozzle geometry has to be determined on a duty cycle basis. The most favorable nozzles have been used as initial hardware configuration for the multiple injection studies, described in the next section.

Multiple Injection

Multiple injection strategies have been explored for both piston crown geometries. Piston crown geometries A and B vary mainly by their extent of re-entrant shape. In the third quarter of 2006 we had completed a screening study to efficiently explore the multiple injection design space using piston A. In the forth quarter of 2006, the injection strategy, which gave the best results for the old nozzle/orifice plate configuration, was repeated with a new injector configuration. The trends observed by changing between single injection and multiple injections were found to be fairly similar. This indicates that the performance shift between multiple injections and single injections is consistent, even with small fuel injector nozzle/orifice plate changes. Note that the performance shifts between single and multiple injections were not found to be transferable across piston bowl geometries. While certain multiple injection commands offered benefits using piston A, the performance shift was not observed with piston B.

Using piston B, we explored in detail single-pilot and single-post injection schemes. In order to find the optimum pilot injection strategy, we explored a wide range of pilot injection durations and dwell times. For post injections the injection duration and location was varied in a similar fashion as for the pilot injection. The studies were carried out for several rail pressure levels and a range of main injection advance angles. In order to understand to what extend the benefits observed for pilot and post injections are additive, selected cases of combinations therefore have been tested.

For selected cases, we showed that the addition of pilot injections provides a SFC benefit (at constant NOx level) over the single injection. The addition of pilot injections was found to have little impact on PM emissions. For single injections, the rail pressure was found to have a strong effect on SFC. For rail pressures levels leading to a higher SFC with a single injection, the SFC benefits observed for adding on a pilot injection where larger. At full-load, pilot injection strategies have shown an improvement for limited NOx levels over the UPS. At part-load, pilot injections improved the NOx-SFC tradeoff compared to the UPS over a wider range of NOx levels.

The addition of post injections allowed for significant reduction in PM. In selected cases at part-load a simultaneous benefit in SFC was observed. The relative PM reduction using post injection was approximately twice at part-load than at full-load. The post injection duration was found to have a strong impact on the engine performance at all loads tested. While larger fuel quantities in the post injection decreased the PM emissions further in our study, the NOx-SFC tradeoff turned unfavorable for prolonged post injection durations. For specific load conditions, the engine performance was found to be fairly insensitive to the location of the post injection. In order to achieve NOx parity with an additional post injection, the main injection timing had to be slightly advanced.

Fuel Type

Three different fuels with sulfur levels changing by more than a factor of 200 where tested. As expected, a linear dependence of PM emissions on fuel sulfur level was found. The quantitative results at hand now allow for a better comparison of the data taken on the single-cylinder engine to data taken on other engines run with different sulfur levels.

Conclusions and Future Work

Changes in nozzle geometry have been proven to allow for further engine performance benefits. Clear trends have been identified and quantified. For the range studied, the number of holes seemed to have the strongest effect on PM, followed by rail pressure and nozzle flow. Changing the spray cone angle was found to have monotonic but opposing trends for SFC and PM. In this case, a trade-off function between SFC and PM was identified. Multiple injection strategies have been shown to allow for additional fuel and emission benefits over the optimized nozzle geometry single injection results. Pilot injections have been successfully proven to reduce NOx emissions, especially at part-load. Post injections have been shown to give significant reduction in PM, without imposing a measurable SFC penalty. Additional diagnostics, like in-cylinder visualization of the combustion event and particle size measurements in the engine exhaust, allow for further understanding and guidance of future engine developments. Future work is needed to optimize the combination of post and pilot injections for the most favorable hardware combination. Furthermore, we will expand the studies over the entire engine duty cycle.

II.A.21 Stretch Efficiency in Combustion Engines with Implications of New Combustion Regimes

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Objectives

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

Approach

- Use literature study to reevaluate prior work on improving engine efficiency.
- Exercise appropriate engine models to define the greatest opportunities for further advancement.
- Develop improvements to those models as needed to address the impact of new approaches to combustion.
- Conduct availability (exergy) analyses using the Second Law of Thermodynamics as well as the First Law to study where the large losses inherent in conventional and alternative combustion approaches lie.
- Design and conduct proof-of-principle experiments.

Accomplishments

- Designed and constructed a bench-top experimental apparatus for demonstrating low-irreversibility combustion based on the concept referred to as counterflow-preheat with near-equilibrium reaction (CPER).
- Continued exploring better ways for recuperating exhaust heat and utilizing compound cycles for extracting work.
- Continued exercising engine and combustion models to identify combustion modifications that would mitigate exergy losses.
- Continued collaborating with Texas A&M in analyzing case studies of the major exergy losses during diesel engine operation.

Future Directions

- Shakedown and experimentally demonstrate low-irreversibility combustion in the CPER bench-top apparatus.
- Continue analyses of data from CPER experiments to determine efficiency implications and appropriate ways to model exergy losses under different operating modes.
- Continue exploring better ways for recuperating exhaust heat and utilizing compound cycles for extracting work.
- Continue exercising engine and combustion models to identify combustion modifications that would mitigate exergy losses.

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Introduction

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

In conventional engines the largest efficiency losses (approximately 20-25%) occur in the combustion process itself and are difficult to mitigate. Such losses are not due to unburned fuel, which is a relatively small loss, but they are instead due to the generation of thermodynamic entropy by unrestrained chemical reactions. The net effect is to divert some of the fuel energy into molecular motion and heat. This diverted energy becomes unavailable to produce useful work according to the Second Law of Thermodynamics. Simple energy balances, which reflect the First Law of

Thermodynamics, don't distinguish between available energy (energy that can produce work) and unavailable energy (energy that can only make heat). However, as we discuss below, it is theoretically possible to carry out our combustion reactions in a more restrained way that produces less entropy and preserves more of the original fuel energy for work.

Typically, processes that generate entropy are referred to as thermodynamically irreversible. Detailed analyses of the irreversibility of unrestrained combustion have shown that it comes mostly from 'internal heat transfer' between the products (exhaust gases) and reactants (fuel and air). Such heat transfer is inevitable in both pre-mixed and diffusion flames, where highly energetic product molecules are free to exchange energy with unreacted fuel and air [2]. Since these molecules have large energy (i.e., temperature) differences, considerable entropy is generated when they interact. In general, combustion irreversibility is mitigated if the reactions take place nearer chemical equilibrium. This requirement can be accomplished when the reactants are preheated reversibly (slowly, with small temperature gradients) such that they are brought closer to the temperature of the products [3].

Approach

We previously conducted analytical studies of the exergy losses in current internal combustion engines in collaboration with Professors Jerald Caton (Texas A&M University) and David Foster (University of Wisconsin). Based on these studies, we have identified the irreversibility of the combustion step as the largest single contributor to fuel exergy loss. In response, we have shifted our efforts to experimental evaluation of novel approaches to combustion that can reduce this inherent irreversibility. A common theme of all the novel approaches being considered is that they attempt to create conditions under which the combustion reactions occur closer to a state of chemical equilibrium.

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

- Counterflow preheating of the inlet fuel and air with exhaust, and;
- Introduction of a reforming catalyst to stimulate reforming of the fuel as it is preheated.

These two concepts are specific implementations of more general concepts emerging from our previous analytical and literature investigations referred to as CPER [3] and thermo-chemical recuperation (TCR) [4].

A bench-top experimental apparatus is being constructed to allow direct comparisons between conventional atmospheric combustion of hydrocarbon fuels and atmospheric combustion based on CPER-TCR. Measurements from the bench-top combustor will be used to validate the theoretical predictions and also explore practical ways to maximize the benefits.

Results

The majority of the FY 2007 effort has focused on the design and construction of a bench-top experiment that can be used to demonstrate the feasibility of more reversible combustion based on CPER-TCR. The basic concept behind CPER-TCR is illustrated schematically in Figure 1, where more reversible combustion is achieved by preheating the inlet fuel and air in counterflow to the exhaust to reduce the average temperature difference associated with internal heat transfer. In addition, the reversibility of the fuel preheating is enhanced by catalytically promoting simultaneous reforming reactions which occur closer to chemical equilibrium than the fuel decomposition reactions occurring in the flame.

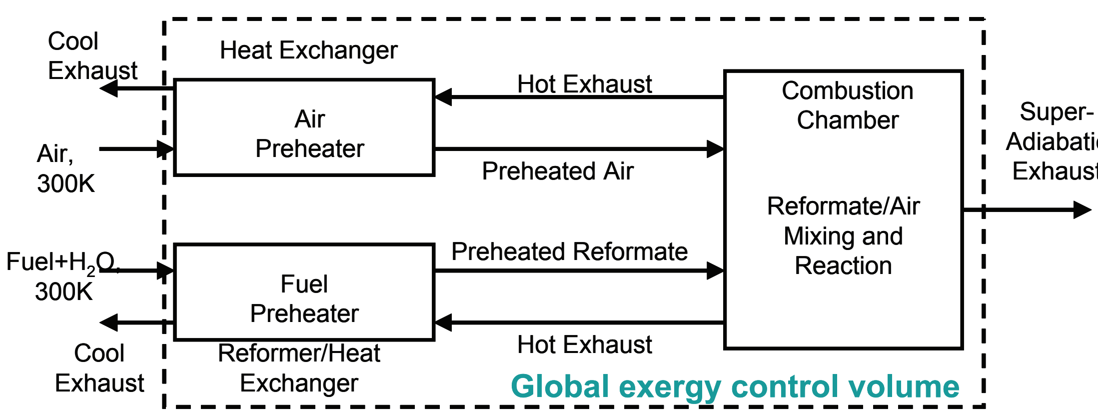

FIGURE 1. Conceptual schematic for restrained combustion by CPER and TCR. Fuel and air are preheated prior to combustion by counterflow heat transfer with exhaust. Additional exhaust exergy is retained in thermo-chemical form due to simultaneous reforming of the fuel.

Theoretical analyses suggest that as much as two-thirds of the fuel exergy normally lost during combustion can be retained through this type of process. For the experiment, all stages of preheating and combustion are designed to be carried out at nearly constant pressure. The two initial fuels being considered for shakedown experiments are methane and ethanol.

The experimental combustor is designed to burn fuels within an enclosed, insulated combustion chamber as schematically illustrated in Figure 2. Fuel and air can be delivered at constant flow into the chamber through vertical feed lines that pass through the upper plate of the combustion chamber, flow through counter-current heat exchangers, and finally into a small burner at the base of the upper plate assembly. The combustion exhaust gases exit from the top of the chamber through three separate vertical exhaust tubes as illustrated in the assembly photograph in Figure 3. One of the exhaust tubes vents directly from the combustion chamber into the atmosphere, while the other two discharge from the hot-side outlets of the fuel and air preheaters, respectively. Pressure regulators at the end of the exhaust lines control the rate of reaction products flowing through each exhaust outlet, permitting the degree of air and fuel preheating to be independently controlled.

Details of the air and fuel preheaters are illustrated in Figures 4 and 5, respectively. As noted in these figures, the fuel and air lines are introduced through the top plate via the corresponding exhaust vents. Fins and helical coils are used to enhance the counterflow heat transfer, and in addition, there is provision to include a reforming catalyst (either in pellet or monolithic form) on the cool side of the fuel preheater. The latter is intended to promote endothermic reforming reactions that recuperate additional exhaust heat in the form of thermo-chemical exergy, which is then returned to the combustor.

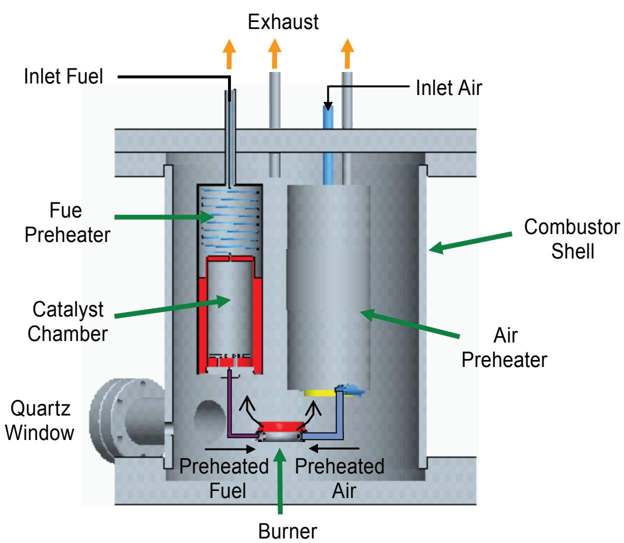

FIGURE 2. Schematic of the experimental CPER-TCR combustor. Incoming air and fuel are preheated by exhaust, and the fuel is partially reformed. Exhaust exits the top via three separate vents. Two quartz windows provide optical access.

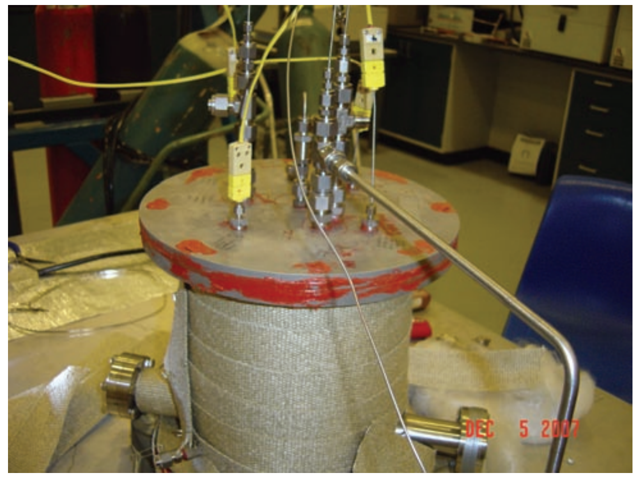

FIGURE 3. Photograph of the assembled experimental CPER-TCR combustor.

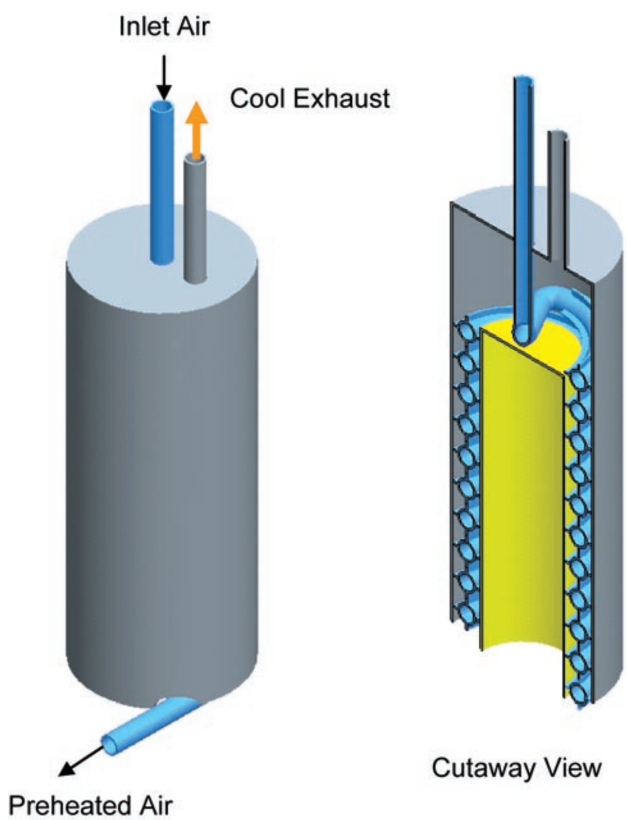

FIGURE 4. Schematic showing details of the air preheater. Heat is transferred from the hot exhaust in the surrounding manifold through the finned coil into the incoming air.

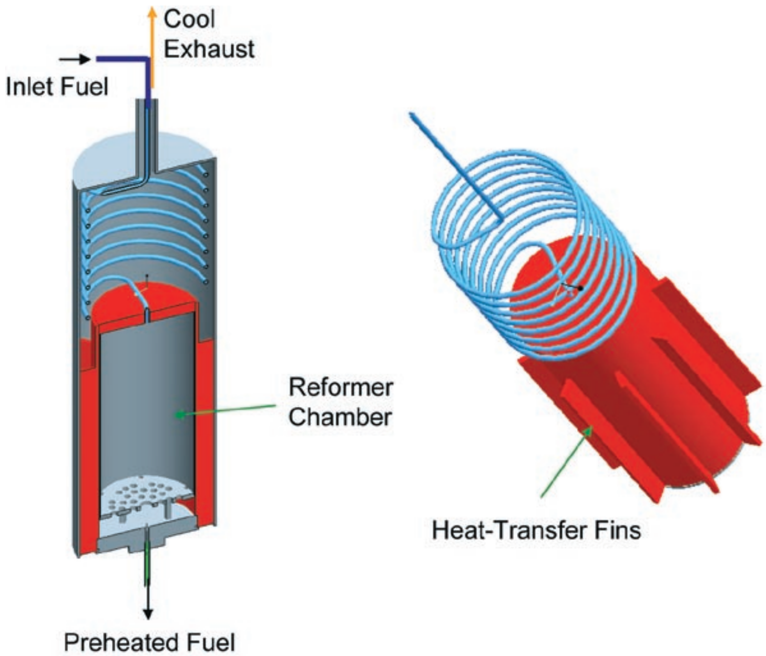

FIGURE 5. Schematic showing details of the fuel preheater. Heat is transferred from the hot exhaust in the surrounding manifold through the coiled tubing and canister into the fuel and refoming catalyst. The catalyst promotes endothermic reforming reactions that produce H_2 and CO from the raw fuel.

Details of the burner, which is located at the bottom of the combustion chamber, are still being resolved. It is expected that the burner will utilize some type of porous metal distributor (e.g., sintered metal) with a catalyst to stabilize the combustion at very lean conditions. While the irreversibility of lean combustion is known to be higher than for stoichiometric combustion, it is also recognized that the current materials of construction would be inadequate to sustain the temperatures involved in stoichiometric combustion. Since the current objective is to show the exergy advantage of the CPER-TCR configuration, it is sufficient to compare the combustor exergy performance at lean fueling conditions with and without preheating and reforming.

The fuel and air flows are controlled and measured by electronic control valves and flow transmitters, respectively. Water or steam can be added as needed to promote reforming reactions. The temperature of each stream (inlet and outlet) is monitored with thermocouples, and the composition of exhaust gas is monitored for unburned hydrocarbons and CO. The above measurements will be sufficient to develop global energy and exergy balances over the combustor at each steady-state operating condition.

Conclusions

An experimental bench-top CPER-TCR combustor has been constructed and is awaiting shakedown testing and demonstration of combustion with significantly reduced thermodynamic irreversibility. This combustor should provide the opportunity for the first experimental demonstration of a thermal combustion process that can retain a significant fraction of the exergy now destroyed in conventional combustors and combustion engines.

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II.A.22 Advancements in Engine Combustion Systems to Enable High-Efficiency Clean Combustion for Heavy-Duty Engines

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Objectives

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

Accomplishments

- Successfully completed the first part of the Near-Zero Emissions at 50 Percent Thermal Efficiency (NZ-50) project. It demonstrated 50.2% thermal efficiency with integrated experimental and analytical technologies at Environmental Protection Agency (EPA) 2010 emissions levels at a single operating condition in a multi-cylinder engine configuration.
- Successfully launched the second part of the NZ-50 project in March of 2007, which focuses on high efficiency clean combustion.
- Identified an advanced fuel injection system with variable nozzle technology, genetic combustion optimization, and advanced control and calibration optimization as three key enabling technologies.
- Successfully completed project annual review with DOE in August, passing the first "Go/No-Go" decision point by developing a technical roadmap to achieve project objectives.
- Evaluated a new dual combustion mode concept using variable fuel nozzle technology. Analytically characterized the benefits of the dual combustion modes, demonstrating 12% improvement in brake specific fuel consumption (BSFC), 96% reduction in NOx, and 54% reduction in soot compared to the baseline engine at the A25 operating point. NOx and PM emissions are below the EPA 2010 emissions standard.
- Demonstrated and explored genetic combustion optimization and identified the best possible combinations of fuel injector hole size, numbers of holes, fuel spray angles, piston bowl geometry, injection timing, and swirl ratio.
- Developed and validated sophisticated advanced control logic through a large variety of offline simulations and optimizations. Down-selected a few calibration packages over hundreds of offline optimizations in a transient engine testing cell, achieving excellent trade-off between emissions and BSFC, thus saving significant time and resources.

Future Directions

- Procure advanced next generation fuel injection system including variable nozzles that can greatly enhance fuel injection flexibility.
- Develop a master plan on consolidation of fuel injection strategy and dual combustion modes to minimize cylinder-out emissions.
- Continue steady-state advanced combustion development. Implement genetic optimization recommendations for hardware procurement.
- Continue transient combustion and control development on a next generation of heavy-duty engine platform.

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Introduction

Detroit Diesel Corporation is conducting the NZ-50 multi-year cooperative agreement. This project consists of two major parts. The first part started in 2000. This part emphasizes fuel economy in developing and integrating commercially viable, on-highway truck engine technology while demonstrating near zero emissions and 50% thermal efficiency. The first part of the project was successfully completed, demonstrating 50.2% thermal efficiency with integrated experimental and analytical technologies at EPA 2010 emissions regulation levels at a single operating condition in a multi-cylinder engine configuration [1]. The second part of the project started in March of 2007, focusing on engine combustion systems using HECC techniques to minimize cylinder-out emissions. Throughout the project, integrated analytical tool box with hardware experiments has been developed to define various most potential conceptual engine system technologies and component enhancements, and then tested. The key enabling technologies have been aggressively pursued, making significant progresses. This annual report will primarily focus on the progress of the second part of the NZ-50 project.

Approach

Detroit Diesel Corporation has developed a proven concept and methodology of combining experimental and analytical tools to facilitate integrated engine, aftertreatment and vehicle development. It uses integrated analytical and experimental tools for subsystem component optimization encompassing advanced fuel injection, increased exhaust gas recirculation (EGR) cooling capacity and combustion process optimization. Model-based controls employing multiple input and output techniques enable efficient integration of the various subsystems and ensure optimal performance of each system within the total engine package. Project assessment and milestone achievement are based on the context of the total engine package with subsystem components that are capable of integration into a production feasible multi-cylinder engine product. This system approach benefits substantially from an integrated experimental and analytical approach to technology development. This results in a shortened developmental cycle, and substantial NOx-PM trade-off and fuel economy improvement in both engines and vehicles.

Moving to the second part of the project with the focus on HECC, the technical approach is tailored to key combustion enabling technologies in addition to the system approach mentioned above. One of the key enabling technologies is the fully flexible fuel injection system, which can facilitate different advanced combustion modes. Working with fuel injection suppliers, a highly flexible fuel injection system with variable nozzle technology is being developed, which results in an unprecedented technical road map. Displayed in Figure 1 is the technology map developed for this project. As can be seen in Figure 1, highly flexible fuel injection system can greatly simplify the combustion strategy into three combustion zones, which feature emerging dual mode combustion. Introduction of a generic combustion optimization technique in conjunction with advanced control technology that has been consistently developed can considerably enhance the project.

Results

Achievement of 50.2% thermal efficiency in the first part of the project required significant technology building blocks [1], which laid out a strong foundation for this current combustion focused project. Carrying this strong momentum with further identification of key enabling technologies, a new dual combustion strategy is emerging. This is done with an advanced fuel injection system in conjunction with highly flexible variable nozzle technology. This variable nozzle technology features a moving needle and nozzle body that can generate a micro-variable circular orifice (MVCO), which is equivalent to a 6~50 variable micro-hole nozzle. It can also generate a conical spray only or mixed-mode conical-multi-jet spray patterns to meet the needs of different engine operating conditions.

Use of an advanced three-dimensional computational program with sophisticated combustion and spray models was made to evaluate this dual mode combustion concept. Table 1 shows the simulated results for a low load point at the A25 operating point (25% load and A engine speed). As can be seen, with this dual combustion mode resulted from a high flexible variable nozzle with 12% improvement in BSFC, 96% reduction in NOx, and 54% reduction in soot are obtained, and NOx and soot emissions are below EPA 2010 emissions standards.

While focusing on analytical evaluation of the emerging dual mode combustion, two other key technical areas were also conducted in parallel. Genetic combustion optimization is one area, while advanced control and calibration optimization is another. Figure 2 shows the comparisons between traditional and genetic combustion optimization. The key difference between

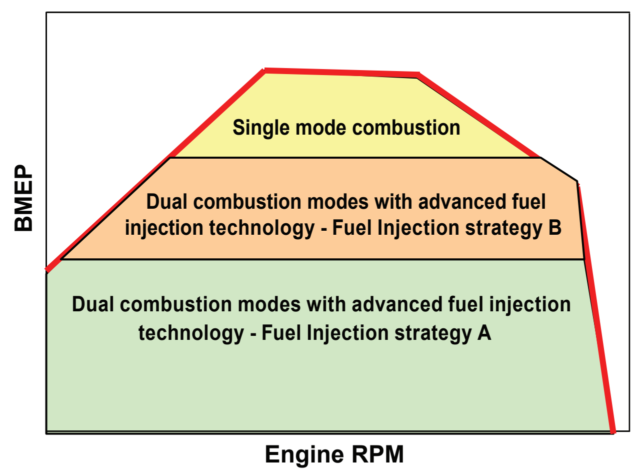

FIGURE 1. Strategy for Combustion Concepts Integration

TABLE 1. Emerging Dual Model Combustion with Variable Fuel Injection System

	Case	BSFC [g/kW·hr]	NOx [g/hp·hr]	Soot [mg/m³]	CO [g/hp·hr]	HC [g/hp·hr]
Baseline	Baseline	222	1.592	0.767	0.47	0.071
MVCO	MVCO (Dual Injection Mode)	195.2	0.07	0.349	0.473	0.189
	Improvement	12%	96%	54%	-1%	-166%

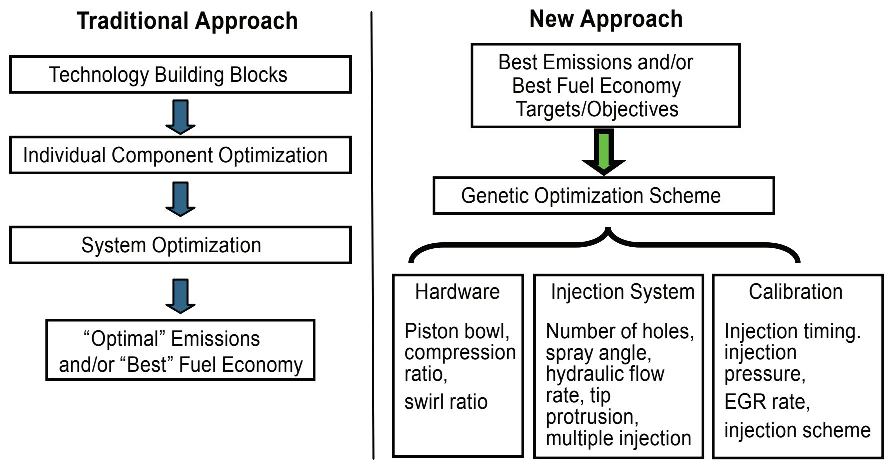

FIGURE 2. Innovative System Optimization Methodologies Emerging

these two approaches is that there is no guarantee for optimal results with the traditional approach since testing matrix is so large that it is virtually impossible to test all points. In contrast, the genetic optimization approach starts with top levels of objective definition, and then randomly selects testing matrix points, following well proven mathematical procedures to down-select optimal points. Figure 3 shows the genetic combustion optimization results at the A25 operating point. As can be seen, the pareto citizens that represent the optimal boundary among a large number of testing points are found, thus locating a trade-off between emissions and BSFC depending on applications.

Realizing that transient engine control is critical to proper torque response over the road, fuel economy and emissions, DDC continues spearheading development of next generation engine control techniques including model-based approaches, on-board setpoint adaptation and observer models. Experimental and simulation results help to quantify the benefits of nonlinear control techniques, both from a stability and response time standpoint. Displayed in Figure 4 is the trade-off between BSFC and NOx using advanced control logic to down-select a few optimal points through a large number of offline simulation points. More detailed descriptions of DDC's sophisticated control technology are available [2].

Conclusions

- Successfully completed the first part of the project with achievement of the March 2007 objective, demonstrating 50.2% thermal efficiency with integrated experimental and analytical technologies at EPA 2010 emissions regulation levels at a single operating condition in a multi-cylinder engine configuration.

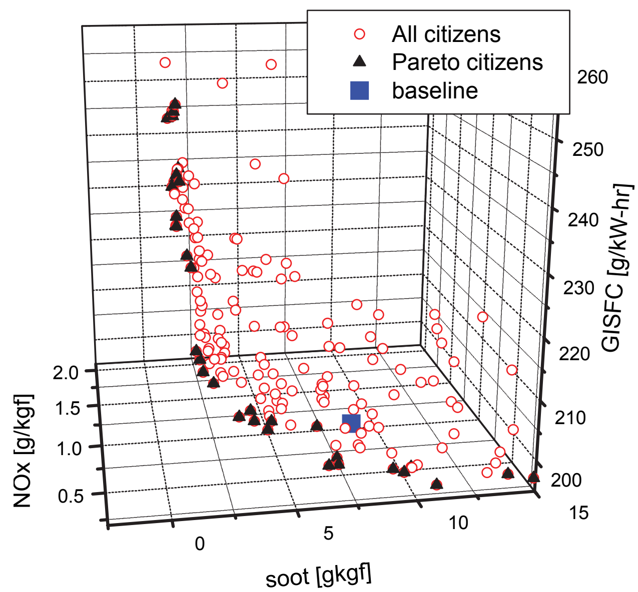

FIGURE 3. Genetic Combustion Optimization for A25

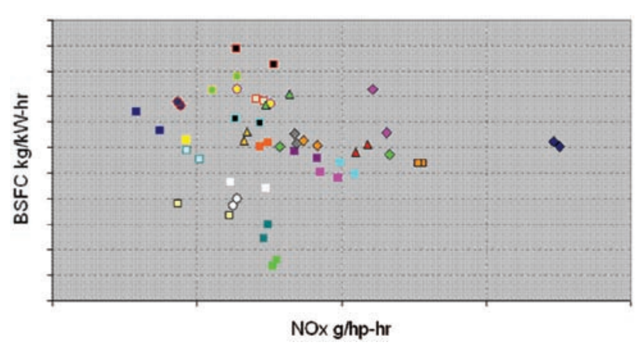

FIGURE 4. Advanced Control and Calibration Optimization (Each point marker designates one calibration FTP set point.)

- Successfully launched the second part of the project in March of 2007, focusing on HECC.
- Identified variable nozzle technology, genetic combustion optimization, and advanced control and calibration optimization as key enabling technologies in achieving the project objectives.
- Analytically characterized dual-combustion modes with an advanced fuel injection system, demonstrating 12% improvement in BSFC, 96% reduction in NOx, and 54% reduction in soot compared to a baseline engine at the A25 operating point. The NOx and soot emissions are below EPA 2010 emission regulations.
- Explored genetic combustion optimization for combinations of fuel injector hole size, numbers of holes, fuel spray angles, piston bowl geometry, injection timing, and swirl ratio.
- Validated advanced control logic through a variety of offline optimizations. Considerably simplified the calibration process to obtain optimal calibration packages in transient engine testing cells, and excellent trade-off between emissions and BSFC were obtained.

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2. Guangsheng Zhu and Houshun Zhang, "Invention of Squish-Induced Mixing-Intensified Low Emission Combustion (SIMILECOM)." Record of invention was submitted on August 16, 2007.

3. Jack Peckham, "Next-Generation Computer Controls Can Boost Diesel Fuel Efficiency without Compromising Emissions, Performance," Diesel Fuel News, Volume 11, issues 20, September, 2007.

II.A.23 Development of High Efficiency Clean Combustion Engine Designs for Spark-Ignition and Compression-Ignition Internal Combustion Engines

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Objectives

- Develop and demonstrate prototype gasoline and diesel engine hardware which enables operation of homogeneous charge compression ignition (HCCI) combustion for improved fuel efficiency and emissions performance.
- Understand and reduce the risks and roadblocks associated with this new combustion system by designing and demonstrating hardware solutions.
- Demonstrate enabling system on a 2.0-2.4L inline four-cylinder (I4) gasoline engine in a mid-size car.
- Demonstrate fully flexible system on a 2.0-2.4L I4 gas engine in a mid-size car.
- Demonstrate simple variable valve actuation system on a 4.5L dual overhead camshaft (DOHC) V8 engine in a mid-size sport utility vehicle.
- Demonstrate fully flexible system on a single-cylinder diesel engine.
- Demonstrate fully flexible system on a 4.5L DOHC V8 engine in a mid-size sport utility vehicle.

Accomplishments

Gasoline Systems

- Functional performance of key components and subsystems that enable HCCI operation have been tested and documented.
- Enabling system (2-step valvetrain) concept has been built, tested, and continues development work:
  - Engine dynamometer testing ongoing.
  - Mule and demonstration vehicle builds assembled, basic functions demonstrated, limited amount of vehicle calibration work done.
- Fully-flexible system concept single valve test fixture has been built, and initial testing is underway with basic concept functions demonstrated.
- Fully-flexible multi-cylinder design effort continues with focus on part count, part complexity, packaging, assembly, service.

Diesel Systems

- Fully flexible variable valve actuation (VVA) system in use on single-cylinder engine.
- Late intake valve closing has been demonstrated to:
  - Increase premixed charge compression ignition (PCCI) load range, which gives fuel consumption improvement.
  - Reduce exhaust gas recirculation (EGR) requirement at Tier 2 Bin 5 oxides of nitrogen (NOx) level.
  - Reduce particulates.
  - Increase in boost pressure and hydrocarbon (HC) emissions.
- Demonstrated functionality of the cam phaser VVA system over required operating range on multi-cylinder engine.
- Discovered discrepancy between the GT-Power model predictions and actual test results that caused lower than expected air flow and EGR rates.

Future Directions

Gasoline Systems

- Continue development and calibration work on vehicles with enabling system.
- Continue work on fully-flexible system to understand part variation, dynamic range, and energy consumption.
- Continue to refine the fully-flexible system design for multi-cylinder engines, especially valve lift sensing from a function/cost/packaging standpoint.

Diesel Systems

- Investigate internal EGR benefits using fully flexible system.
- Investigate other efficiency improvements using VVA.
- Rectify turbo-machinery problems and procure a new high-pressure stage turbocharger that meets air flow and EGR requirements.
- Integrate VVA controls into electronic control unit for transient testing.

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Introduction

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

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

Approach

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

Results

Gasoline Systems

The focus of the gasoline hardware development is on generating designs that reduce costs, reduce technical risks, and demonstrate hardware systems. Two valvetrain variants are under development. The simpler system uses a 2-step valvetrain design that enables some level of HCCI operation, and its focus is on identifying cost-effective component solutions. The fully flexible concept uses an electro-hydraulic camless VVA system design that is less limited in terms of operating strategy, and its focus is on developing the VVA system and quantifying potential benefits. Other hardware systems to be evaluated as part of this hardware development include direct fuel injection and cylinder pressure sensing.

In order to design and develop engine systems that enable HCCI operation, an important intermediate step is to evaluate the functional performance of some key engine components and subsystems. This step is also important for the integration of the components into a well-balanced engine design which has the desired capabilities. The performance of the following key components and subsystems were tested: the 2-step oil control valve; the 2-step switching roller finger follower; the cam phaser; the cam phaser control system; and the cylinder pressure sensor. The results of these tests were documented in a project milestone report, and they strongly influenced the design and development of both the enabling and fully flexible VVA systems.

The enabling VVA system and the fully flexible VVA system provide the ability to deliver appropriate quantities of fuel at the appropriate times. They also have the ability to robustly measure cylinder pressure with mass production-viable sensing hardware under normal vehicle operating conditions. The enabling VVA system has the ability to deliver desired HCCI valve events with a low-friction, reliable 2-step switching valvetrain, which also provides the ability to mechanically switch from HCCI valve events to normal spark ignition valve events in a fast, robust, and predictable manner.

The fully flexible VVA system has several capabilities beyond those of the enabling VVA system. The drawing in Figure 1 shows the mechanism for electrically actuated cam phasing, which provides for a high range of authority and very fast response in HCCI mode. It has the ability to provide complete control of valve motion, including lift, timing, and closing velocity. It has the ability to meet system performance requirements under normal and extreme vehicle operating conditions, while reducing system energy consumption. It has the ability to meet basic packaging, assembly, and service requirements with mass-production-viable hardware. Finally, it has the ability to meet noise and vibration requirements.

In addition to the bench testing of most components, the enabling system has been incorporated into engines and vehicles where the testing and development has continued. Engine dynamometer

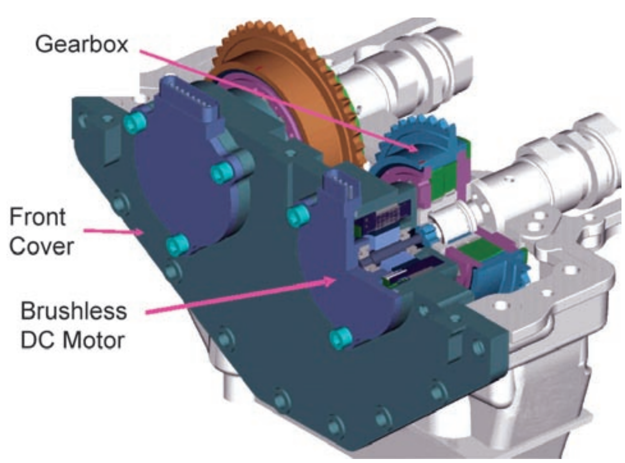

FIGURE 1. Mechanism for Electrically Actuated Cam Phasing

testing using this enabling system is ongoing. Mule and demonstration vehicles have been assembled, and they demonstrate basic functions by utilizing some limited vehicle calibration work.

For the fully flexible VVA system concept, a test fixture has been built as shown in Figure 2, and the basic concept functions have been demonstrated. Testing of this fixture and other aspects of the design are underway. The design for the fully-flexible multi-cylinder application continues with the focus on part count, part complexity, packaging, assembly, and service. However, more development work and testing must be performed to understand part variation, dynamic range, and energy consumption.

Diesel Systems

The single-cylinder diesel engine development has focused on testing a fully flexible electro-hydraulic VVA system. A schematic for this fully flexible system appears in Figure 3, which shows how the control system uses a servo valve to hydraulically control engine valve lift and duration. The benefit of this fully flexible VVA work is to improve our understanding of the upper bound efficiency potential of the diesel engine. This type of work is demonstrated in Figure 4, which shows how the system can adjust the intake valve closing (IVC) angle to control the effective compression ratio (CR).

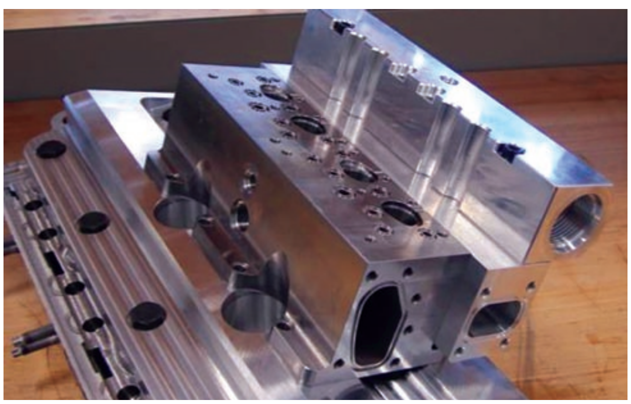

FIGURE 2. Test Fixture for Fully Flexible VVA Concept

Work on the multi-cylinder diesel engine has focused on the development of a production viable VVA system. In this system, a driveshaft within the cam is rotated to control intake valve timing. The benefit of testing this type of cam phaser system is to improve our understanding of the requirements and performance capabilities of a production viable VVA system. Both the single-cylinder and the multi-cylinder work are important for the development of technologies needed to achieve our goal of ultra-low engine-out NOx levels approaching Tier 2 Bin 5.

The fully flexible system on the single-cylinder engine has been used to investigate the potential benefits of various VVA strategies, such as late IVC. In theory, late IVC could increase the load range where PCCI occurs. Testing of late IVC has demonstrated the following:

- Increase in the PCCI load range, which produces fuel consumption improvement.
- Reduce EGR requirement at Tier 2 Bin 5 NOx level.
- Reduce particulates.
- Increase in boost pressure and hydrocarbon emissions.

For the multi-cylinder diesel application, the cam phaser VVA system demonstrated functionality over the required engine operating range. However, a discrepancy was found between the GT-Power model predictions and the actual multi-cylinder engine test results. As shown in Figure 5, this discrepancy caused lower than expected airflow and EGR rates. Further development will be required to resolve this air handling issue.

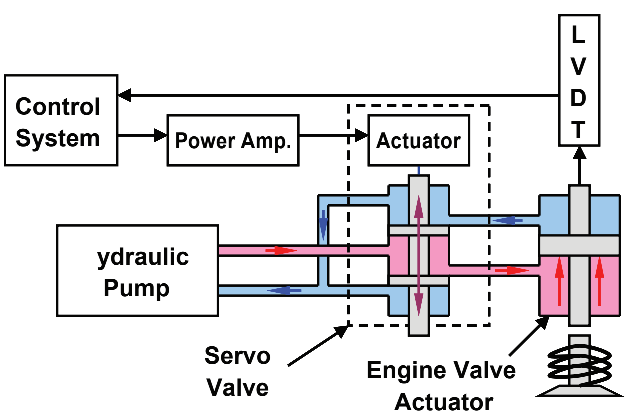

FIGURE 3. Schematic for Fully Flexible VVA System

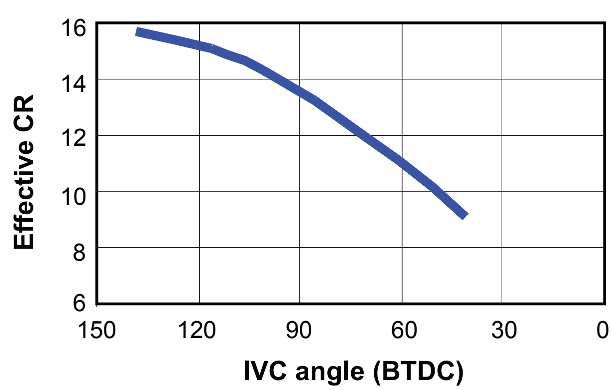

FIGURE 4. Impact of Late IVC to Reduce Effective CR

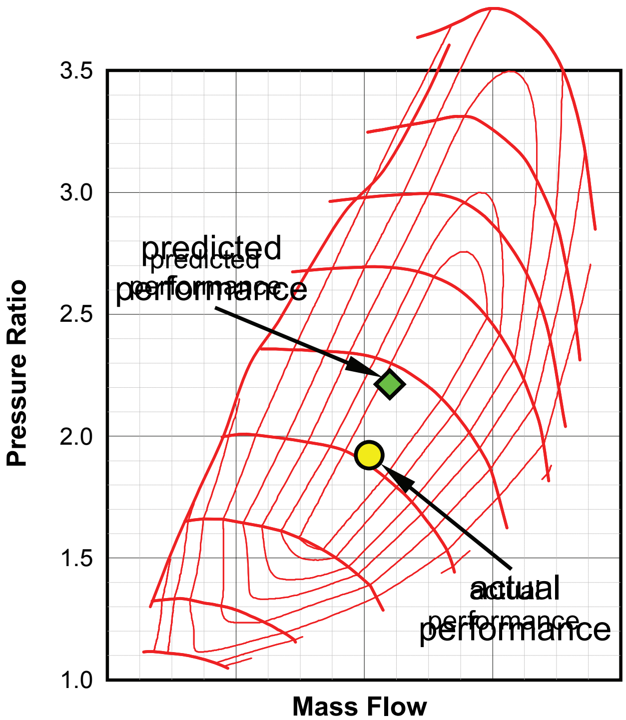

FIGURE 5. Difference between Predicted and Actual Performance of Cam Phaser System

Conclusions

Based on the successful demonstration of the "enabling" design on the gasoline HCCI engine in dynamometer testing and in vehicles, work on the enabling system should be continued. Based on the progress made on the fully-flexible design for the gasoline HCCI engine, the next steps of executing a multi-cylinder design should be taken.

For the diesel HCCI engine, significant progress has been made on both the simple and the fully-flexible designs. Both systems should continue to be developed, so that their potential performance, efficiency, and cost effectiveness can be properly assessed.

FY 2007 Publications/Presentations

Report at the DOE Merit Review – May 2007.