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

Accomplishments

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

Future Directions

- Increase the relevance of our measurements by studying sprays under conditions even closer to those of modern diesel engines. We have made steady progress over the course of the project, continually increasing the ambient pressure and enabling the use of production nozzles. In FY 2006 we achieved 30 bar ambient pressure; in FY 2007 we plan to make measurements at 35 bar. This will be comparable to top dead center (TDC) density conditions inside a boosted light-duty diesel engine.
- Increase the impact of our work by fostering collaboration with outside groups. Our collaborations with modeling groups allow our work to increase the fundamental understanding of the mechanics of the spray event, while our collaborations with industry enable us to develop a technique that is useful as a diagnostic for injection system manufacturers. Both of these expand the impact of our research, and help to meet the program objectives of decreased emissions and increased efficiency.
- Improve the measurement technique. While we produce useful results today, improvements to the measurement technique will increase its applicability and accessibility in the future. Such improvements include faster data acquisition, processing, and analysis, improved x-ray detector systems, increased x-ray intensity, and greater automation.

Introduction

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

Approach

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

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

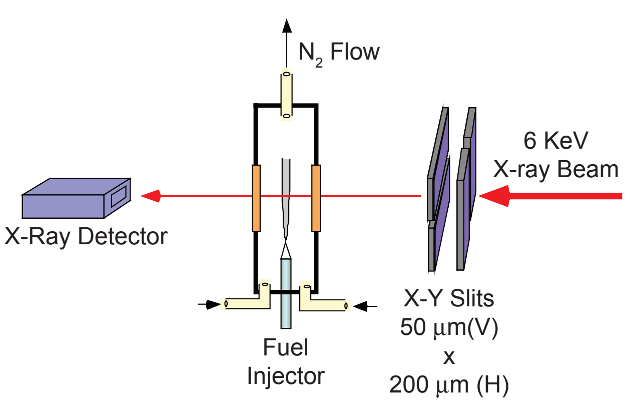

FIGURE 1. Schematic of the Experimental Setup

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

Results

In FY 2006 we made significant advances in effort to make measurements of sprays under conditions similar to those in a real engine. For the first time, x-ray measurements were performed under ambient density conditions comparable to those at start-of-injection in a modern light-duty diesel engine. These measurements represent a significant increase in our capability to measure sprays under high-pressure conditions, and enable the results to be directly applied to modern engines and computational models.

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

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

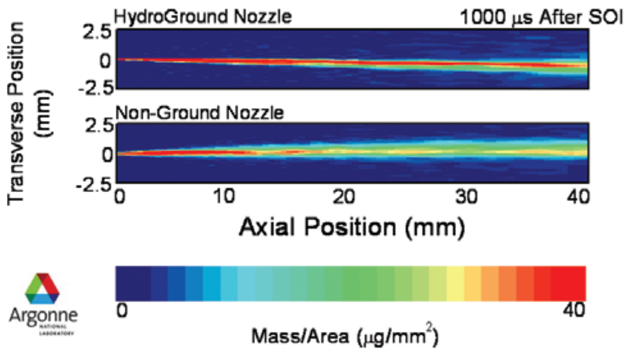

FIGURE 2. Spray images reconstructed from x-ray measurements of sprays from nozzles with different internal geometries.

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

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

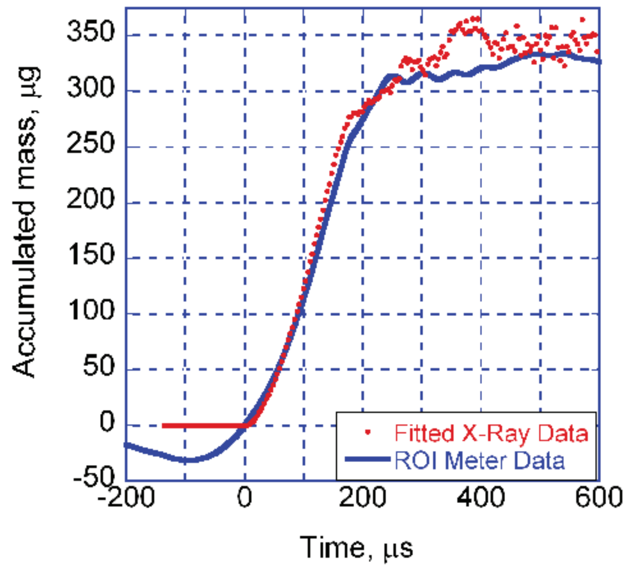

FIGURE 3. Comparison of the rate of injection measured using x-ray radiography and a commercial rate meter.

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

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

Conclusions

- The x-ray technique can be used to observe subtle changes in the spray structure resulting from different nozzle geometries. These changes are not apparent using other imaging techniques. This is a very useful diagnostic tool to fuel system manufacturers when designing and testing new injection systems.
- The time-dependent mass measurements provide unique information to spray modelers, and allow them to test their models in the near-nozzle region of the spray, something that was impossible

previously. This data is crucial for the development of accurate spray models and for the detailed understanding of spray behavior. The quantitative measurements that we have provided may help to elucidate the mechanisms of spray atomization. This could ultimately lead to the design of cleaner, more efficient engines.

- The impact of our work on the engine community is shown by the expanding list of collaborators and by the significant in-kind contributions to our work that are being made by fuel system and engine manufacturers.

References

1. C. F. Powell, Y. Yue, R. Poola, and J. Wang, J. Synchrotron Rad. 7:356-360 (2000).

2. C. F. Powell, Y. Yue, R. Poola, J. Wang, M.-C. Lai, J. Schaller, SAE 2001-01-0531, (2001).

FY 2006 Publications/Presentations

1. "Diesel Spray Characterization Using Synchrotron X-Rays", C. F. Powell, A. Kastengren, T. Riedel, J. Wang, S.-K. Cheong, K.-S. Im, X. Liu, Presentation to the Combustion MOU Partners, Sandia National Laboratory, February 2006.

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

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

4. "Spray Density Measurements Using X-Ray Radiography" A. L. Kastengren, C. F. Powell, Submitted to Journal of Automotive Engineering, July 2006.

5. "Spray Structure Measured With X-Ray Radiography", A. L. Kastengren, C. F. Powell, T. Riedel, J. Wang, S.-K. Cheong, K.-S. Im, X. Liu, DEER Conference, Detroit, MI, August 2006.

6. "The Structure of High-Velocity Dense Sprays in the Near-Nozzle Region" F. X. Tanner, K. A. Feigl, S. A. Ciatti, C. F. Powell, S. –K. Cheong, J. Liu, J. Wang., Atomization and Sprays 16 (2006) 579-597.

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

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

Future Directions

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

Introduction

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

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

Approach

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

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

Results

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

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

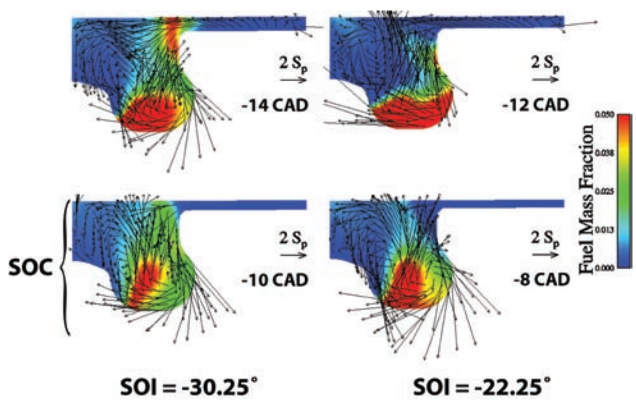

FIGURE 1. With earlier injection, the initial splitting of the fuel between the squish volume and the bowl leads to a broader fuel distribution at the start of combustion (SOC) and less CO formation.

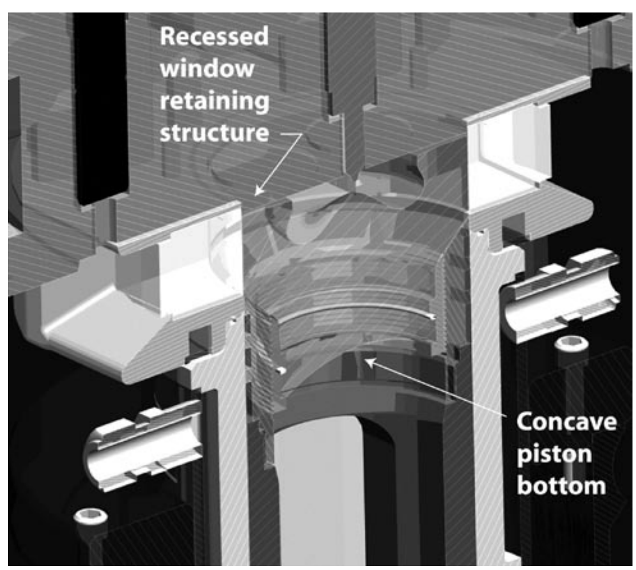

FIGURE 2. Representation of the new optical engine design, incorporating the GM 1.9 liter production head. Significantly enhanced optical access was achieved as compared to previous designs.

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

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

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

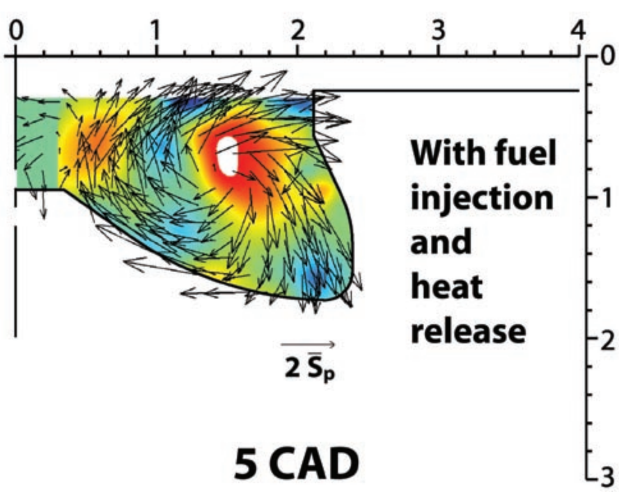

FIGURE 3. Bulk flow structures measured in a fired diesel engine. The flow divergence, indicated by the false color background, identifies regions of large volume expansion (heat release).

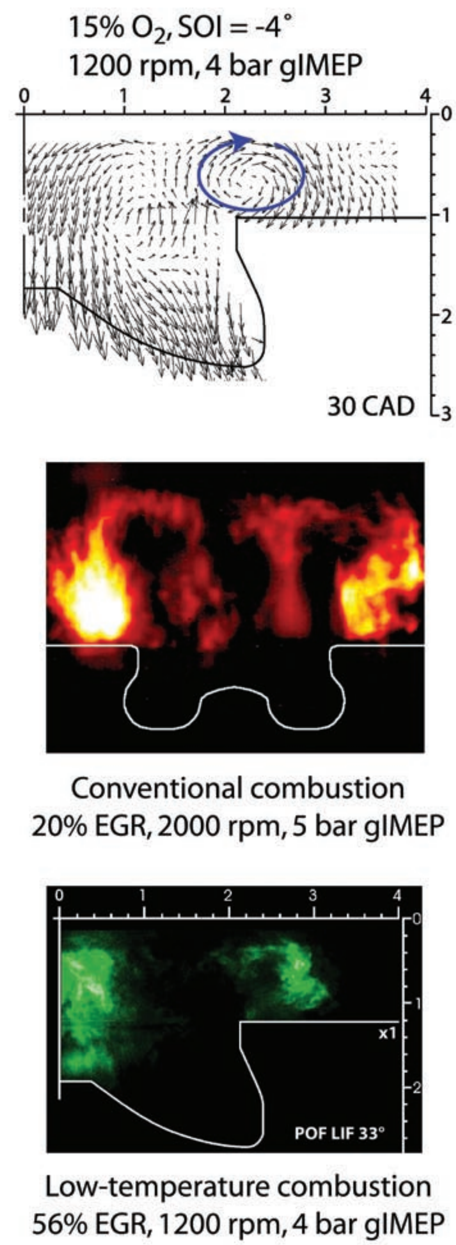

FIGURE 4. Toroidal vortex formed at the bowl exit during the expansion stroke. Either soot or partially-oxidized fuel may be trapped within this vortex for conventional or low-temperature combustion systems, respectively.

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

Conclusions

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

References

1. Miles, PC (2005) US Department of Energy, Office of FreedomCar and Vehicle Technology, 2005 Annual Progress Report.

2. Miles, PC (2004) US Department of Energy, Office of FreedomCar and Vehicle Technology, 2004 Annual Progress Report.

FY 2006 Publications/Presentations

1. Yu R, Bai XS, Hildingsson L, Hultqvist A, Miles PC (2006) Numerical and Experimental Investigation of Turbulent Flows in a Diesel Engine, ***SAE 2006 Fall Powertrain and Fluid Systems***, Oct. 16-19, Toronto, SAE Paper: 2006-01-3436.

2. Hildingsson L, Hultqvist A, Miles PC (2006) The Effect of Swirl and Injection Phasing on Flow Structures and Mixing in an HSDI Diesel Engine. ***Thermo-and Fluid-dynamic Processes in Diesel Engines****: THIESEL2006*, Sept. 13-15, Valencia, Spain

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

4. Miles PC, Hildingsson L, Hultqvist A (2006) The Influence of Fuel Injection and Heat Release on Bulk Flow Structures in a Direct-Injection, Swirl-Supported Diesel Engine. ***13th Int. Symp. on Applications of Laser Tech. to Fluid Mech.***, 26–29 June, Lisbon, Portugal.

5. Kook S, Bae C, Miles PC, Choi D, Bergin M, Reitz RD (2006) The Effect of Swirl Ratio and Fuel Injection Parameters on CO Emission and Fuel Conversion Efficiency for High-Dilution, Low-Temperature Combustion in an Automotive Diesel Engine, ***SAE World Congress***, SAE Paper: 2006-01-0197.

6. Kook S, Bae C, Choi D, Miles PC, Pickett LM (2005) The Influence of Charge Dilution and Injection Timing on Low-Temperature Diesel Combustion. ***SAE Fall Powertrain and Fluid Systems Conf***., SAE Paper 2005-01-3837 *(**2005 SAE Horning Memorial Award winner**)*

7. Miles PC. (2007) In-Cylinder Turbulent Flow Structure in Direct-Injection, Swirl-Supported Diesel Engines, Ch. 1 in **Flow and Comb. in Automotive Engines**, C. Arcoumanis, ed. Springer-Verlag. (*in press)*

8. Choi D, Miles PC, Yun H, Reitz RD (2005) A Parametric Study of Low-Temperature, Late-Injection Combustion in an HSDI Diesel Engine. ***JSME International Journal***, Ser. B, 48:656-664.

9. Colban W, Miles PC, Collin R, Hildingsson L, Hultqvist A, Andersson Ö. Combined Measurements of Flow Structure, Partially-Oxidized Fuel, and Soot in a High-Speed, Direct Injection Diesel Engine. Presented at the ***DOE OFCVT Advanced Engine Combustion Meeting***, June 2006.

10. Miles PC, Oh S, Kook S, Reitz RD, Bergin M, Hultqvist A, Hildingsson L. Automotive Low-Temperature Diesel Combustion Research, ***DOE OFCVT Peer/Merit Review,*** May 2006.

11. Miles PC, Choi D, Kook S, Bergin M., Reitz RD. Factors Affecting CO Emissions in Low-Temperature Combustion Regimes of HSDI Diesel Engines. ***DOE OFCVT Advanced Engine Combustion Meeting***, Feb. 2006.

Special Recognitions & Awards

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

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

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

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

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

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

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

Approach

This project utilizes an optically-accessible, heavy-duty, direct-injection diesel engine for in-cylinder measurements of compression-ignition spray, combustion, and pollutant formation processes. A cut-away cross-sectional schematic of the engine is shown in Figure 1. An extended piston with a large window located in the bowl of the piston provides primary imaging access to the combustion chamber. A portion of the piston bowl-

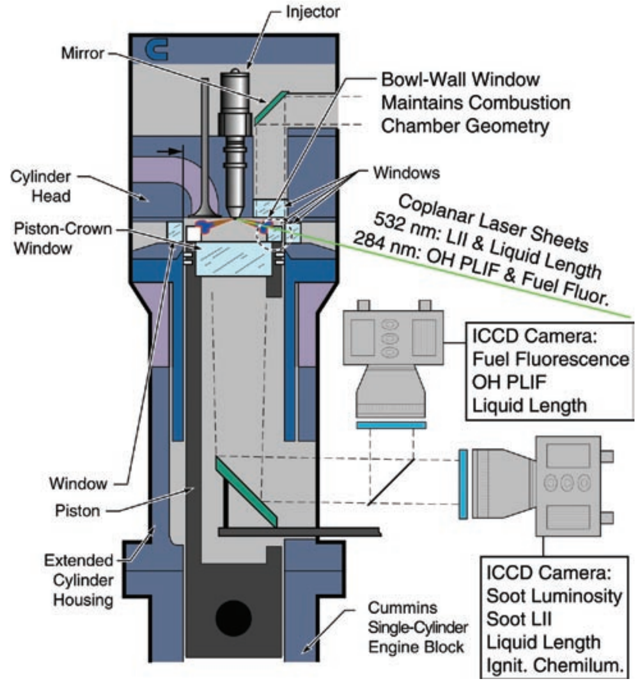

FIGURE 1. Schematic Diagram Showing Optical Engine and Laser/Imaging Diagnostics

wall is fitted with an optical window that matches the contours of the bowl-rim, in-line with one of the cylinder-wall windows, as shown in Figure 1. This window allows laser-sheet access into the combustion bowl of the piston, along the axis of one of the injector fuel-jets. Windows inserted in the cylinder wall provide cross-optical access for the laser diagnostics.

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

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

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

Results

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

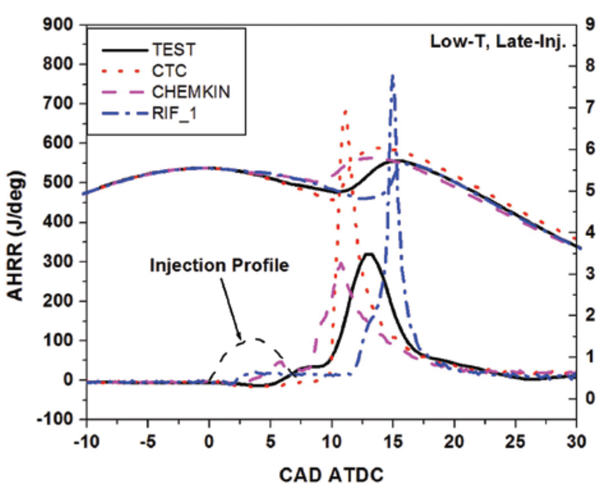

FIGURE 2. Experimentally measured and modeled cylinder pressure (top) and AHRR (bottom), and measured mass rate of injection profile (bottom).

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

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

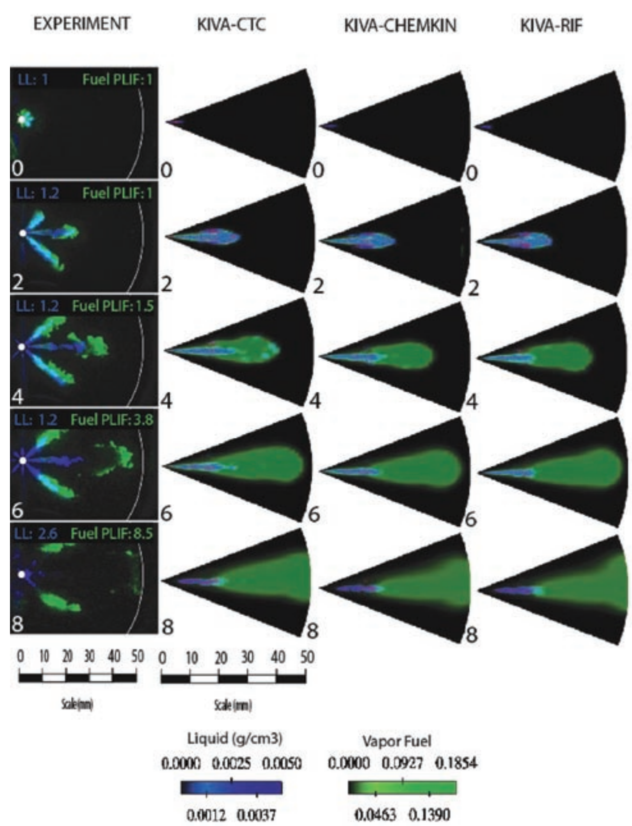

FIGURE 3. Experimentally observed liquid fuel (blue) and vapor-fuel fluorescence (green) and model-predicted liquid-fuel (red circles and blue color) and vapor-fuel mass fraction (green). The relative camera gains are indicated at the top of each experimental image, and the crank angle (°ATDC) is indicated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

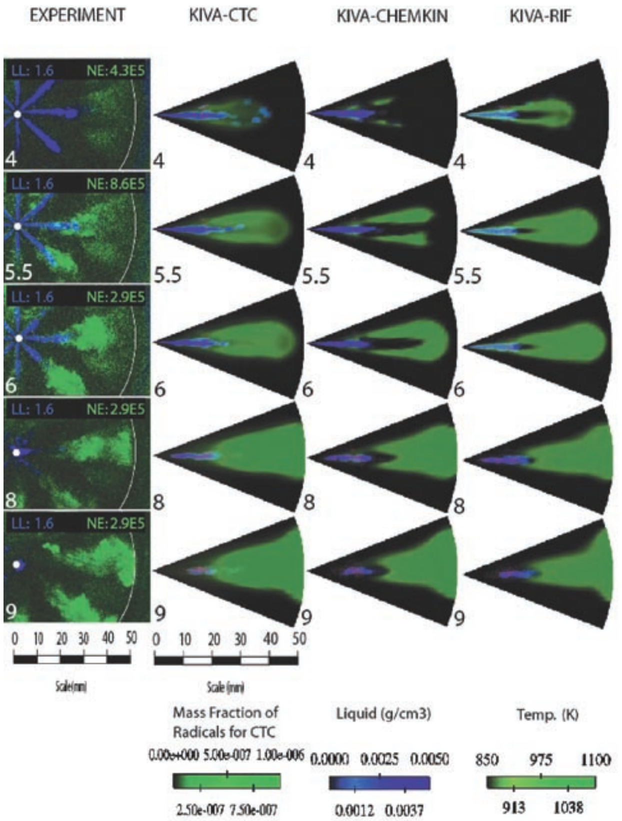

FIGURE 4. Experimentally observed liquid fuel (blue) and natural emission (green) and model-predicted liquid-fuel (red circles and blue color) and either ignition radical concentration (KIVA-CTC, green) or local gas temperature (KIVA-CHEMKIN and KIVA-RIF, green). Labeling is the same as Figure 3.

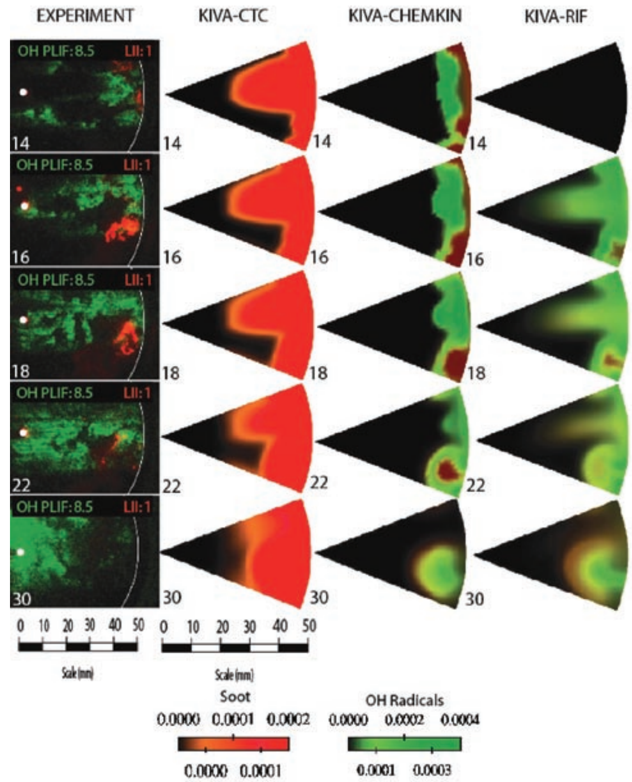

FIGURE 5. Experimentally observed OH-PLIF (green) and soot LII (red) and model-predicted OH (green) and soot (red) mass fractions. Labeling is the same as Figure 3.

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

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

Conclusions

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

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

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

Other activities on this project can be summarized as follows:

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

References

1. Kanda, T., Hakozaki, T., Uchimoto, T., Hatano, J., Kitayama, N., and Sono, H., "PCCI Operation with Early Injection of Conventional Diesel Fuel," SAE Paper 2005-01-0378, 2005.

2. Minato, A., Tanaka, T., and Nishimura, T., "Investigation of Premixed Lean Diesel Combustion with Ultra High Pressure Injection," SAE Paper 2005-01-0914, 2005.

3. Kimura, S., Aoki, O., Ogawa, H., Muranaka, S., and Enomoto, Y., "New Combustion Concept for Ultra-Clean and High-Efficiency Small DI Diesel Engines," SAE Paper 1999-01-3681, SAE Transactions, 108, No. 3, pp. 2128-2137, 1999.

4. Kimura, S., Aoki, O., Kitahara, Y., and Aiyoshizawa, E., "Ultra-Clean Combustion Technology Combining a Low-Temperature and Premixed Combustion Concept for Meeting Future Emission Standards," SAE Paper 2001-01-0200, SAE Transactions, 110, No. 4, pp. 239-248, 2001.

5. Yanagihara, H., Satou, Y., and Mizuta, J., "A Simultanoues Reduction of NOx and Soot in Diesel Engines under a New Combustion System (Uniform Bulky Combustion System - UNIBUS)," 17th International Vienna Motor Symposium, 1996.

6. Hasegawa R. and Yanagihara, H., "HCCI Combustion in a DI diesel engine," SAE Paper 2003-01-0745, SAE Transactions, 112, No. 3, 2003.

FY 2006 Publications/Presentations

1. "End-of-Injection Over-Mixing and Unburned Hydrocarbon Emissions in Low-Temperature-Combustion Diesel Engines," M. P. B. Musculus, T. Lachaux, L. M. Pickett, and C. Idicheria, Submitted to 2007 SAE International Congress and Exposition.

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

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

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

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

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

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

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

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

10. "Measurements of the Influence of Soot Radiation on In-Cylinder Temperatures and Exhaust NOx in a Heavy-Duty DI Diesel Engine," M. P. B. Musculus, SAE paper 2005-01-0925, SAE Transactions 114, No. 3, 845-66.

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

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

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

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

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

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

Emissions regulations coming into force over the coming decade, increasing costs of imported petroleum, and concerns about global climate change are driving the development of cleaner, more-efficient engine technologies using non-traditional and renewable fuels. One promising approach to achieving the desired efficiency and emissions targets without the use of costly exhaust-aftertreatment systems is high efficiency clean combustion (HECC). HECC is achieved when in-cylinder temperatures are low enough that high nitrogen oxide (NOx) emissions are avoided, and high particulate matter (PM) emissions are avoided by premixing the fuel/oxidizer mixture to overall lean conditions, decreasing in-cylinder temperatures below those required for soot formation, or enhancing late-cycle soot oxidation. An incomplete understanding of fuel effects on HECC has been one barrier to it being successfully implemented and optimized in production engines. Tasks during fiscal year 2006 (FY 2006) focused on enhancing the understanding of fuel effects on advanced engine processes by: 1) using fuel composition changes to overcome the critical barrier of elevated soot emissions under HECC and conventional combustion strategies, and 2) evaluating the validity of prevailing hypotheses to explain the observed increased NOx emissions with biodiesel fueling, so that this barrier to using this important renewable fuel can be eliminated.

Approach

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

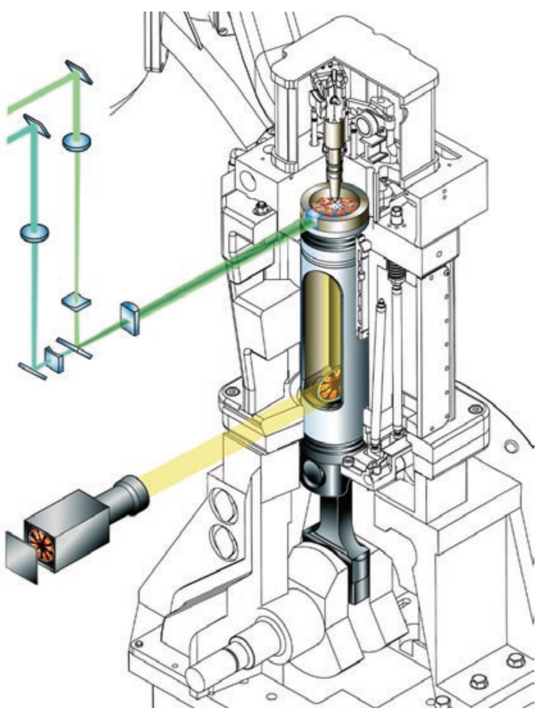

FIGURE 1. Schematic of Sandia Compression-Ignition Optical Research Engine (SCORE)

TABLE 1. SCORE Specifications

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

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

Results

Can near-term non-traditional fuels enable mixing-controlled HECC? FY 2005 results showed that mixing-controlled HECC (*i.e.*, operation compliant with EPA 2010 on-highway emissions targets and achieving >42% indicated efficiency) is possible without the use of aftertreatment through a strategy employing a highly oxygenated fuel (diethylene glycol diethyl ether, DGE), conventional injection timing, and exhaust gas recirculation (EGR) levels sufficient to drive the oxygen mole fraction in the intake mixture to 10-12% [2,3]. This approach avoids the control, pressure-rise-rate, and light-load emissions problems commonly experienced with premixed HECC strategies like HCCI. FY 2006 experiments focused on determining whether near-term fuels such as neat soy biodiesel (B100) and a Fischer-Tropsch-like paraffinic fuel (CN80) could achieve similar mixing-controlled HECC performance. Figure 2 shows that the smoke emissions for these fuels, while up to a factor of two lower than for the #2 diesel reference fuel (D2), were still at least an order of magnitude higher than the 2010 emissions target at the dilution levels required for NOx compliance. This indicates that additional in-cylinder strategies are required to enable HECC with these near-term fuels [4].

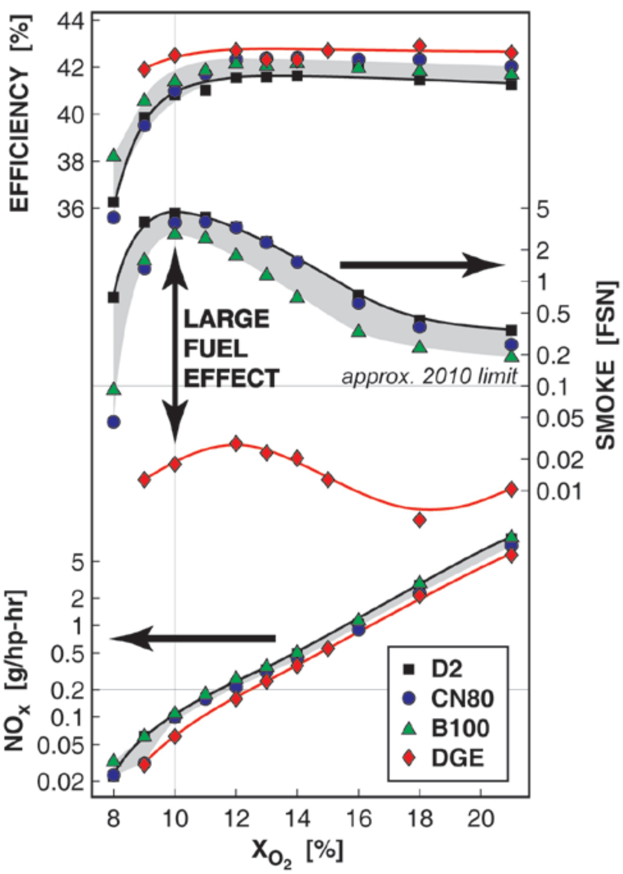

FIGURE 2. Engine-out NOx and smoke emissions, and indicated efficiency, for four different fuels over a range of intake-O_2 mole fractions (X_{O2}). The fuels are a low-sulfur #2 diesel reference fuel (D2), an 80-cetane blend of diesel primary reference fuels (CN80 = 76.5 vol% n-hexadecane + balance 2,2,4,4,6,8,8-heptamethylnonane), a neat soy biodiesel (B100 = Nexsol BD-0100 from Peter Cremer NA), and diethylene glycol diethyl ether (DGE). The gray, shaded regions show the ranges achievable with the near-term fuels. It is evident that B100, CN80, and D2 have excessive smoke emissions at dilution levels required for NOx compliance while maintaining reasonable efficiency. X_{O2} was adjusted by diluting the intake mixture with nitrogen gas. The injector nozzle had six, 0.163-mm-diameter orifices with a 140° included angle, and the single injection began within 5 crank-angle-degrees before TDC. The engine load was held constant at 6.7 bar gross indicated mean effective pressure (IMEP).

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

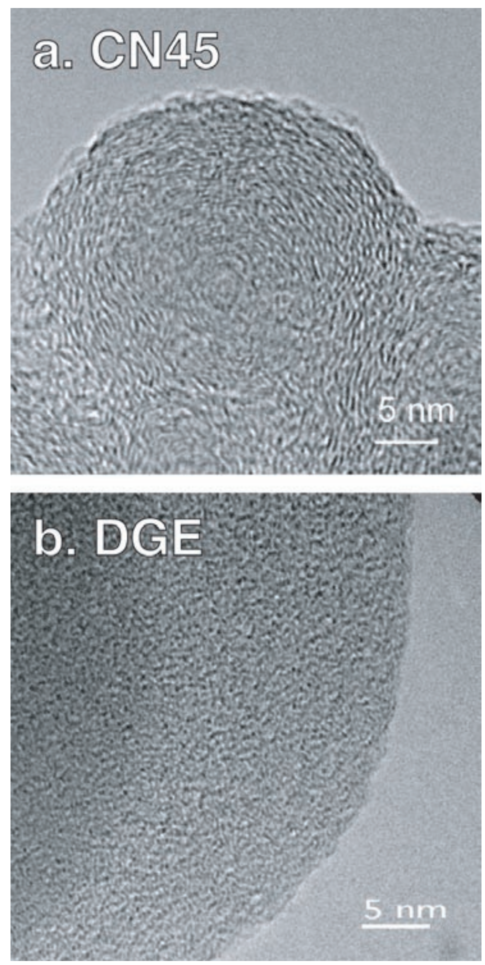

FIGURE 3. High resolution transmission electron micrographs of soot produced by a) CN45 hydrocarbon reference fuel and b) DGE. Note that the DGE soot has a highly disordered nanostructure (*i.e.*, no evidence of concentric carbon layer planes), which is correlated with oxidation rates up to five times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

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

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

Conclusions

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

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

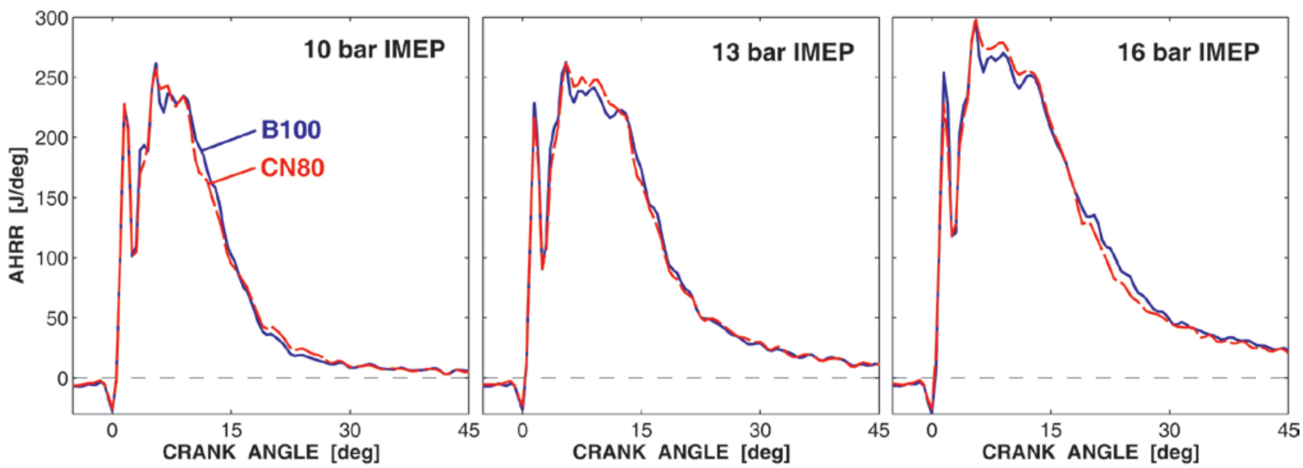

FIGURE 4. Apparent heat-release rate (AHRR) profiles showing matching between B100 and CN80 at three different engine loads.

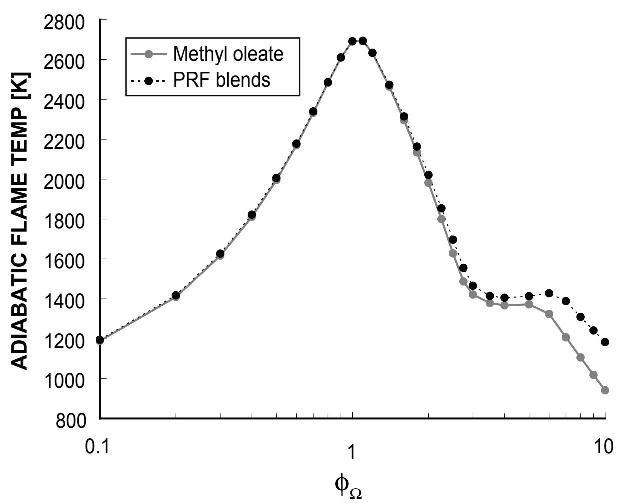

FIGURE 5. Adiabatic flame temperature as a function of mixture stoichiometry for mixtures of diesel primary reference fuels (PRFs) and methyl oleate (a surrogate for B100). The stoichiometric adiabatic flame temperature values are identical for all of the fuels. The oxygen equivalence ratio, ϕ_Ω, is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

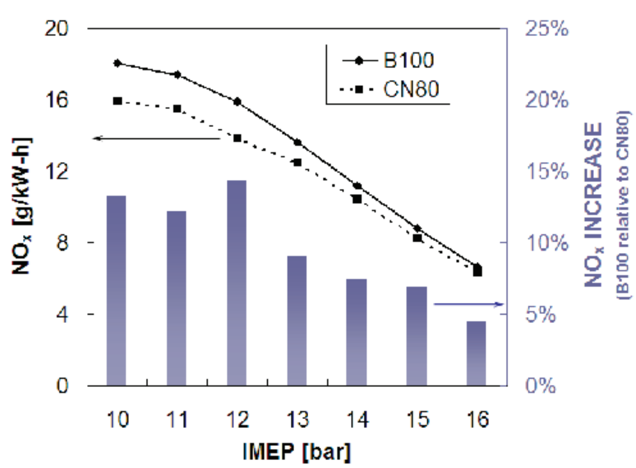

FIGURE 6. Fueling with B100 produces a load-averaged 10.5% NOx increase relative to CN80, even though start of injection, ignition delay, premixed-burn magnitude, heat-release rate, and stoichiometric adiabatic flame temperature are matched between the two fuels at each load.

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

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

References

1. Mueller, C.J., Martin, G.C., Briggs, T.E., and Duffy, K.P., "An Experimental Investigation of In-Cylinder Processes under Dual-Injection Conditions in a DI Diesel Engine," SAE Paper 2004-01-1843, *SAE Trans.*, Vol. 113, Sect. 3 (2004).

2. Upatnieks, A. and Mueller, C.J., "Clean, Controlled DI Diesel Combustion Using Dilute, Cool Charge Gas and a Short-Ignition-Delay, Oxygenated Fuel," SAE Paper 2005-01-0363 (2005).

3. Upatnieks, A., Mueller, C.J., and Martin, G.C., "The Influence of Charge-Gas Dilution and Temperature on DI Diesel Combustion Processes Using a Short-Ignition-Delay, Oxygenated Fuel," SAE Paper 2005-01-2088, *SAE Trans.*, Vol. 114, Sect. 4 (2005).

4. Cheng, A.S., Upatnieks, A., and Mueller, C.J., "Investigation of Fuel Effects on Dilute Combustion in an Optical Direct-Injection Diesel Engine," manuscript in preparation (2006).

5. Vander Wal, R.L. and Mueller, C.J., "Initial Investigation of Effects of Fuel Oxygenation on Nanostructure of Soot from a Direct-Injection Diesel Engine," *Energy & Fuels* **20**:2364-2369 (2006).

6. Mueller, C.J., "The Quantification of Mixture Stoichiometry When Fuel Molecules Contain Oxidizer Elements or Oxidizer Molecules Contain Fuel Elements," SAE Paper 2005-01-3705, *SAE Trans.*, Vol. 114, Sect. 4 (2005).

7. Cheng, A.S., Upatnieks, A., and Mueller, C.J., "Investigation of the Impact of Biodiesel Fuelling on NO_x Emissions Using an Optical Direct Injection Diesel Engine," *Int. J. Engine Research* **7**:297-318 (2006).

FY 2006 Publications

1. Vander Wal, R.L. and Mueller, C.J., "Initial Investigation of Effects of Fuel Oxygenation on Nanostructure of Soot from a Direct-Injection Diesel Engine," *Energy & Fuels* **20**: 2364-2369 (2006).

2. Cheng, A.S., Upatnieks, A., and Mueller, C.J., "Investigation of the Impact of Biodiesel Fuelling on NO_x Emissions Using an Optical Direct Injection Diesel Engine," *Int. J. Engine Research* **7**:297-318 (2006).

3. Martin, G.C., Mueller, C.J., and Lee, C., "Two-Photon Nitric Oxide Laser-Induced Fluorescence Measurements in a Diesel Engine," *Applied Optics* **45**:2089-2100 (2006).

4. Mueller, C.J., "An Introduction to Biodiesel," *CRF News* **28**, May/June (2006).

5. Martin, G.C., Mueller, C.J., and Lee, C., "Two-Photon Laser-Induced Fluorescence of Nitric Oxide in a Diesel Engine," SAE Paper 2006-01-1201 (2006).

6. Mueller, C.J. and Martin, G.C., "Sandia Optical Experiments," *DOE High Efficiency Clean Combustion Phase I Topical Report*, NETL Annual Report (2005).

7. Mueller, C.J., "Using Non-Traditional Diesel Fuels and Optical Diagnostics to Understand and Optimize In-Cylinder Processes," *Proc. of DOE Advanced Engine Combustion and Fuels Program Review*, DOE/OFCVT Annual Report (2005).

8. Mueller, C.J., "The Quantification of Mixture Stoichiometry When Fuel Molecules Contain Oxidizer Elements or Oxidizer Molecules Contain Fuel Elements," SAE Paper 2005-01-3705, *SAE Trans.*, Vol. 114, Sect. 4 (2005).

9. Upatnieks, A., Mueller, C.J., and Martin, G.C., "The Influence of Charge-Gas Dilution and Temperature on DI Diesel Combustion Processes Using a Short-Ignition-Delay, Oxygenated Fuel," SAE Paper 2005-01-2088, *SAE Trans.*, Vol. 114, Sect. 4 (2005).

10. Mueller, C.J., "Diesel-Like Oil-Sands-Derived Fuels," *Proc. of Oil Sands Chemistry and Engine Emissions Roadmap Workshop*, Edmonton, Alberta, Canada (2005).

FY 2006 Presentations

1. "Investigation of Fuel and Oxygen-Concentration Effects on Combustion and Emissions Using an Optical Direct-Injection Diesel Engine," Advanced Engine Combustion Working Group Meeting, Detroit, MI (June 29, 2006).

2. "Conventional and Alternative Fuels Low-Temperature Combustion Research," DOE Advanced Engine Combustion and Fuels Annual Review Meeting, Argonne, IL (May 18, 2006).

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

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

5. "Establishing a Conceptual Framework to Help Identify Paths to Optimal HCCI Operating Regimes," Caterpillar Advanced Combustion Section Meeting, Peoria, IL (Dec. 1, 2005).

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

7. "The Quantification of Mixture Stoichiometry When Fuel Molecules Contain Oxidizer Elements or Oxidizer Molecules Contain Fuel Elements," SAE Powertrain and Fluid Systems Meeting, San Antonio, TX (Oct. 24, 2005).

8. "An Overview of Sandia National Laboratories with a Focus on Recent Advanced Engine Combustion and Fuels Research Results," Univ. of Wisconsin – Madison Mechanical Engineering Dept. invited Lindbergh Lecture, Madison, WI (Oct. 13, 2005).

9. "An Overview of Sandia National Laboratories with a Focus on Recent Advanced Engine Combustion and Fuels Research Results," Caterpillar Advanced Combustion Section Meeting, Peoria, IL (Oct. 12, 2005).

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

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

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

Approach

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

The PLRS technique is illustrated in Figure 2, which is a composite image of a vaporizing n-heptane fuel jet visualized using two different techniques. The left image (till 16 mm) shows Mie scattering from the liquid-phase of the vaporizing fuel jet. The right image is Rayleigh scattering from the ambient and the vapor-phase of the fuel jet. Scattering from liquid fuel extends only to 9 mm. Positioning of the PLRS laser sheet and camera field-of-view downstream of the liquid penetration ensured no interference from liquid droplets. The method for conversion to equivalence ratio is given in Ref. [1].

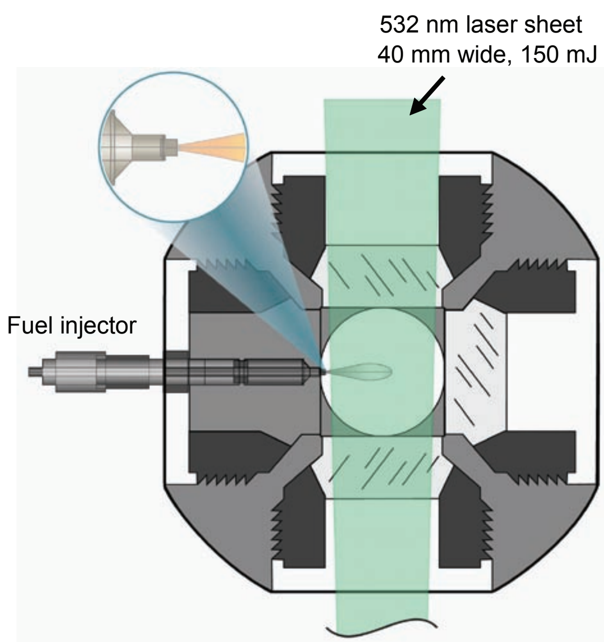

FIGURE 1. Schematic of the combustion vessel and optical setup for planar diagnostics. A 532 nm, 40 mm wide, collimated laser sheet is used for Rayleigh scattering measurements.

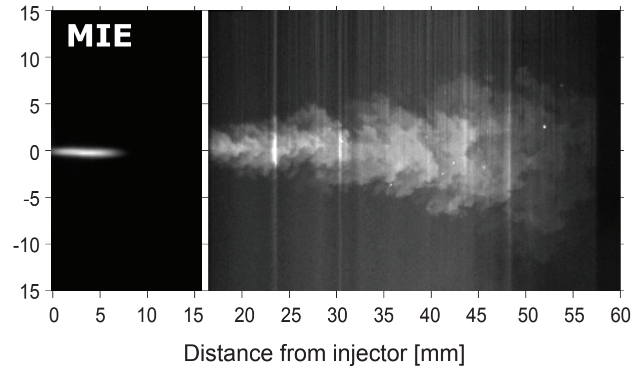

FIGURE 2. A diesel spray injected into the constant-volume combustion vessel visualized using two diagnostic techniques. On the left is the liquid phase visualized using Mie scattering and on the right is the vapor phase visualized by Rayleigh scattering. The two images are obtained from separate injection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

Results

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

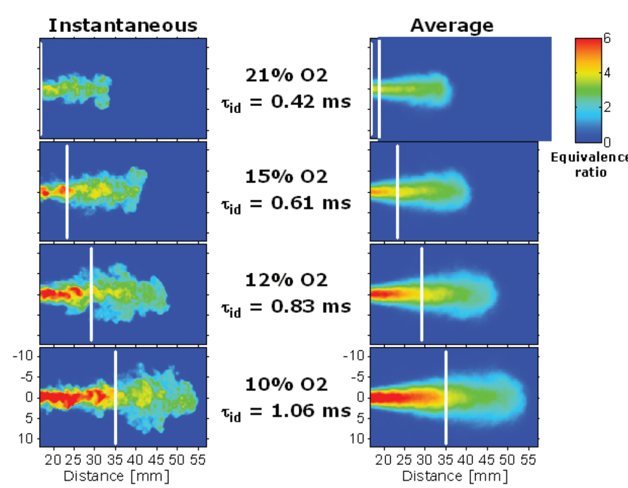

FIGURE 3. Mean (left) and instantaneous (right) equivalence ratio images for the different EGR conditions at time of ignition. Dashed line is lift-off length. (Conditions of Fig. 2)

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

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

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

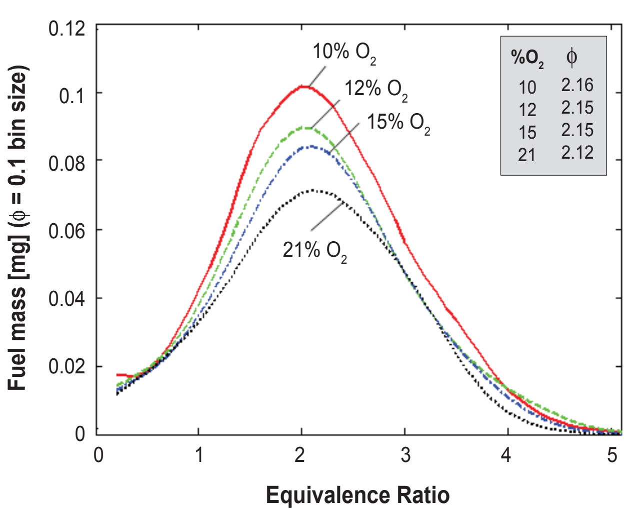

FIGURE 4. Fuel mass distributions in the premixed-burn region for different EGR conditions. The bin size used was Δϕ=0.1.

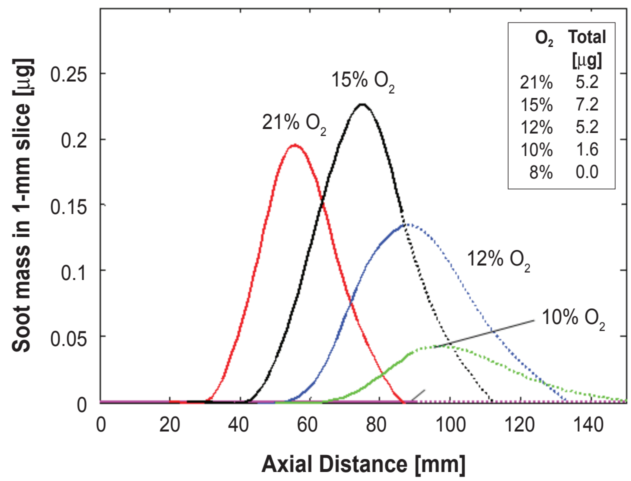

FIGURE 5. Soot mass in thin (1 mm) radial cross-sections of the jet as a function of axial distance. (Fig. 2 conditions)

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

Conclusions

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

References

1. Idicheria, C.A., and Pickett, L.M., "Effect of EGR on Diesel Premixed-Burn Equivalence Ratio," Proc. Combust. Inst. doi:10.1016/j.proci.2006.08.022.

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

FY 2006 Publications/Presentations

1. 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.

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

3. Pickett, L.M., Caton, J.A., Musculus, M.P.B., Lutz, A. E. "Two-Stage Lagrangian Modeling of Soot Precursor Formation at Diesel Engine Operating Conditions," accepted to International Journal of Engine Research, 2006.

4. Pickett, L.M., Siebers, D.L., Idicheria, C.A. "Relationship Between Ignition Processes and the Lift-Off Length of Diesel Fuel Jets," SAE Paper 2005-01-3843, 2005.

5. Idicheria, C.A., and Pickett, L.M. "Soot Formation in Diesel Combustion under High-EGR Conditions," SAE Paper 2005-01-3834, 2005.

6. Kook, S., Bae, C., Choi, D., Miles, P.C., and Pickett, L.M. "The Influence of Charge Dilution and Injection Timing on Low-Temperature Diesel Combustion and Emissions," SAE Paper 2005-01-3837, 2005.

Special Recognitions & Awards/Patents Issued

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

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

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

For further clarification, the term HECC was first introduced in the FreedomCAR Advanced Combustion and Emissions Control Tech Team and Diesel Crosscut Team in 2003. The intent was to convey the objectives of advanced combustion research in a fresh, all-encompassing name in a time when low-temperature combustion (LTC), premixed charge compression ignition (PCCI), homogeneous charge compression ignition (HCCI), Modulated Kinetics (MK), and many more acronyms were in use, but conveyed nothing about the advantages and/or were aligned with certain companies.

Approach

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

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

Results

Major challenges to evaluating HECC strategies on an engine dynamometer are selecting representative experiment conditions and then relating the results to drive cycle emissions. Four speed-load conditions which were originally defined by an industry working group to be representative of light-duty diesel engine operation were selected for use in this study [1-2]. The working group also assigned weights to each mode for estimating the magnitude of drive cycle emissions. While this approach does not take into account cold-start or other transient phenomena, the metric has been successfully used by others for comparison purposes and to demonstrate potential improvements from one technology to another. The four modes used in this study are summarized in Table 1.

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

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

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

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

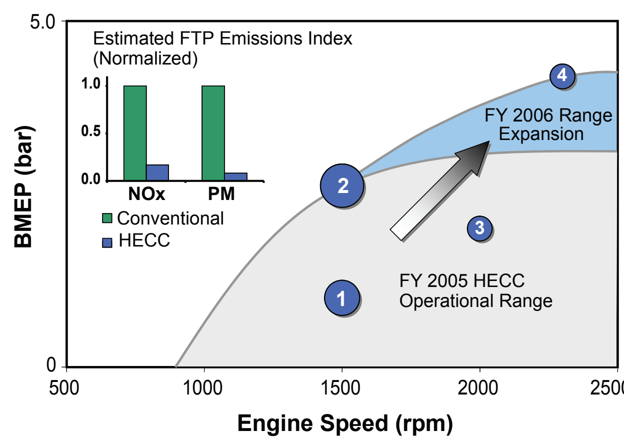

FIGURE 1. Expansion of Usable HECC Speed-Load Range Using Low-Pressure EGR

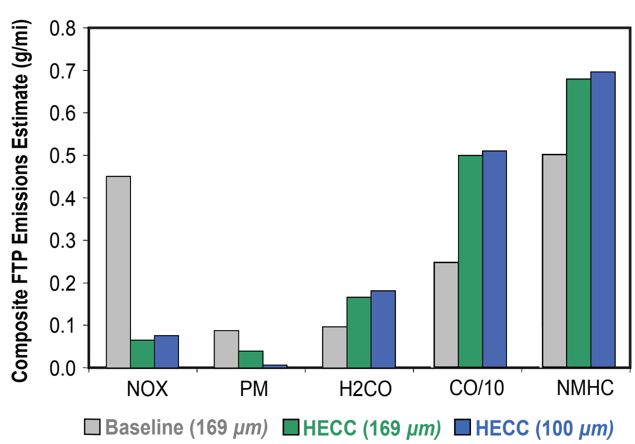

FIGURE 2. Composite Emissions Estimates Based on Light-Duty FTP Modal Conditions (Injector orifice diameter in parentheses.)

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

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

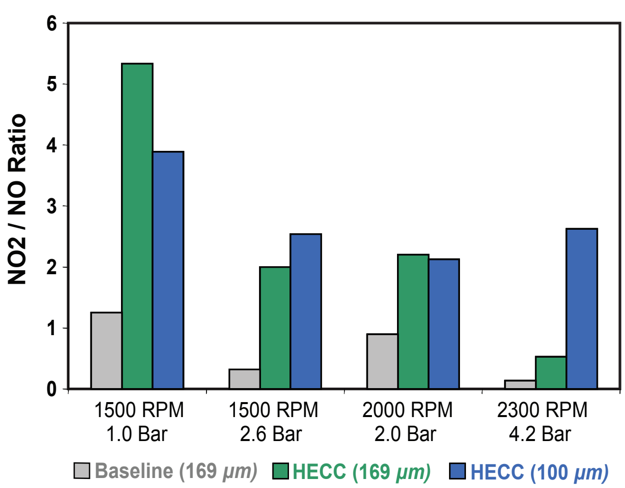

FIGURE 3. NO_2/NO Ratio for Conventional and HECC Operating Conditions (Injector orifice diameter in parentheses.)

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

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

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

Conclusions

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

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

References

1. Kenney, T., Gardner, T., Low, S., Eckstrom, J., Wolf, L., Korn, S., and Szymkowicz, P., "Overall Results: Phase 1 Ad Hoc Diesel Fuel Test Program," SAE Paper Number 2001-01-0151. Society of Automotive Engineers, Warrendale, 2001.

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

FY 2006 Publications/Presentations

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

2. R. M. Wagner, C. S. Sluder, “Evaluation of High Efficiency Clean Combustion Strategies for Meeting Future Emissions Regulations in Light-Duty Diesel Engines”, DEER 2006 (Detroit, MI; September 2006).

3. R. M. Wagner, C. Scott Sluder, “Update on Light-Duty Multi-Cylinder HECC Research at ORNL”, 2006 AEC Working Group Meeting at USCAR (Southfield, MI; June 2006).

4. R. M. Wagner, C. S. Sluder, “High Efficiency Clean Combustion (HECC) in Light-Duty Multi-Cylinder Diesel Engines”, 2006 DOE National Laboratory ACE Merit Review & Peer Evaluation at Argonne National Laboratory (Argonne, IL; May 2006).

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

6. C. S. Sluder, R. M. Wagner, J. M. Storey, and S. A. Lewis, “Implications of Particulate and Precursor Compounds Formed During High-Efficiency Clean Combustion in a Diesel Engine”, SAE 2005-01-3844 (San Antonio, TX, USA; October 2005).

Special Recognitions & Awards/Patents Issued

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

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

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II.A.7 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.
- Directly complement optical engine experiments being conducted at the Combustion Research Facility (CRF) by performing identical companion simulations.
- Focus initially on optical hydrogen-fueled internal combustion engine (H2-ICE) experiment, and then systematically extend focus to low temperature combustion (LTC) applications.

Accomplishments

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

Future Directions

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

Introduction

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

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

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

Approach

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

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

Results

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

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

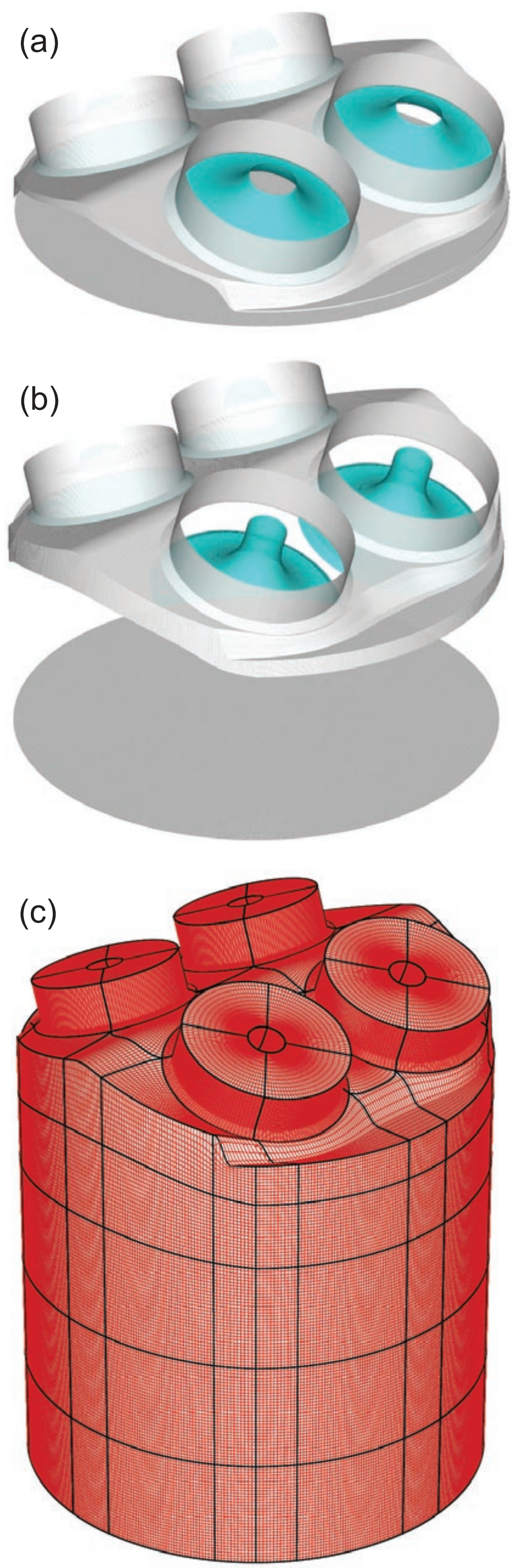

FIGURE 1. Generalized time-varying multiblock grid at 360, 432, and 540 CAD (intake stroke) used for LES of the CRF H2-ICE engine (3-million cells, 137 blocks, ports removed from images).

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

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

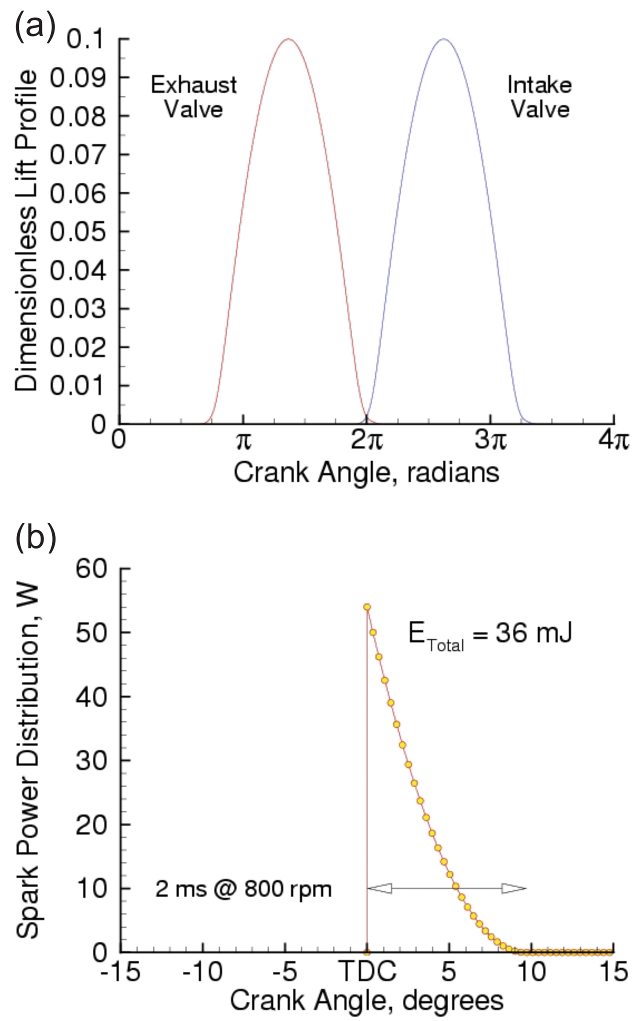

FIGURE 2. Valve and Spark Timing Profiles

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

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

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

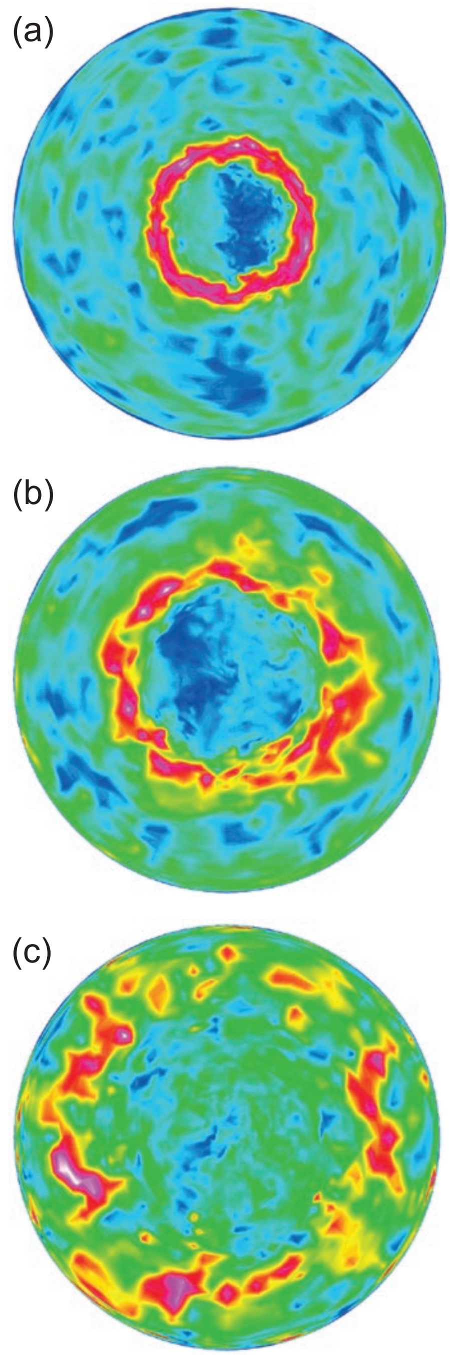

FIGURE 4. Instantaneous H_2O production rate at 4, 8, and 12 CAD, respectively, after spark.

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

Conclusions

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

FY 2006 Publications/Presentations

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

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

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

4. Oefelein, J. C., Schefer, R. W. and Barlow, R. S. (2006). Toward validation of large eddy simulation for turbulent combustion (invited), AIAA Journal, 44(3) 418-433.

5. Oefelein, J. C. (2006). Mixing and combustion of cryogenic oxygen-hydrogen shear-coaxial jet flames at supercritical pressure (invited). Combustion Science and Technology, 178(1-3): 229-252.

6. Oefelein, J. C. (2005). Thermophysical characteristics of LOX-H2 flames at supercritical pressure. Proceedings of the Combustion Institute, 30: 2929-2937.

7. Chiu, H.-H. and Oefelein, J. C. (2005). Chapter 6: Modeling liquid-propellant spray combustion processes (invited). Liquid rocket thrust chambers, aspects of modeling, analysis and design. AIAA Progress in Astronautics and Aeronautics, New York, New York.

8. Segura, J. C., Eaton, J. K. and Oefelein, J. C. (2005). Predictive Capabilities of Particle-Laden Large Eddy Simulation, Technical Report TSD-156, Dept. of ME, Stanford University Stanford, California.

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

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

Presentations at Conferences and Project Meetings

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

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

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

4. DOE Headquarters, September 2005.

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

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

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

8. Supercomputing 2005, Seattle WA, November 2005.

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

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

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

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

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

14. BMW, Sandia CRF, March 2006.

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

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

17. SciDAC 2006, Denver CO, June 2006.

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

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

Objectives

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

Accomplishments

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

Future Directions

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

Introduction

Modeling the premixed charge compression ignition (PCCI) engine requires a balanced approach that captures both fluid motion as well as low- and high-temperature fuel oxidation. A fully integrated computational fluid dynamics (CFD) and chemistry scheme (i.e. detailed chemical kinetics solved in every cell of the CFD grid) would be the ideal PCCI modeling approach, but is computationally very expensive. As a result, modeling assumptions are required in order to develop tools that are computationally efficient, yet maintain an acceptable degree of accuracy. Multi-zone models have been previously shown by the authors to be accurate to capture geometry-dependent processes in homogeneous charge compression ignition (HCCI) engines [1]. We have been testing methodologies for multi-zone analysis of PCCI combustion that show promise for delivering accurate results within a reasonable computational time. We are also developing new tools of analysis that apply to different aspects of HCCI/PCCI operation.

Approach

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

Results

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

KIVA3V-ANN has been validated by comparison with iso-octane HCCI experiments in two different

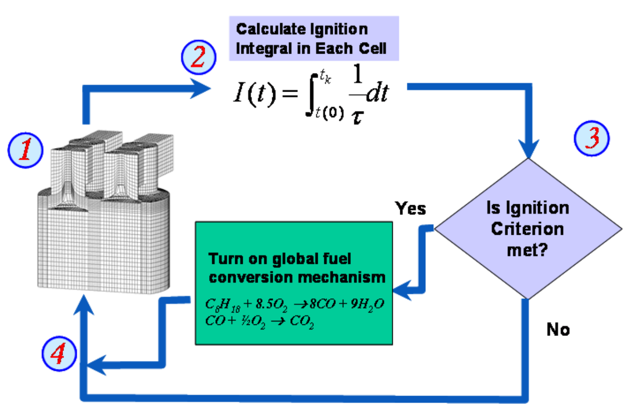

FIGURE 1. Schematic of the analysis procedure used for neural network based analysis of HCCI/PCCI combustion. The neural network is trained for predicting combustion delay. Ignition in individual cells is predicted through the use of the autoignition integral. Ignited cells then react according to a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

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

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

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

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

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

The approach consists of injecting the gaseous fuel using the KIVA3V liquid injection model. The resulting "gaseous spheres" evaporate after a short distance, producing a gaseous jet. The gaseous spheres are fully coupled with the gas phase species with respect to energy and momentum, and therefore simulate entrainment and mixing. "Evaporation" of the gaseous spheres, i.e., their transition from being treated as distinct entities to being part of the combustion chamber gas is based on gas dynamics and empirical relations.

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

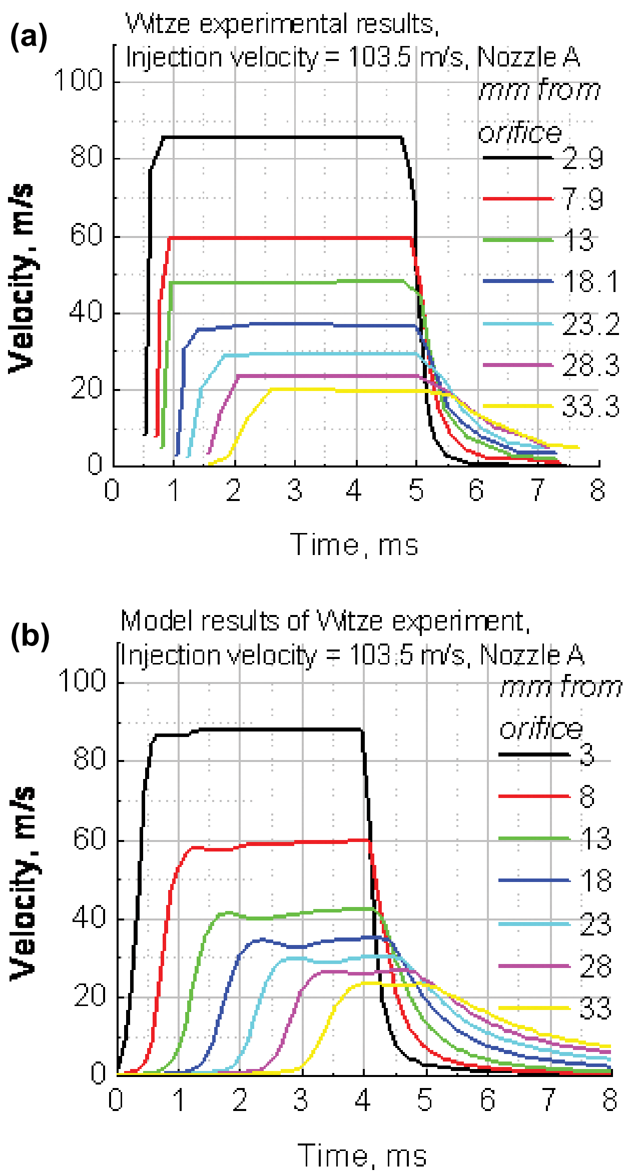

FIGURE 2. Measured (top) and calculated (bottom) velocity histories at seven locations downstream of the injector, for fully expanded experiments with air injected into air.

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

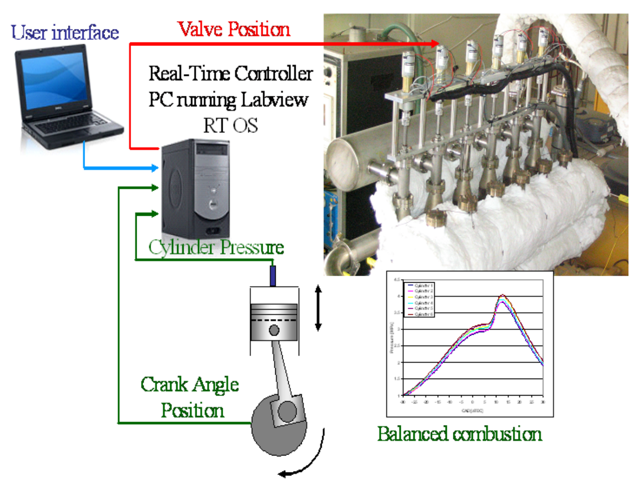

FIGURE 3. Control system for experimental Caterpillar 3406 HCCI engine based on blending a hot stream and a cold stream in a cylinder-by-cylinder basis.

Conclusions

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

References

1. Salvador M. Aceves, Daniel L. Flowers, Francisco Espinosa-Loza, Joel Martinez-Frias, Magnus Christensen, Bengt Johansson, Randy Hessel, "Analysis of the Effect of Geometry Generated Turbulence on HCCI Combustion by Multi-Zone Modeling," SAE Paper 2005-01-2134.

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

3. Patric Ouellette, "Direct Injection of Natural Gas for Diesel Engine Fueling," Ph. D. Thesis, University of British Columbia, February, 1996.

FY 2006 Publications/Presentations

1. A Fully Integrated CFD and Multi-zone Model with Detailed Chemical Kinetics for the Simulation of PCCI Engines, Aristotelis Babajimopoulos, Dennis N. Assanis, Daniel L. Flowers, Salvador M. Aceves, and Randy P. Hessel, International Journal of Engine Research, Vol. 6, pp. 497-512, 2005.

2. Improving Ethanol Life Cycle Energy Efficiency by Direct Combustion 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.

3. Development and Testing of a 6-Cylinder HCCI Engine for Distributed Generation, Joel Martinez-Frias, Daniel Flowers, Salvador M. Aceves, Francisco Espinosa-Loza, Robert Dibble, Paper ICEF2005-1342, Proceedings of the 2005 Fall Technical Conference, ASME Internal Combustion Engine Division, October 2005.

4. Experimental and Kinetic Investigation of Effect of Fuel on Ion Sensor Signal to determine Combustion Timing in HCCI Engines, Parag Mehresh, Jason Souder, Daniel Flowers, Uwe Riedel, Robert W. Dibble, International Journal of Engine Research, 2005.

5. Effect of the Di-Tertiary Butyl Peroxide (DTBP) additive on HCCI Combustion of Fuel Blends of Ethanol and Diethyl Ether, J. Hunter Mack, Daniel L. Flowers, Bruce A. Buchholz, Robert W. Dibble, SAE 2005 Fuels & Lubricants Meeting.

6. Source Apportionment of Particulate Matter from a Diesel Pilot-Ignited Natural Gas Fuelled Heavy Duty DI Engine, H.L. Jones, G. McTaggart-Cowan, S.N. Rogak, W.K. Bushe, S.R. Munshi, B.A. Buchholz, SAE 2005 Fuels & Lubricants Meeting.

7. Analysis of Premixed Charge Compression Ignition Combustion with a Sequential Fluid Mechanics-Multizone Chemical Kinetics Model, Salvador M. Aceves, Daniel L. Flowers, , Francisco Espinosa-Loza Aristotelis Babajimopoulos, Dennis Assanis, SAE Paper 2005-01-0115, SAE Transactions, 2005.

8. A Detailed Chemical Kinetic Analysis of Low Temperature Non-Sooting Diesel Combustion, Salvador M. Aceves, Daniel L. Flowers, SAE Paper 2005-01-0923, SAE Transactions, 2005.

9. Analysis of the Effect of Geometry Generated Turbulence on HCCI Combustion by Multi-Zone Modeling, Salvador M. Aceves, Daniel L. Flowers, Francisco Espinosa-Loza, Joel Martinez-Frias, Magnus Christensen, Bengt Johansson, Randy Hessel, SAE Paper 2005-01-2134.

10. 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, Accepted for publication, Combustion Theory and Modelling, 2006.

11. 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.

12. 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.

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

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

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

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

Special Recognitions & Awards/Patents Issued

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

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

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

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DOE Technology Development Manager:
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 2006 Objectives

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

Accomplishments

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

Future Directions

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

Introduction

HCCI engines have significant efficiency and emissions advantages over conventional spark-ignition and diesel engines, respectively. However, several technical barriers must be addressed before it is practical to implement HCCI combustion in production engines. One of these barriers is that high-load operation is limited by excessive cylinder-pressure rise rates (PRR) and engine knock. Other issues are improving combustion efficiency and controlling hydrocarbon and carbon monoxide emissions at low loads, and controlling autoignition timing. As outlined under the accomplishment bullets above, several studies have been conducted over the past year (FY 2006) that provide significant new understanding related to overcoming these technical barriers.

Approach

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

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

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

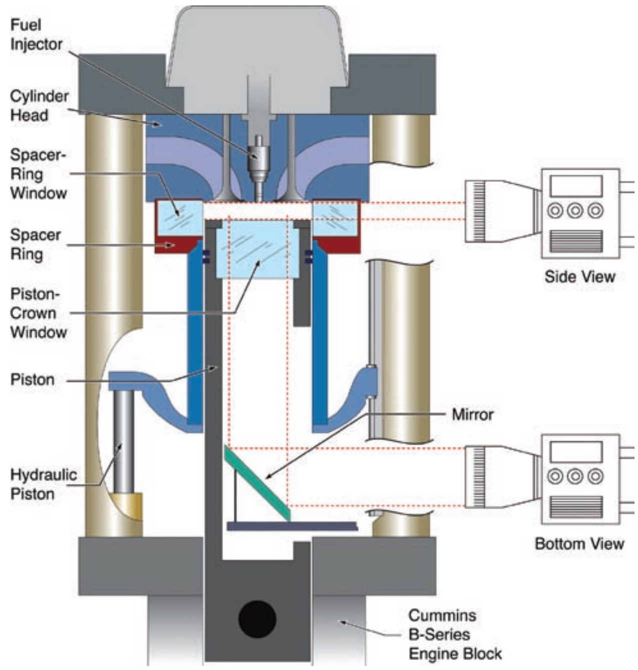


FIGURE 1. Schematic of the optically accessible HCCI engine showing camera views.

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

Results

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

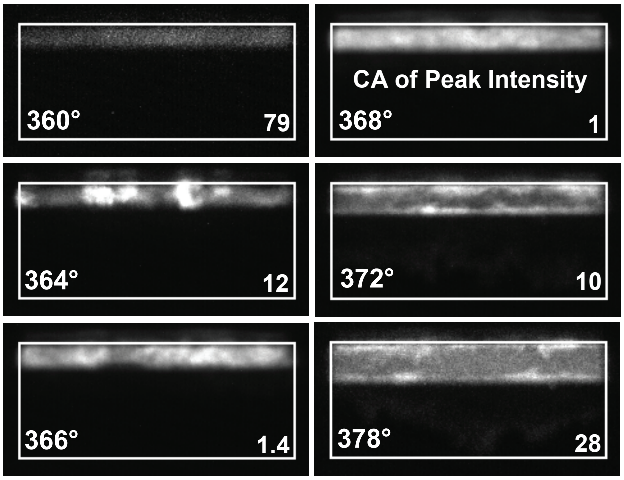


FIGURE 2. A sequence of side-view chemiluminescence images (each from a separate cycle) of HCCI combustion. The crank angle degree ATDC-intake appears in the lower left corner, and the relative intensifier gain is in lower right.

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

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

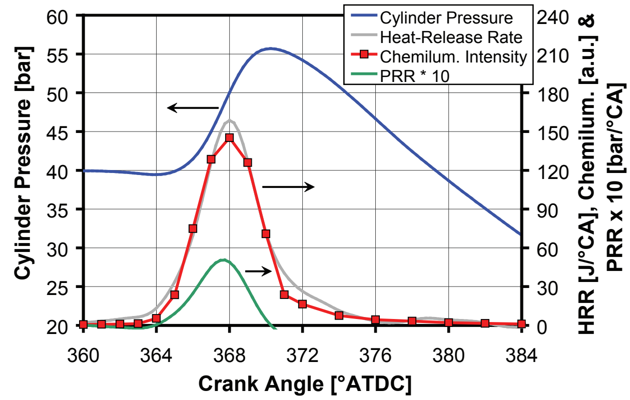


FIGURE 3. Cylinder pressure, HRR, average chemiluminescence intensity and PRR for the same conditions as the images in Figure 2 ($\phi = 0.38$, CA50 = 368°). The data are ensemble-averaged over 20 engine cycles.

and thermal stratification in the boundary layer has only a secondary effect. Based on these results, for enhanced thermal stratification to be effective in further reducing the maximum PRR and allowing higher loads, it must also be distributed throughout the bulk gas. A complete discussion can be found in Ref. [2].

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

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

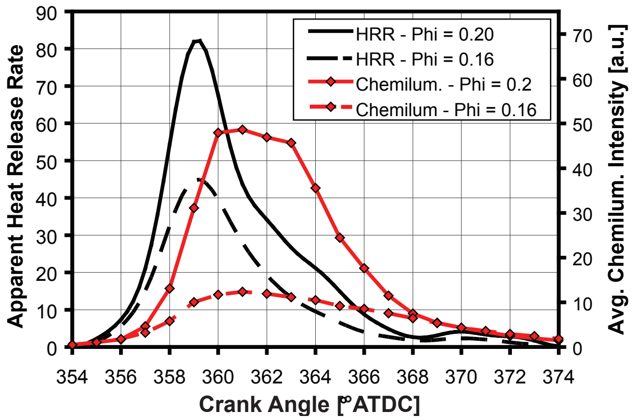
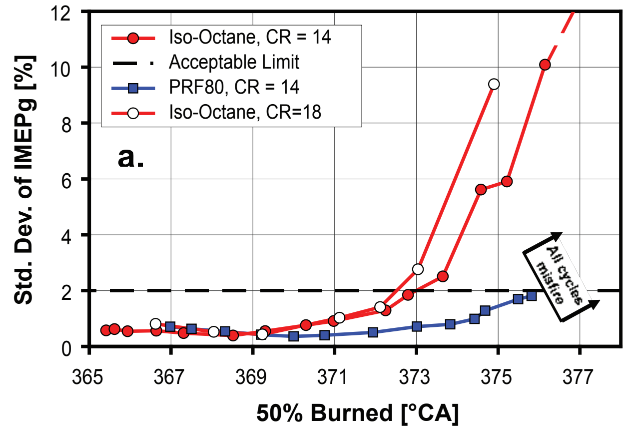


FIGURE 4. Comparison of chemiluminescence intensity and HRR for $\phi = 0.2$ and 0.16. The data are ensemble-averaged over 20 cycles.

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

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



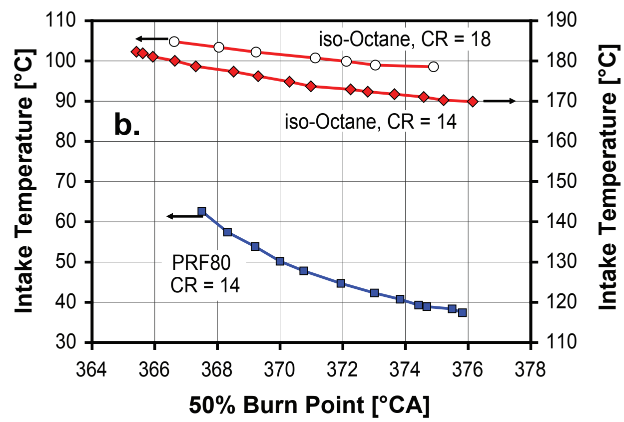


FIGURE 5. Standard deviation of the IMEP (a) and intake temperatures (b) as a function of combustion phasing (50% burn point) for PRF80 and iso-octane.

Conclusions

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

References

1. Sjöberg, M., Dec, J. E., and Cernansky, N. P., "The Potential of Thermal Stratification and Combustion Retard for Reducing Pressure-Rise Rates in HCCI Engines, based on Multi-Zone Modeling and Experiments," *SAE Transactions*, Vol. 114, Sec 3, pp. 236-251, paper no. 2005-01-0113, 2005.

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

3. Heywood, J. B., Internal Combustion Engine Fundamentals, McGraw-Hill, New York, 1988.

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

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

FY 2006 Publications/Presentations

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

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

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

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

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

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

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

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

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

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

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

Special Recognitions & Awards/Patents Issued

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

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

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

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

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

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

II.A.10 Automotive HCCI Combustion Research

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Objectives

This project comprises optical-engine investigations designed to enhance our understanding of in-cylinder processes in automotive-scale homogeneous charge compression ignition (HCCI) engines. Objectives for FY 2006 include:

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

Accomplishments

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

Future Directions

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

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

Introduction

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

Approach

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

Results

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

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

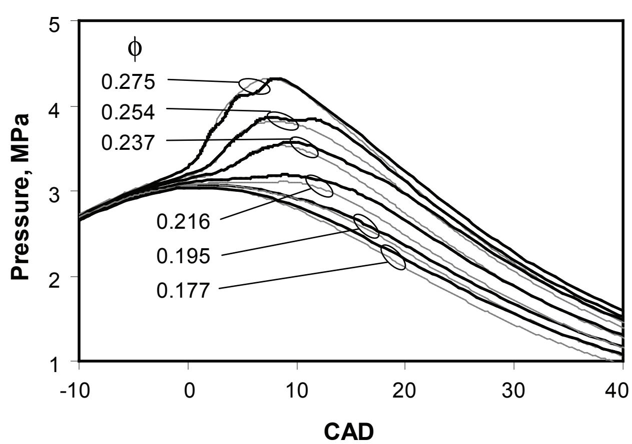

FIGURE 1. CHEMKIN predictions (dark lines) compared to measured pressure data (light lines) for homogeneous HCCI operation over a range of equivalence ratios. Fuel = PRF50, intake pressure = 120 kPa, intake temperature = 120°C, speed = 1200 rpm.

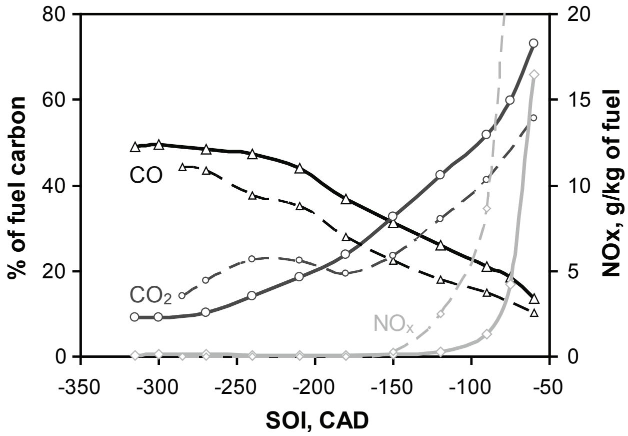

FIGURE 2. Emission predictions (dashed lines) from LIF-based PDF statistics compared to low-load HCCI measurements (solid lines) for CO, CO_2, and NOx. Data are plotted as a function of start-of-injection timing. Swirl injector; global equivalence ratio = 0.2; other conditions as in Fig. 1.

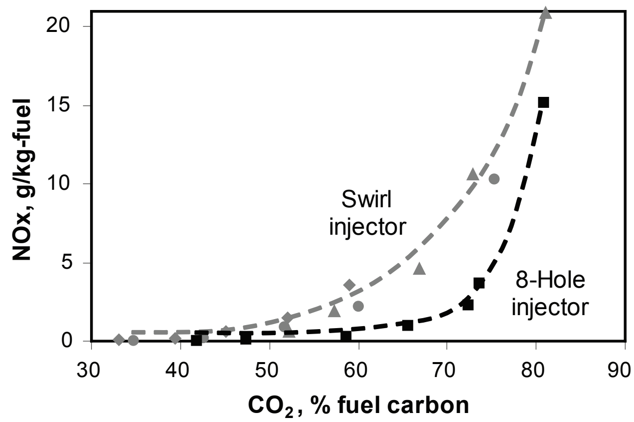

FIGURE 3. NOx-CO_2 trade-off plot for swirl and 8-hole injectors. Different shaped symbols for the swirl injector represent different injection strategies mentioned in the text. Dashed lines are visual aids only. Conditions as in Fig. 2.

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

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

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

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

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

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

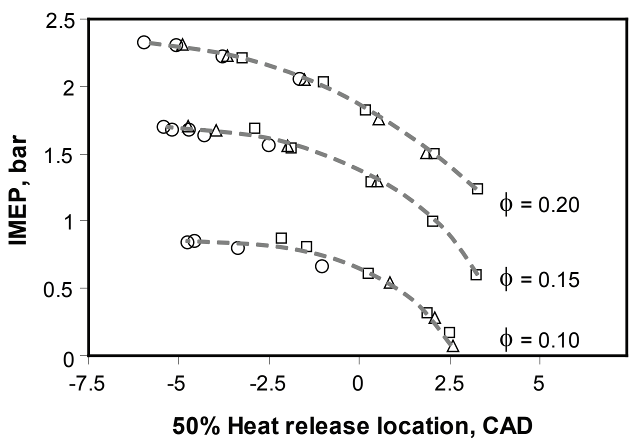

FIGURE 4. Combustion performance of the 8-hole injector for a range of fuel pressures, global equivalence ratios, and start-of-injection timing. Dashed lines are visual aids only. Fuel-pressure symbols: circles = 50 bar; triangles = 100 bar; squares = 150 bar. Other conditions as in Fig. 1.

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

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

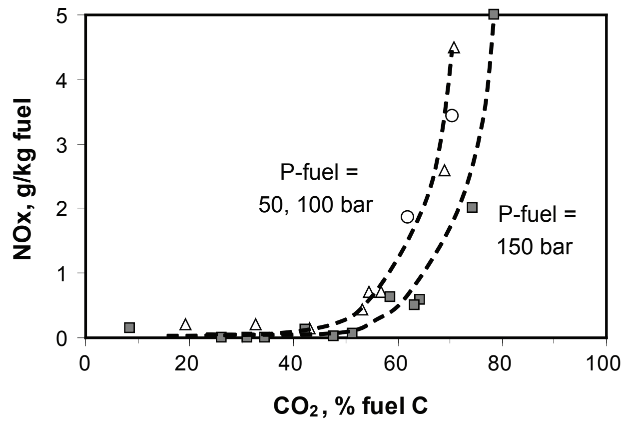

FIGURE 5. NOx-CO_2 trade-off plot for 8-hole injector operating at different fuel pressures. Dashed lines are visual aids only. Symbols as in Fig. 4, with 150-bar symbols filled for visibility.

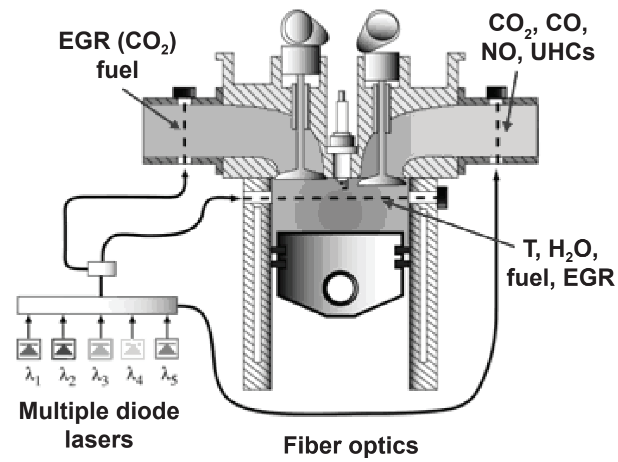

FIGURE 6. Wavelength-multiplexed, TDL sensing for internal combustion engine applications.

and polarization-related interference. The flexibility of the wavelength-multiplexed architecture allows the straightforward addition of wavelengths to potentially measure other important engine parameters as illustrated in Figure 6.

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

Conclusions

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

FY 2006 Publications/Presentations

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

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

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

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

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

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

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

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

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

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

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

II.A.11 Spark-Assisted HCCI Combustion

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

Approach

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

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

Results

In our research, the transition, and hence HCCI, is achieved with high levels of exhaust gas retained in the cylinder through manipulation of the intake and exhaust valve events. Unfortunately, this results in a strong coupling between successive cycles with small variations in the thermal and chemical composition of the retained exhaust gas leading to large variations in the combustion process. Recent results from our research have shown that the SI-HCCI mode transition is very unstable with high torque variations, high unburned hydrocarbon emissions, and potential engine stall. Figure 1 illustrates the trend in engine stability and engine-out NOx emissions during the transition from SI to HCCI operation. Four distinct modes of operation were observed and are labeled in Figure 1. This report will focus on observations from the transition region.

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

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

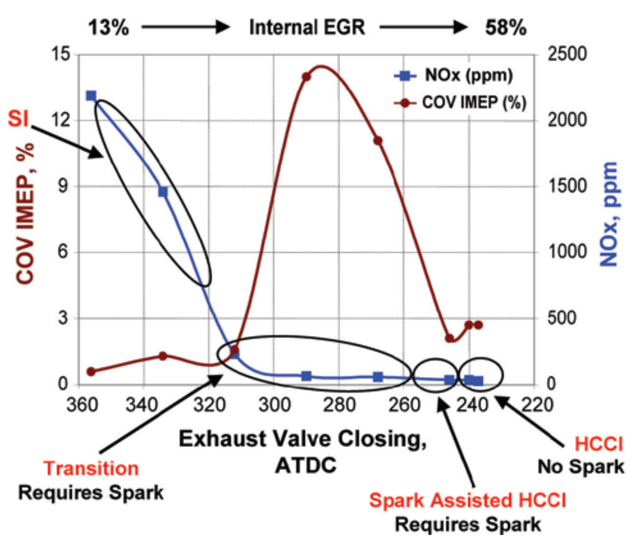

FIGURE 1. Stability and NOx emissions during the transition from SI to HCCI combustion using internal EGR. Engine conditions were 1,600 rpm, 3.4 BMEP.

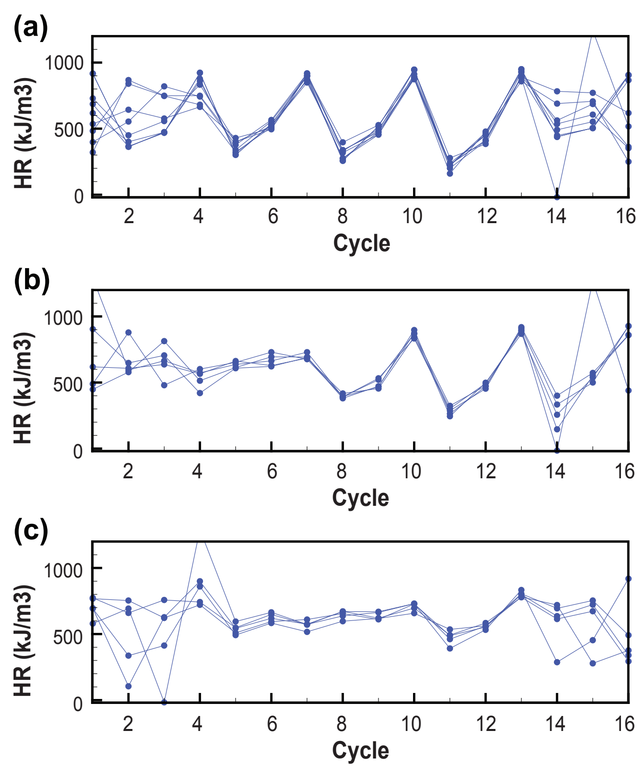

FIGURE 2. Repeating patterns observed for an intermediate EGR level corresponding to the transition region. Engine conditions were 1,600 rpm, 3.4 bar BMEP.

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

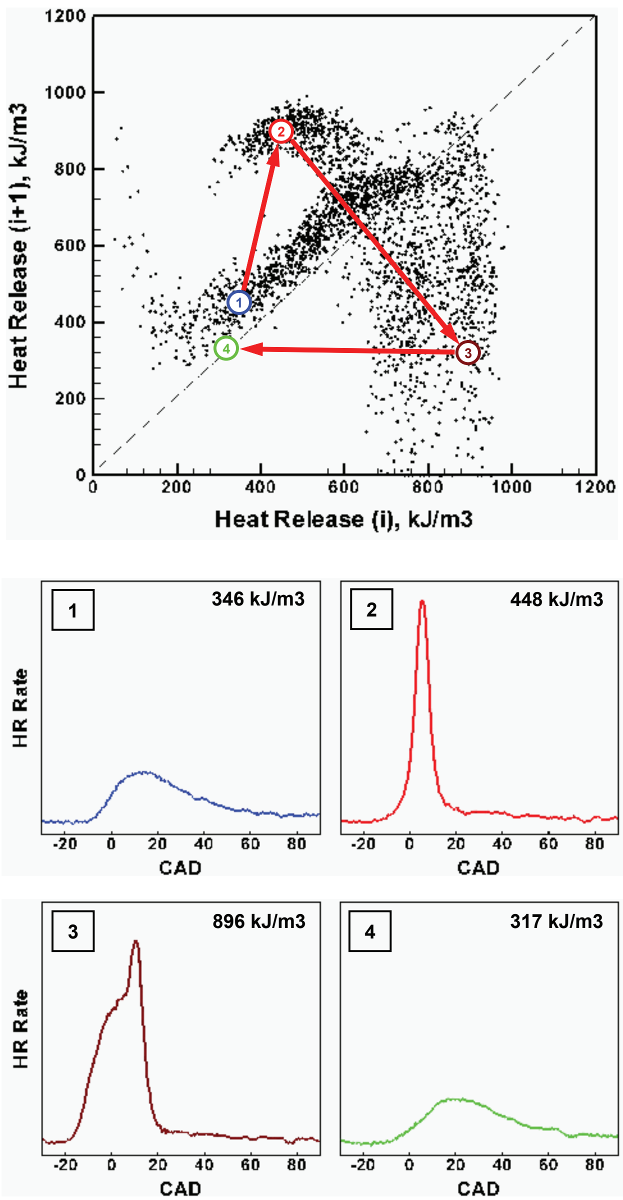

FIGURE 3. Example of the trajectory of the 3-step heat release pattern shown and corresponding heat release rate profiles. Engine conditions were 1,600 rpm, 3.4 BMEP.

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

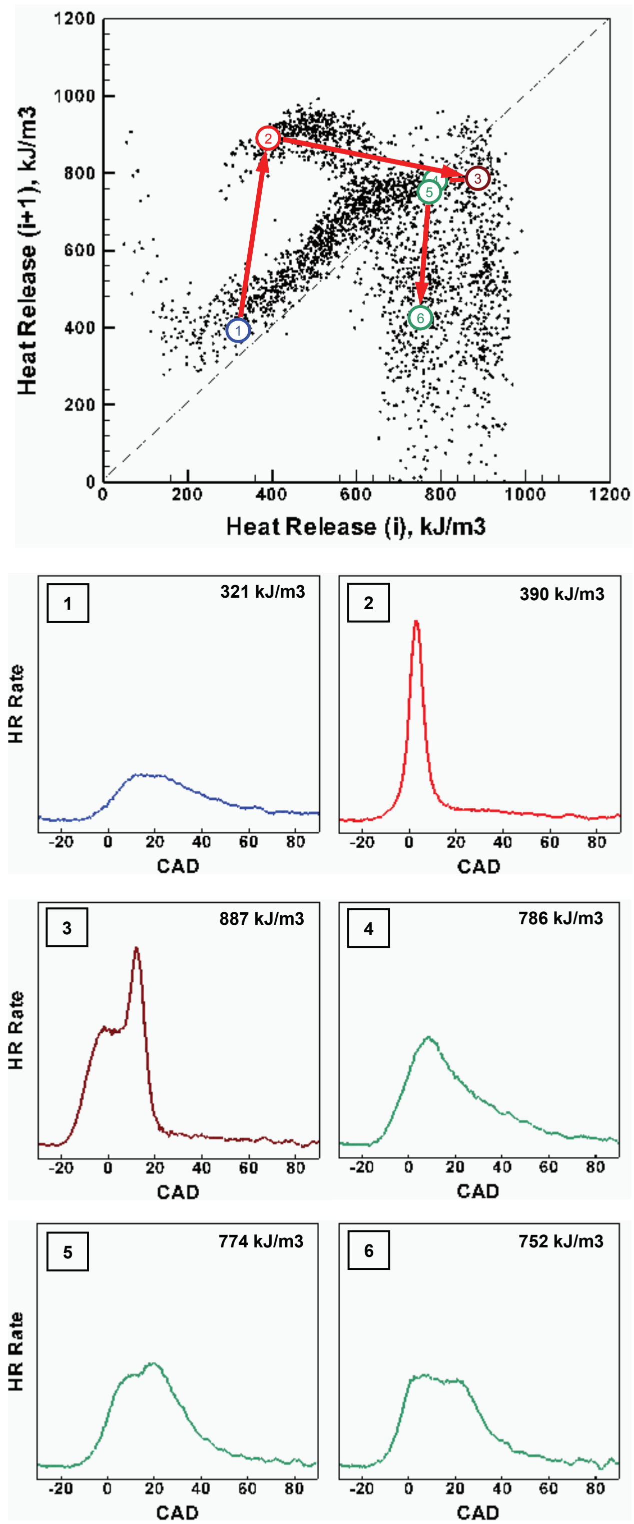

FIGURE 4. Example of temporary entrainment around an unstable fixed point. The unstable fixed point corresponds to a hybrid combustion mode as illustrated in the heat release profiles. Engine conditions were 1,600 rpm, 3.4 BMEP.

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

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

Conclusions

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

FY 2006 Publications/Presentations

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

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

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

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

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

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

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

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

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

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

Special Recognitions & Awards/Patents Issued

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

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

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DOE Technology Development Manager:
Kenneth Howden

NETL Project Manager: Carl Maronde

Subcontractor:
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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 L4 gasoline engine in a mid-size car.
- Demonstrate fully flexible system on a 2.0-2.4L L4 gasoline engine in a mid-size car.
- Demonstrate simple variable valve actuation system on a 4.5L DOHC V8 engine in a mid-size sport utility vehicle.
- Demonstrate fully flexible system on a single-cylinder diesel engine.
- Demonstrate fully flexible system on a 4.5L DOHC V8 engine in a mid-size sport utility vehicle.

Accomplishments

Gasoline Systems

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

Diesel Systems

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

Future Directions

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

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

Introduction

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

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

Approach

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

Results

Gasoline Systems

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

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

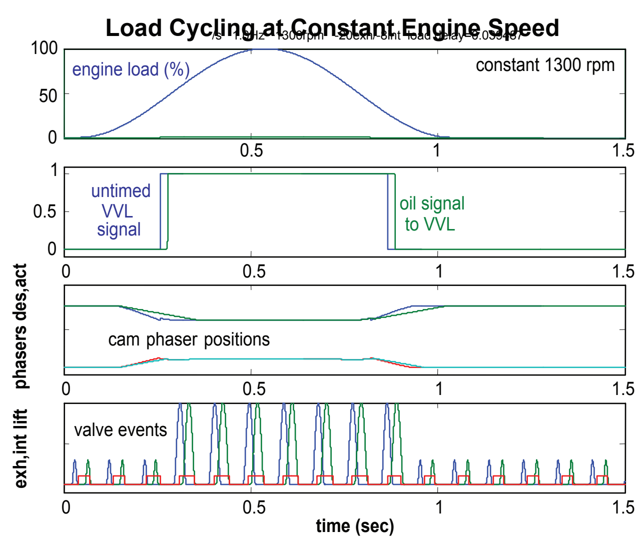

FIGURE 1. System Simulation Analysis of Response of Enabling Valvetrain System to a Load Change at Constant Engine Speed

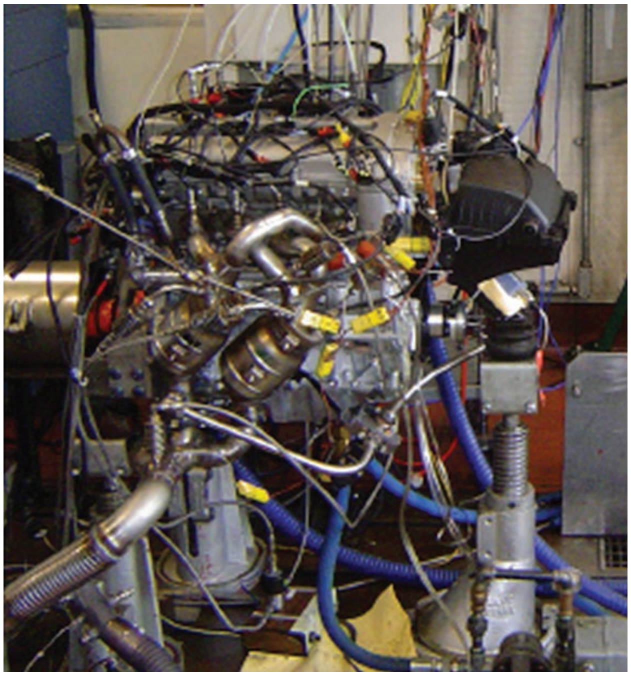

FIGURE 2. Engine with Enabling Valvetrain System Installed on Dynamometer

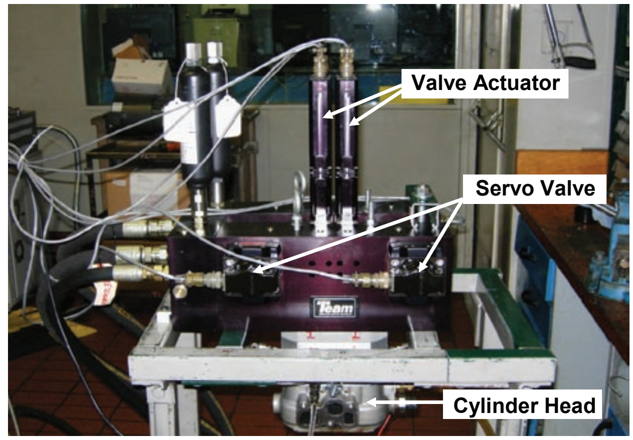

FIGURE 3. Bench Setup for Single-Cylinder Diesel Engine with FVVA System

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

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

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

Diesel Systems

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

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

Conclusion

Based on the progress made on the "enabling" design for the gasoline HCCI engine, a successful demonstration of the flexible valve actuation mechanisms on the diesel engine is expected. For the diesel HCCI engine, significant progress has been made on both the simple and the fully-flexible designs. Multi-cylinder testing of the VCT valve actuation system is underway and initial testing of the single-cylinder engine equipped with the fully flexible valve actuation system has begun. This has allowed issues to be identified and evaluations of preliminary performance to be made. Both systems should continue to be developed, so that their potential performance, efficiency, and cost effectiveness can be properly assessed. The major focus of the upcoming work will be to understand the emissions benefits that are achievable for variable valve actuation mechanisms on the diesel engine.

FY 2006 Publications/Presentations

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

II.A.13 KIVA-4 Development

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DOE Technology Development Manager:
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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

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

Approach

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

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

Realizing that KIVA-4 will be exercised primarily in 3-D engine geometries, we have expanded the suite of 3-D geometries simulated by KIVA-4. We have converted engine meshes from KIVA-3V and tested them with KIVA-4.

Results

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

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

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

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

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

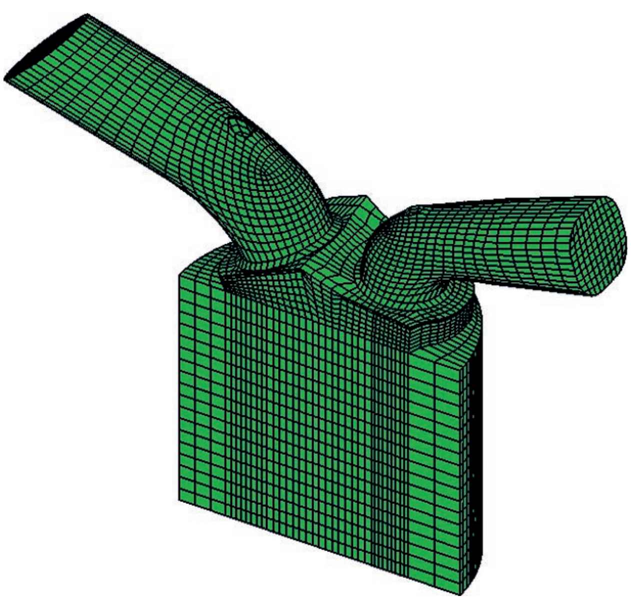

FIGURE 1. A 180° Mesh Simulated with KIVA-4

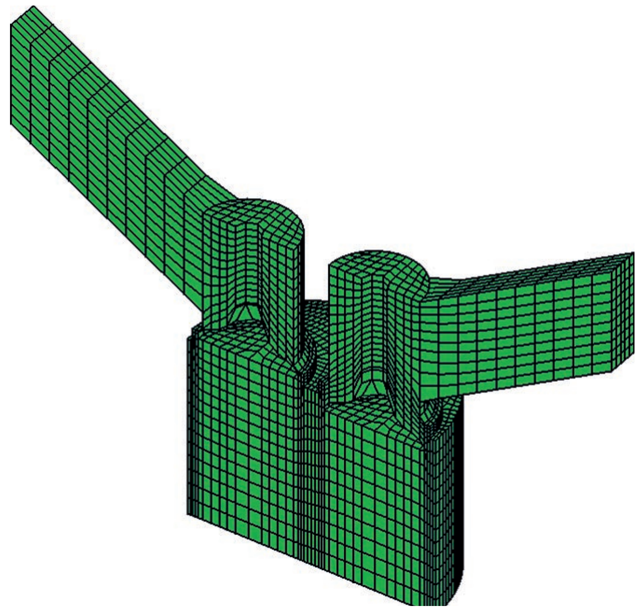

FIGURE 2. A 180° Mesh Simulated with KIVA-4 (provided by Jyh-Yuan Chen of the University of California at Berkeley)

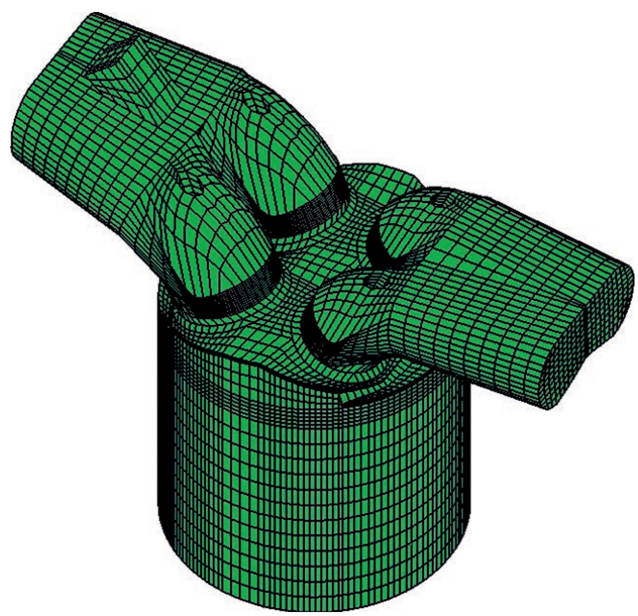

FIGURE 3. A 4-Valve Mesh Simulated with KIVA-4 with Poor Mesh Quality Around Ports

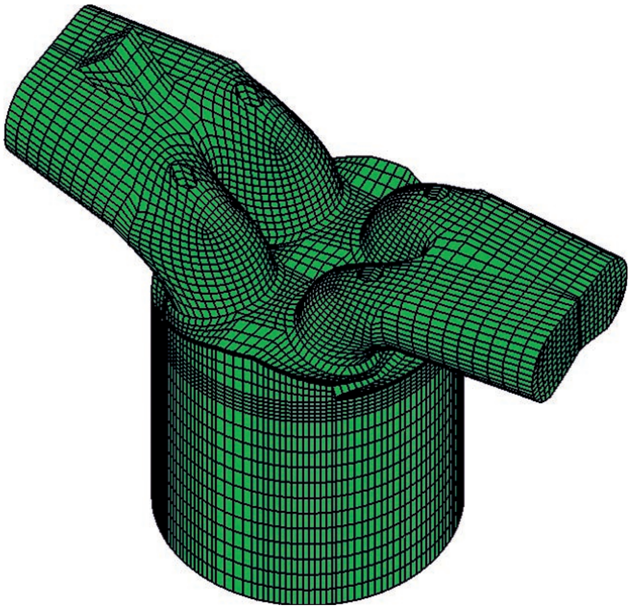

FIGURE 4. The same 4-valve mesh shown in Figure 3 with improved mesh quality around the ports which has been simulated with KIVA-4.

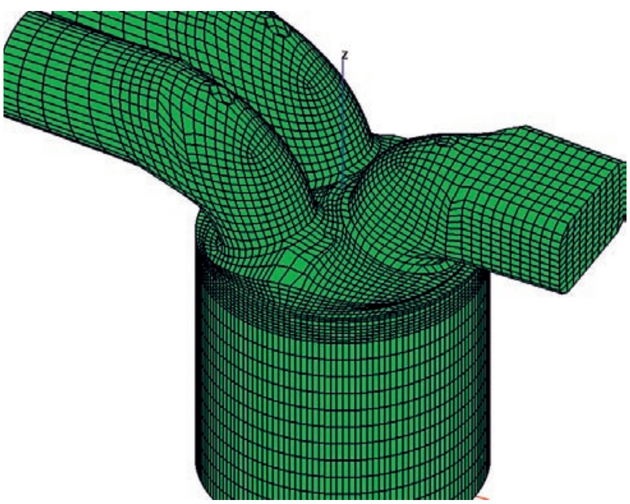

FIGURE 5. A 3-Valve Mesh Simulated with KIVA-4.

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

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

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

Conclusions

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

FY 2006 Publications

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

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

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

FY 2006 Presentations

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

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

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

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

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

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

Approach

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

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

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

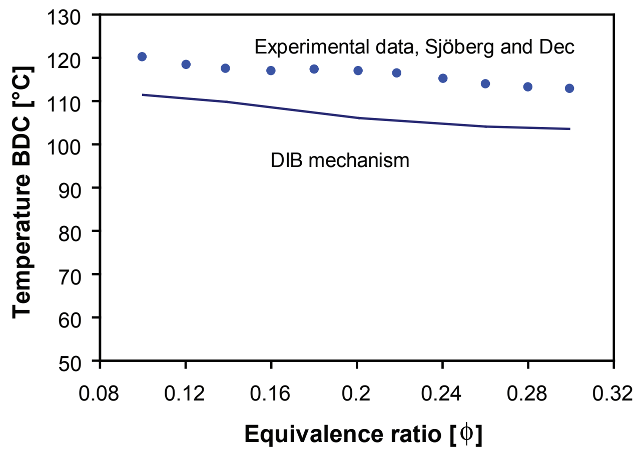

FIGURE 1. The temperature required at bottom dead center to maintain ignition phasing at top dead center in an HCCI engine at Sandia. (Ignition phasing is determined by the 50 percent burn point.) The equivalence ratio is varied by changing the amount of fuel injected into the engine. The fuel is diisobutylene.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

Results

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

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

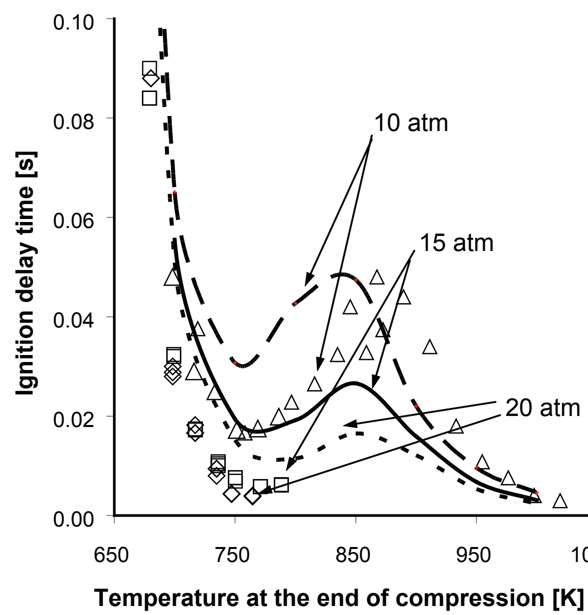

FIGURE 2. Experimental (points) and model-predicted ignition-delay times (curves) at 10, 15 and 20 atm for methylcyclohexane in a rapid compression machine. The experiments were performed at the National University of Ireland in Galway.

further mechanisms for higher molecular weight cycloalkanes. These rules relate particularly to rate constants for reactions responsible for low temperature heat release. It is critical to get these rate constants correct for modeling of combustion in HCCI engines. We collaborated with Magnus Sjöberg and John Dec at Sandia and used our MCH mechanism to model their experiments in an HCCI engine (Figure 3). We used our new MCH mechanism to simulate the ignition phasing of MCH in an HCCI engine as a function of equivalence ratio (Figure 3). The agreement between the predictions and the experiment are quite good. The paper on MCH mechanism development and validation will be published in the Proceedings of the Combustion Institute.

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

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

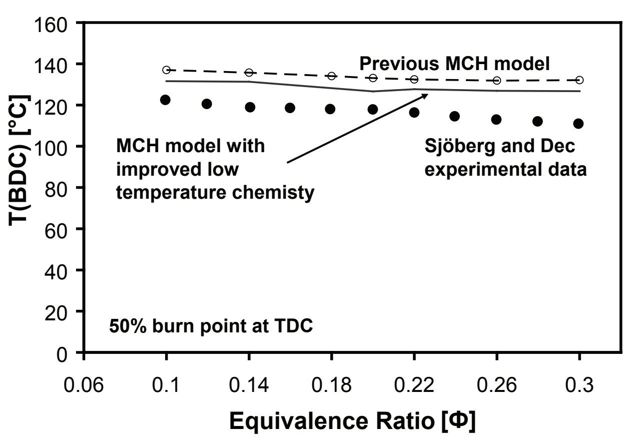

FIGURE 3. The temperature required at bottom dead center to maintain ignition phasing at top dead center in an HCCI engine at Sandia. (Ignition phasing is determined by the 50 percent burn point.) The equivalence ratio is varied by changing the amount of fuel injected into the engine. The fuel is MCH.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

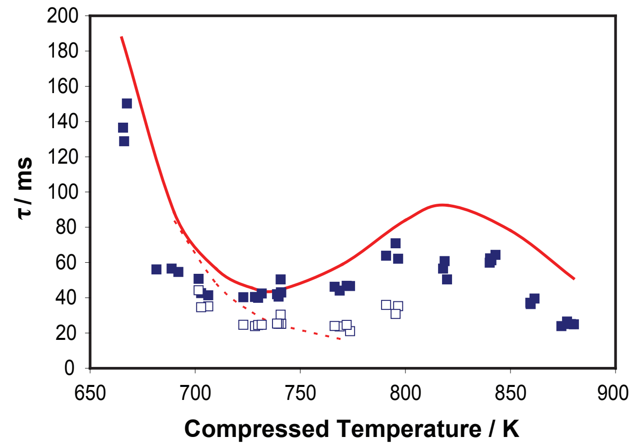

FIGURE 4. Experimental (points) and model predicted ignition delay times (red solid curve) at 7-9 atm for cyclohexane in a rapid compression machine. The experiments were performed at University of Sciences and Technology, Lille, France. Open symbols and the dashed curve correspond to cool flame ignition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

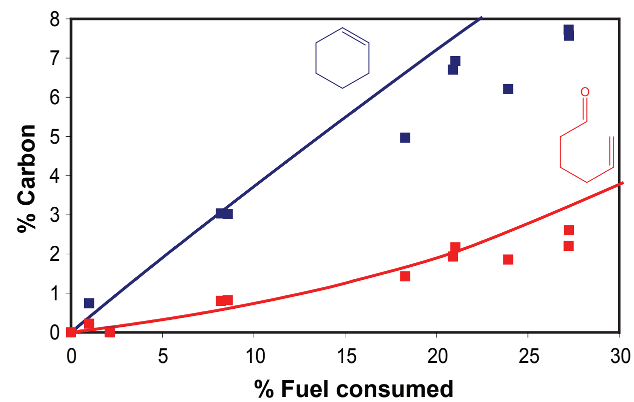

FIGURE 5. Major intermediate products produced in the oxidation of cyclohexane in the rapid compression machine. Cyclohexene (navy blue, experimental (points), model (curve)) and hex-5-enal (red, experimental (points), model (curve)). The percentage of carbon in the fuel that is contained in the intermediate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

Conclusions

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

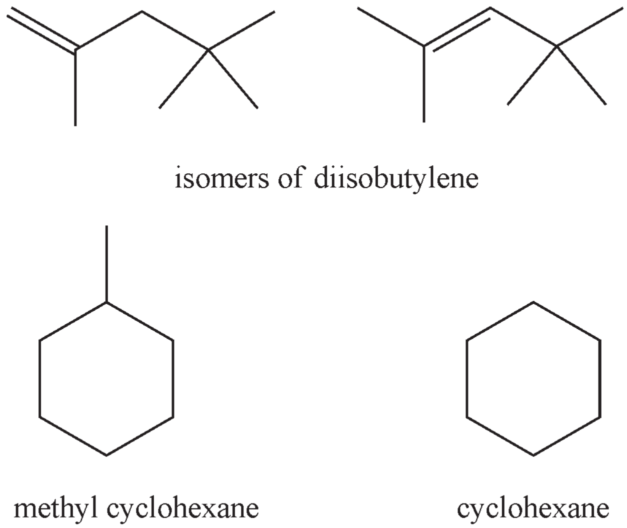

FIGURE 6. Carbon skeletal structures of fuels for which detailed chemical kinetic mechanisms have been developed: diisobutylene, methylcyclohexane and cyclohexane.

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

FY 2006 Publications/Presentations

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

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

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

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

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

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

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

Presentations

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

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

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

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

Special Recognitions & Awards/Patents Issued

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

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

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DOE Technology Development Manager:
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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

Approach

This project leverages several ongoing activities at ORNL involving exploration of new combustion regimes, researching novel approaches to stretch engine efficiency, as well as NOx mitigation technologies. The underpinning philosophy of the effort is that improving efficiency is best approached by thoroughly understanding the mechanisms and magnitudes of the various losses in engines with respect to converting fuel energy to work. Analyses of energy balances (First Law of Thermodynamics) and availability management (Second Law) are both instructive and necessary to identify and assess opportunities for improvements.

The following methodology will be used in this activity:

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

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

Results

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

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

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

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

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

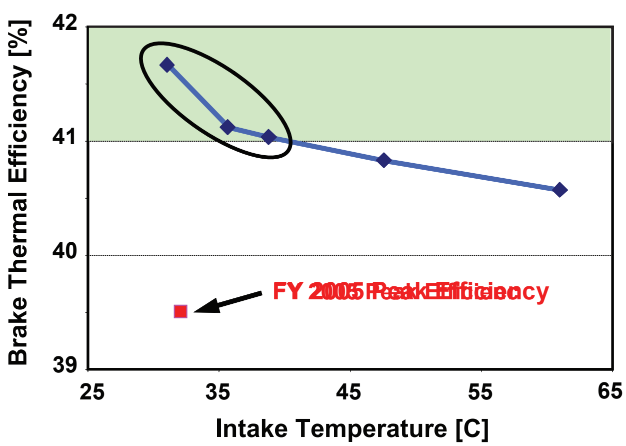

FIGURE 1. BTE as a function of intake charge temperature at 2,000 rpm, 100% load (14.7 bar BMEP). Also shown for reference is the peak BTE achieve in FY 2005.

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

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

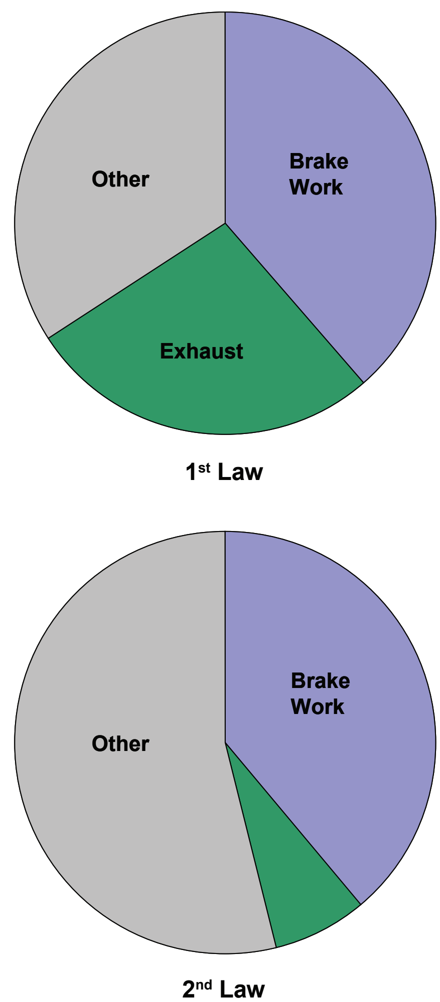

FIGURE 2. First and Second Law analysis of peak BTE conditions to provide better understanding of efficiency opportunities. Note that the first law analysis is based on HHV to be consistent with the second law analysis whereas the BTE calculation is based on LHV as is the convention.

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

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

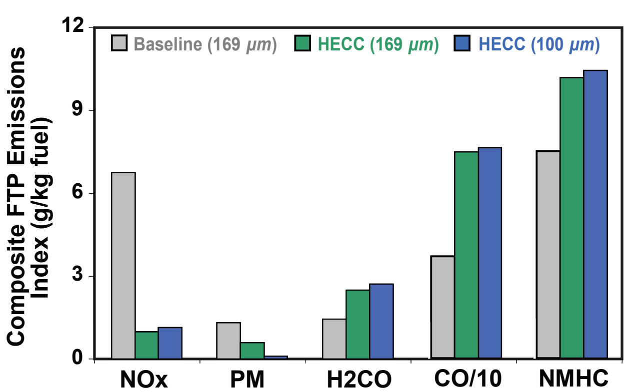

FIGURE 3. Composite emissions indices based on steady-state modal conditions representative of the FTP drive-cycle.

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

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

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

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

Conclusions

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

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

References

1. Kenney, T., Gardner, T., Low, S., Eckstrom, J., Wolf, L., Korn, S., and Szymkowicz, P., “Overall Results: Phase 1 Ad Hoc Diesel Fuel Test Program,” SAE Paper Number 2001-01-0151. Society of Automotive Engineers, Warrendale, 2001.

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

FY 2006 Publications/Presentations

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

II.A.16 Free-Piston Engine Research

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

As fuel efficiency of the typical American automobile becomes more important due to hydrocarbon fuel cost and availability issues, powertrain improvements will require smaller output engines combined with hybrid technologies to improve efficiency. Unfortunately, current crankshaft spark ignition internal combustion engines with optimized power outputs of 30 KW have thermal efficiencies of less that 32%.

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

Approach

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

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

Results

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

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

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

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

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

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

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

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

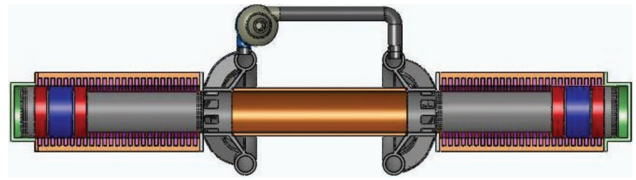

FIGURE 1. Proposed Layout of Sandia's Opposed Piston, Uniflow Scavenged Engine

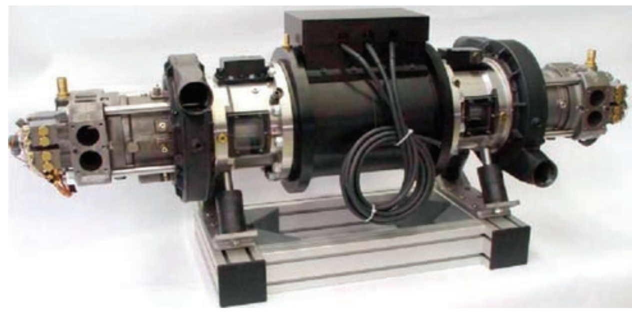

FIGURE 2. The European Union's Free Piston Energy Converter Prototype Engine

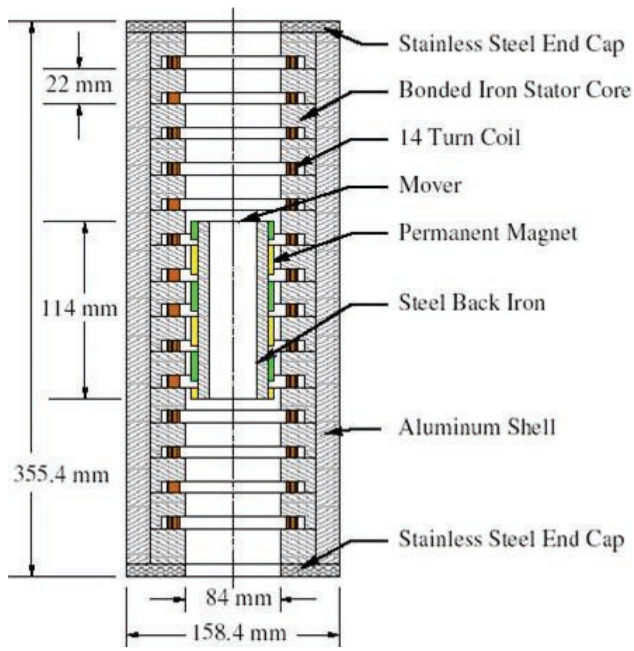

FIGURE 3. Layout of Magnequench International's Linear Alternator In Single-Phase Configuration

Previous and new industrial collaborators are being involved in the prototype design. Sandia continues to expand the concept to other applications. The goal is an operational research prototype by the end of FY2008.

Conclusions

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

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

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

Approach

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

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

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

Results

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

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

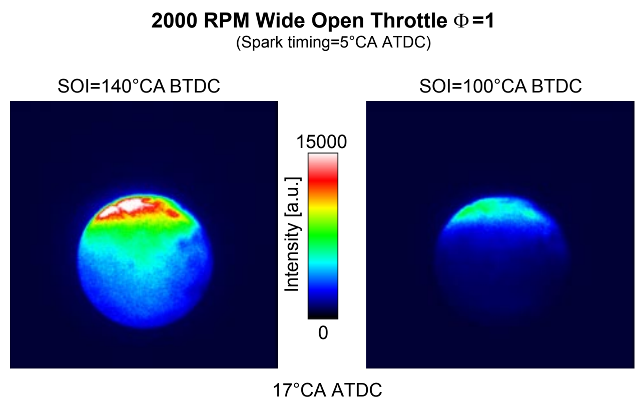

FIGURE 1. Comparison of OH* Intensity at 2,000 RPM and 100% Load for PFI (left) and DI (right) Operation

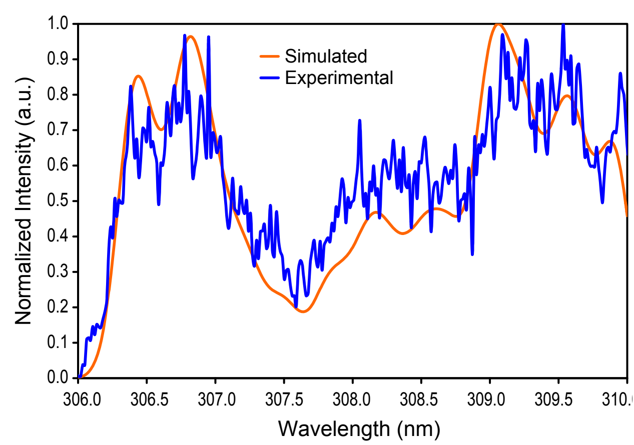

FIGURE 2. Simulated and Experimental Spectral Profiles of OH* Light Intensity during Hydrogen Combustion at 2900K

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

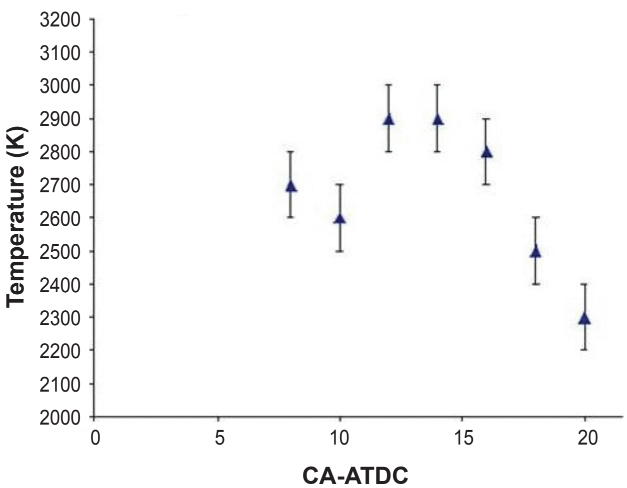

FIGURE 3. Thermal Profile of Hydrogen Combustion as a Function of Engine Crank-Angle Position (Time) for Engine Conditions of 2,000 RPM and 70% Load

Conclusions

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

FY 2006 Publications/Presentations

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

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

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

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

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

Approach

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

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

Results

Sample OH* chemiluminescence images of a single cycle and the ensemble average of 20 single cycles for an equivalence ratio of 0.51 acquired at 0 CAD (11 CAD after spark) are shown in Figure 1(a) and (b), respectively. Images for an equivalence ratio of 0.82

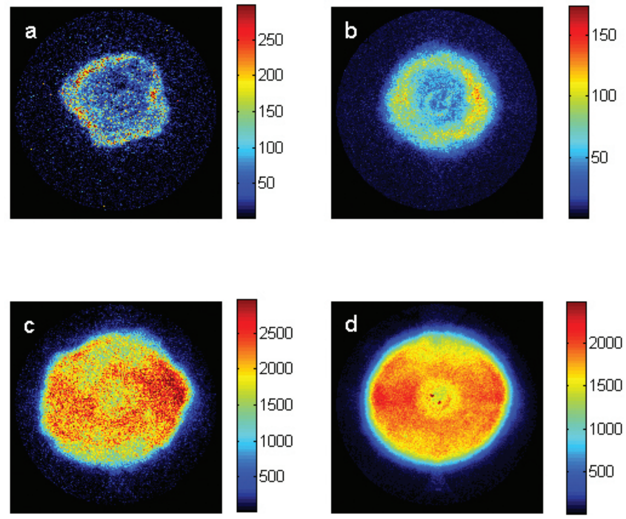

FIGURE 1. Sample OH* chemiluminescence images with pre-IVC injection for $\phi = 0.51$ acquired at 0 CAD (11 CAD after spark) for (a) a representative single cycle and (b) ensemble averaged over 20 single cycles and for $\phi = 0.82$ acquired at 8 CAD (6 CAD after spark) for (c) a representative single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

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

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

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

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

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

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

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

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

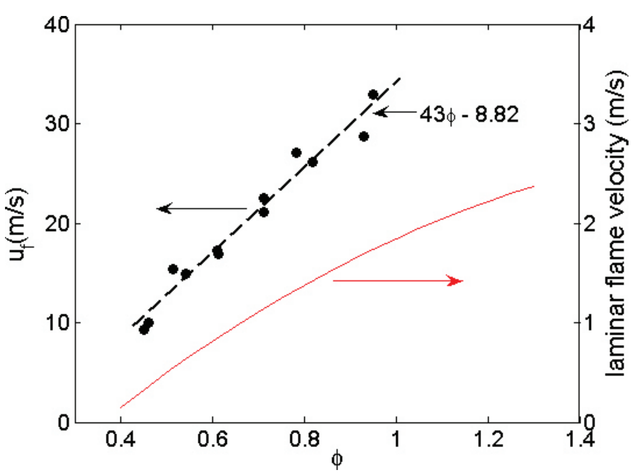

FIGURE 2. Flame front expansion speed (●) plotted against equivalence ratio. The dashed line is a least-squares linear fit to the data. The solid line is the laminar flame velocity versus equivalence ratio for a hydrogen-air mixture at room temperature and atmospheric pressure [8].

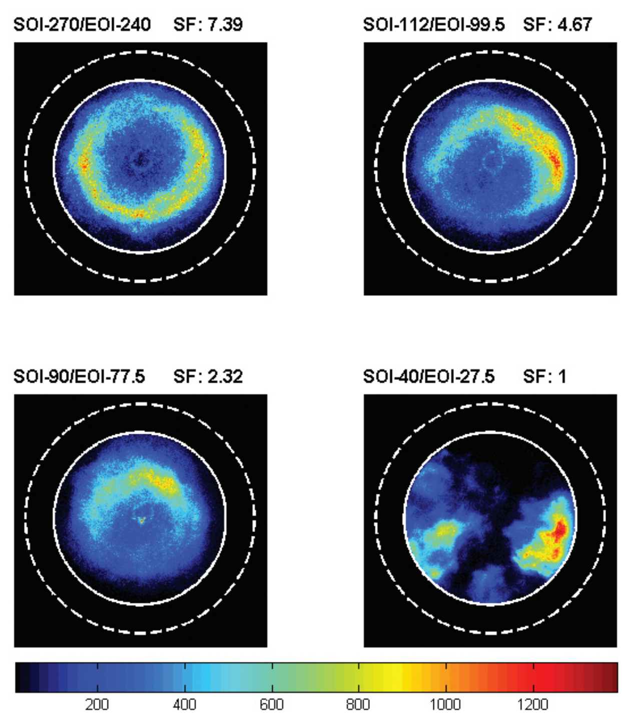

FIGURE 3. Ensemble-averaged OH* chemiluminescence images acquired at the CAD corresponding to the location of approximately 10% of the apparent heat release. Hydrogen injection pressure is 100 bar. The scaling-factor (SF) reported atop each image is a multiplicative factor based on the maximum intensity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

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

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

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

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

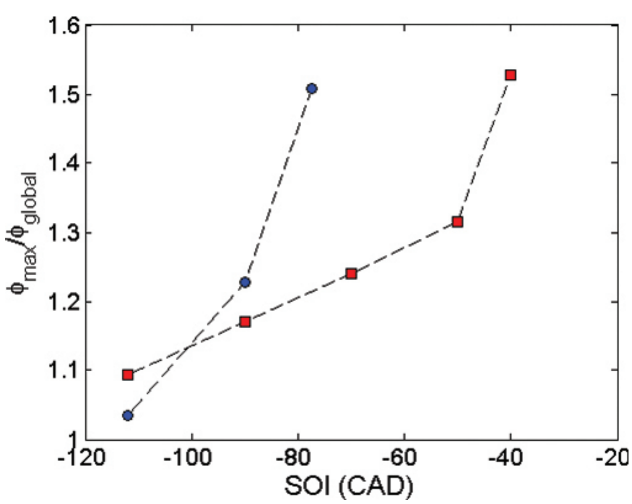

FIGURE 4. The maximum equivalence ratio measured for each SOI normalized by the global equivalence ratio for (●) Pinj = 2.5 MPa and (■) Pinj = 10 MPa.

Conclusions

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

References

1. M. R. Swain, J. M. Pappas, R. R. Adt Jr. and W. J. D. Escher, "Hydrogen-fueled automotive engine experimental testing to provide an initial design-data base," SAE paper 810350, 1981.

2. H. Eichlseder, T. Wallner, R. Freyman and J. Ringler, "The potential of hydrogen internal combustion engines in a future mobility scenario," SAE paper 2003-01-2267, 2003.

3. H. Rottengruber, M. Berckmüller, G. Elsässer, N. Brehm and C. Schwarz, "Direct-injection hydrogen SI-engine operation strategy and power density potentials," SAE paper 2004-01-2927, 2004.

4. C. M. White, R. R. Steeper and A. E. Lutz, "The hydrogen fueled internal combustion engine: A technical review," Int. J. Hydrogen Energy 31:1292-1305, 2006.

5. Department of Energy USA. Hydrogen posture plan: An intergrated research, development and demonstration plan. 2004. URL www.eere.energy.gov\hydrogenandfuelcells\posture plan04.html.

6. T. Clark, "Studies of OH, CO, CH and C2 radiation from laminar and turbulent propane-air and ethylene-air flames," NACA Technical Note 4266, 1958.

7. X. Tang, D. M. Kabat, R. J. Natkin and W. F. Stockhausen, "Ford P2000 hydrogen engine dynamometer development," SAE paper 2002-01-0242, 2002.

8. Lewis, B. and von Elbe, G. Combustion, flames, and explosions of gases. Orlando, Fl: Academic Press, 1987.

FY 2006 Publications/Presentations

1. C. M. White, R. R. Steeper and A. E. Lutz, "The hydrogen fueled internal combustion engine: A technical review," Int. J. Hydrogen Energy 31:1292-1305, 2006.

2. C. M. White, "OH* Chemiluminescence Measurements in a Direct-Injection Hydrogen-Fuelled Internal Combustion Engine," Int. J. Engine Research, in press.

3. C. M. White, A Technical Review of Hydrogen-Fueled Internal Combustion Engines, California Air Resource Board, Sacramento CA, September 2006.

4. C. M. White, Advanced Hydrogen-Fueled Internal Combustion Engine Research, DOE Peer Review, Argonne National Lab, May 2006.

5. C. M. White, Mixture Formation and Combustion in a Hydrogen-Fueled Internal Combustion Engine, International Energy Agency Task Leaders Meeting, Heidelberg, Germany, August 2006.

6. C. M. White, Sandia Hydrogen-Fueled Internal Combustion Engine Program, National Science Foundation Workshop on Hydrogen Combustion, Washington D.C., March 2006.

7. C. M. White, Evaluation of Mixture Formation and Combustion in a H2ICE using OH chemiluminescence, Ford Research Center, Dearborn, Detroit, March 2006.

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

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

Approach

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

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

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

Results

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

Major Accomplishments in 2006

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

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

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

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

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

FIGURE 1. Relative Fuel Consumption Improvement

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

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

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

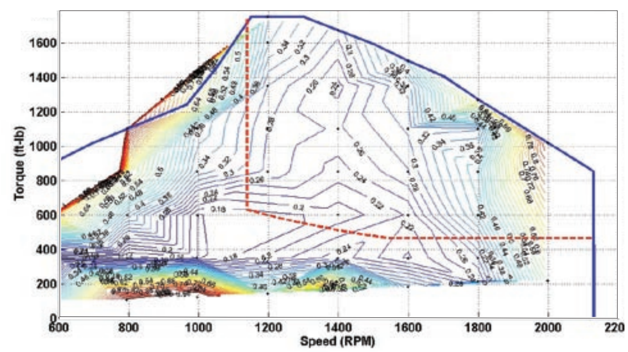

FIGURE 2. ISX High Pressure Injection bsNOx Map

Conclusions

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

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

Our analysis led design commitment has consistently achieved project deliverables.

References

1. Cummins Inc. Quarterly Reports as submitted to the Department of Energy.

FY 2006 Publications/Presentations

1. 'Premix Charge, Compression Ignition Combustion System Optimization' – 2006 Diesel Engine Emissions Reduction (DEER) Conference, Richard J Gustafson.

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

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- Sandia National Laboratories (Livermore, CA)
- IAV Automotive (Detroit, MI)
- Alipro (Peoria, IL)

Objectives

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

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

Accomplishments

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

Future Directions

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

Introduction

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

Approach

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

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

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

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

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

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

Results

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

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

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

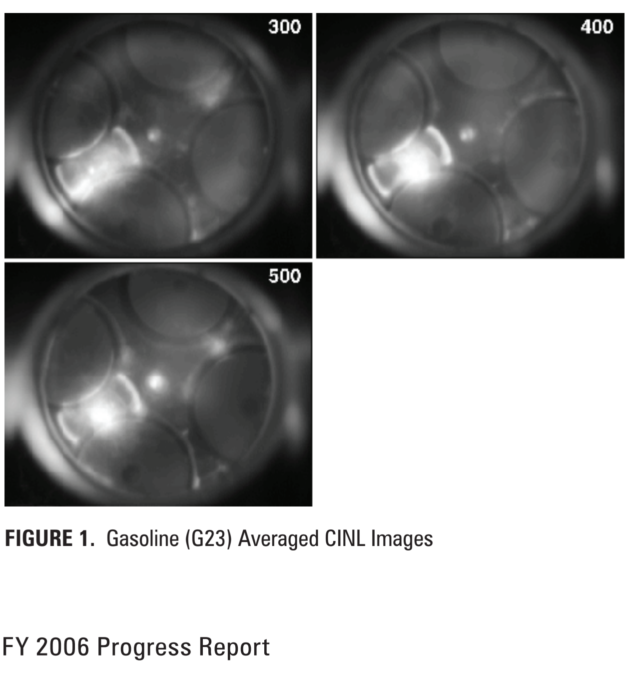

FIGURE 1. Gasoline (G23) Averaged CINL Images

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

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

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

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

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

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

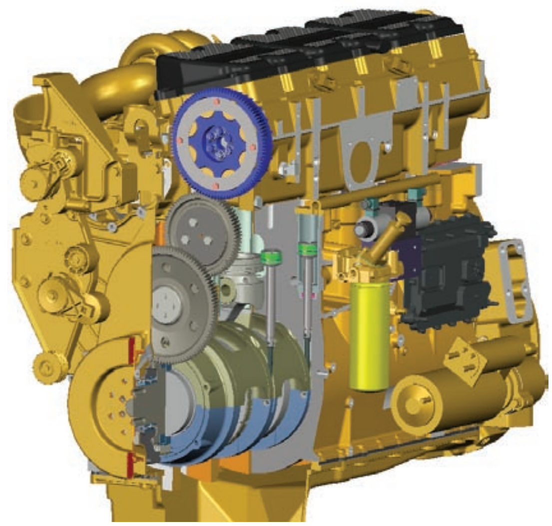

FIGURE 2. Variable Compression Ratio Engine

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

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

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

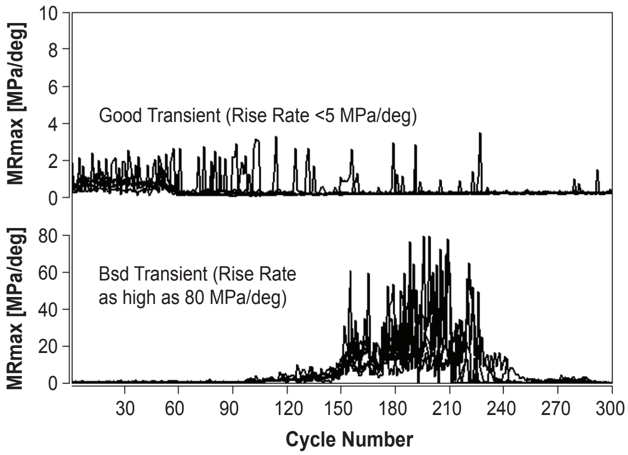

FIGURE 3. Comparison of Rise-Rates Achieved During Two Different Transients in MPa/deg

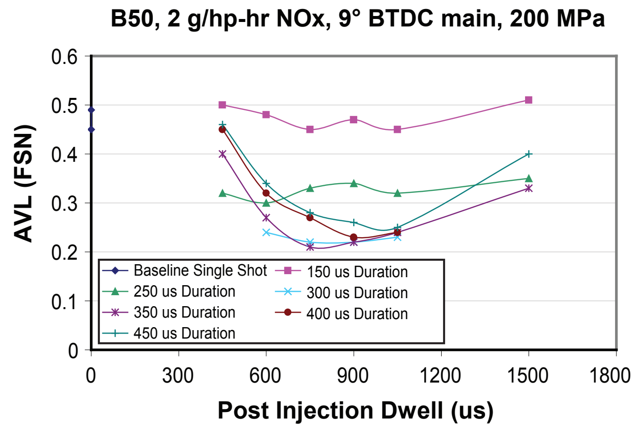

FIGURE 4. Effect of Post Injections on Smoke Reduction Using Advanced Fuel System

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

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

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

FY 2006 Publications/Presentations

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

Special Recognitions & Awards/Patents Issued

Patents Applied for:

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

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

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

Objectives

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

Accomplishments

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

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

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

Control system development items including:

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

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

The following items are in process to be completed:

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

Future Directions

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

Introduction

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

Approach

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

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

Results

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

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

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

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

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

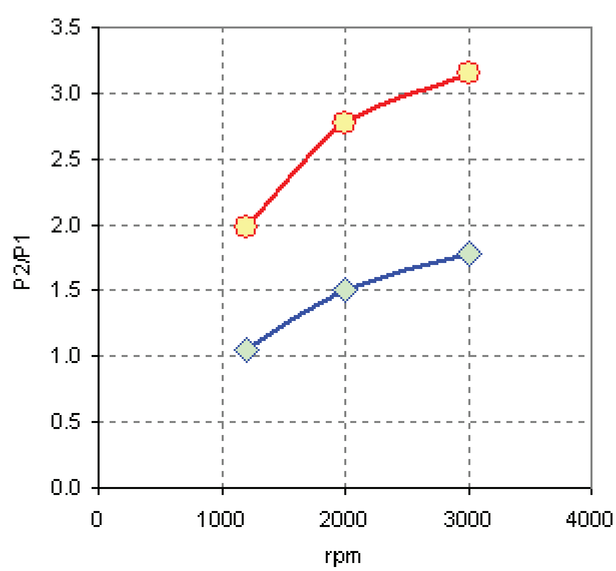

FIGURE 1. Engine Operating Conditions (Turbocharger Compressor Ratio; Top Line: 50% load; Bottom Line: Lug Curve)

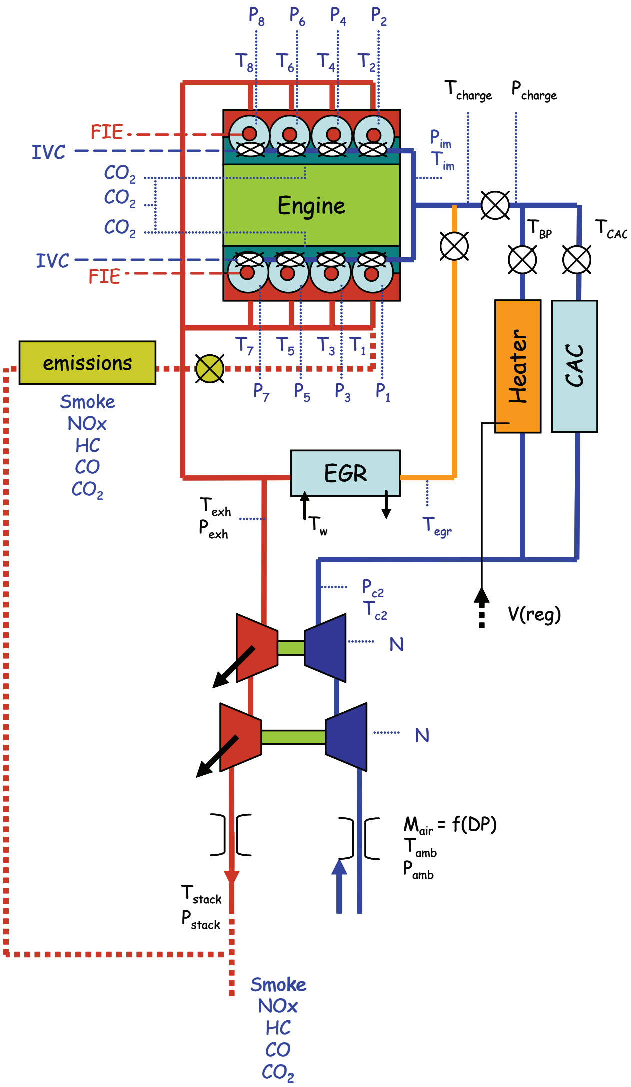

FIGURE 2. Engine Layout

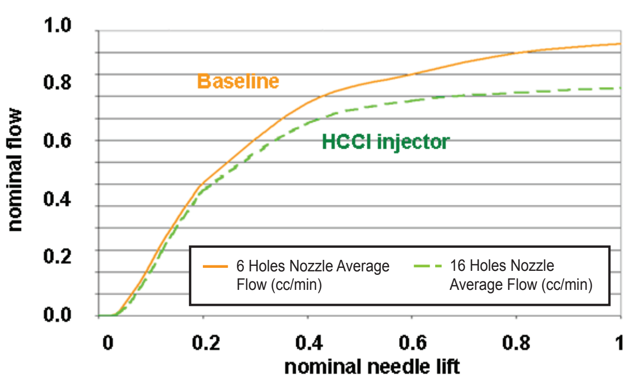

FIGURE 3. Injector Flow Comparison

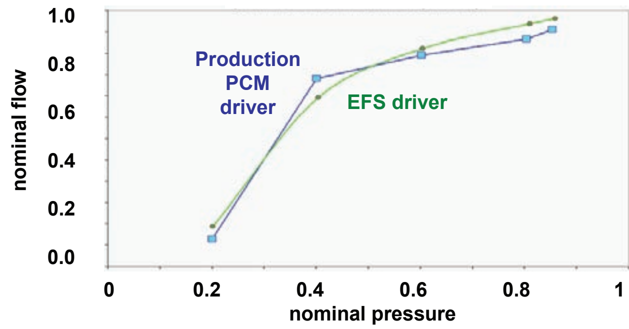

FIGURE 4. Effect of Driver on Injector Characteristics

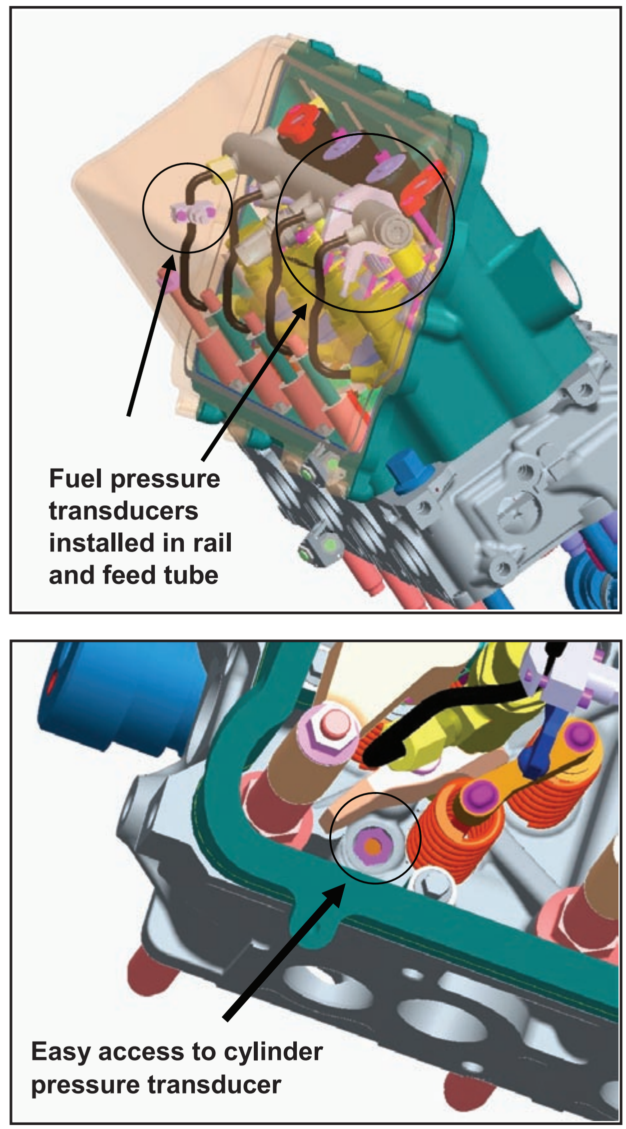

FIGURE 5. JVS Valve Actuation Packaged on a 6.4L V8 Cylinder Head

allows for positioning of pressure sensors on rail and feed tubes. A new valve spacer and cover were adopted to accommodate the increase height (on the order of 50 mm) and allow easy access, including access to pressure transducers (Figure 5).

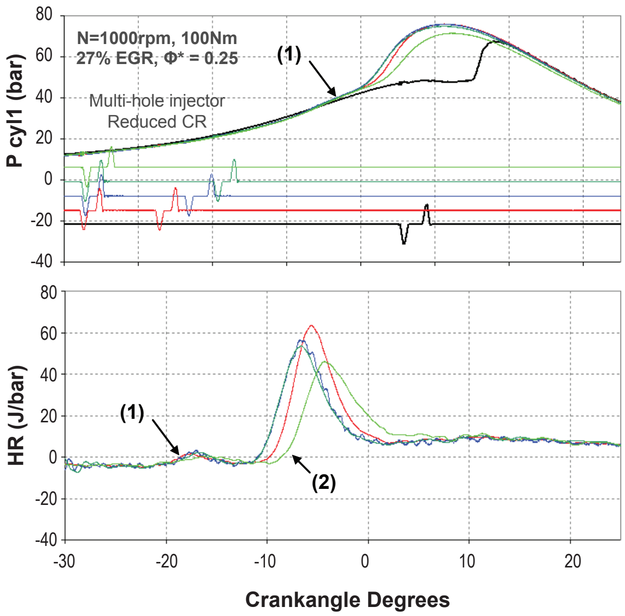

FIGURE 6. HCCI Combustion With Multiple Injection Strategies

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

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

Conclusions

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

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

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

References

1. Gui, Xinqun, "Project Narrative – Low Temperature Combustion Demonstrator for High Efficiency Clean Combustion," International Truck and Engine Corporation, August 9, 2004.

2. Yoshinaka Takeda, Nakagome Keiichi, and Niimura Keiichi, "Emission characteristics of premixed lean Diesel combustion with extremely early staged fuel injection", SAE 961163.

3. Allen W. (Bill) Gray, III and Thomas W. Ryan III, "Homogeneous charge compression ignition (HCCI) of Diesel fuel", SAE 971676.

4. Yoshinori Iwabuchi, Kenji Kawi, Takeshi Shoji, and Yoshinaka Takeda, "Trial of new concept Diesel combustion system – premixed compression ignited combustion", SAE 1999-01-0185.

5. Hisashi Akagawa, Takeshi Miyamoto, Akira Harada, Satoru Sasaki, Naoki Shimazaki, Takeshi Hashizume and Kinji Tsujimura, "Approaches to solve problems of the premixed lean Diesel combustion", SAE 1999-01-0183.

6. Zoldak, P.S., "Design of a Research Engine For Homogeneous Charge Compression Ignition (HCCI) Combustion," Master's Thesis, University of Windsor, September 15, 2005.

7. Shuji Kimura, Osamu Aoki, Hiroshi Ogawa and Shigeo Muranaka, "New combustion concept for ultra-clean and high-efficiency small DI Diesel engines", SAE 1999-01-3681.

8. Naoya Kaneko, Hirokazu Ando, Hideyuki Ogawa, Noboru Miyamoto, "Expansion of the operating range with in-cylinder water injection in a premixed charge compression ignition engine", SAE Paper 2002-01-1743, 2002.

9. Bruno Walter, Bertrnd Gatellier, "Development of the high power NADI concept using dual mode Diesel combustion to achieve zero NOx and particulate emissions", SAE Paper 2002-01-1744, 2002.

FY 2006 Publications/Presentations

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

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

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

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- Sturman Industries, Woodland Park, CO

Objectives

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

Accomplishments

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

Future Directions

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

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

Introduction

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

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

Approach

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

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

Results

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

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

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

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

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

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

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

Meanwhile, further refinement of the engine simulation with low-pressure-loop EGR indicated that 200 g/kWh BSFC (42% brake thermal efficiency) was achievable, although additional backpressure has to be added after the DPF in order to drive the clean EGR to the compressor inlet. Attention was shifted to the water-cooled exhaust manifold without EGR, and the heat release was changed to represent combustion without EGR. The WAVE simulation predicted that without EGR 40 to 42% brake thermal efficiency was achievable even with exhaust aftertreatment. Also, this engine simulation work showed that VTG turbocharger with about twice the flow of the production turbocharger was needed to avoid excessive boost. Unfortunately, no VTG turbocharger was available with suitable turbine and compressor sizes. This is because unusually high exhaust energy is available with the SCI engine while only moderate boost levels and flows are needed from the compressor. Therefore, a larger fixed turbocharger with a pneumatically-operated wastegate on the turbine housing was used for the third series of engine tests. Although the air system was not optimal, the goal was to achieve proper in-cylinder conditions in order to determine the NOx and PM emissions. Then measured engine performance data can be adjusted using simulation to represent an air system designed for the SCI engine concept.

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

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

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

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

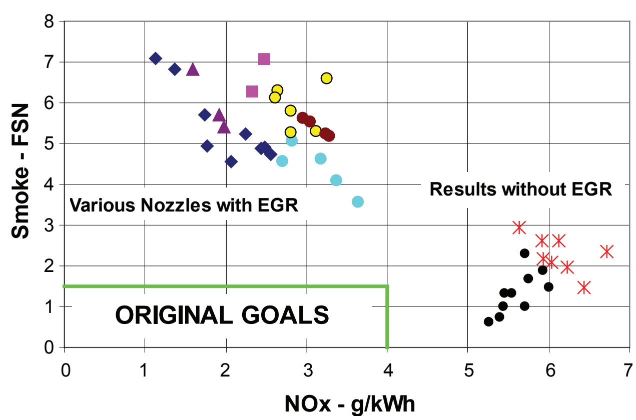

FIGURE 1. Comparison of Results from Second Test with EGR and Third Test without EGR at FLRS

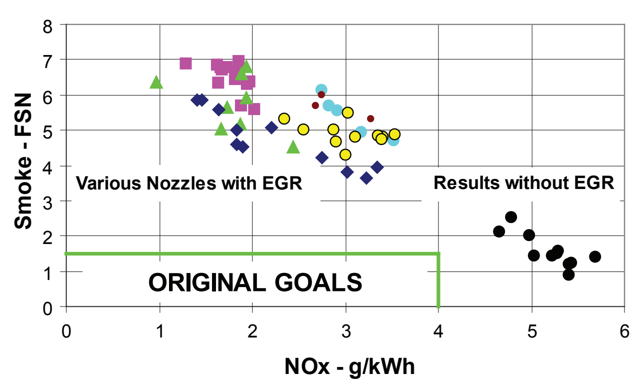

FIGURE 2. Comparison of Results from Second Test with EGR and Third Test without EGR at Peak Torque

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

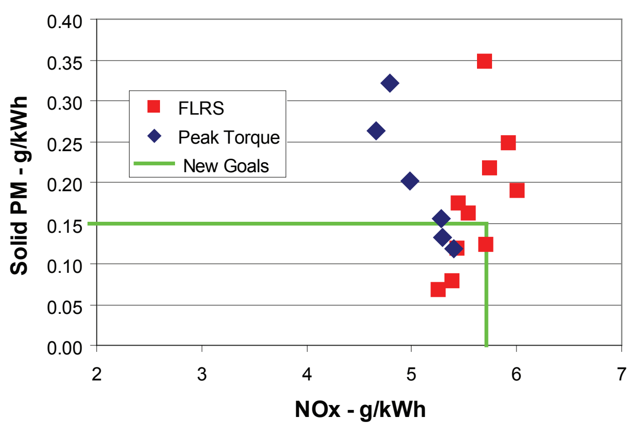

FIGURE 3. Engine-Out Emission Results without EGR

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

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

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

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

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

Conclusions

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

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

FY 2006 Publications/Presentations

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

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

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Objectives

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

Accomplishments

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

Future Directions

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

Introduction

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

Approach

A GT-Power™ engine simulation model was constructed to predict engine efficiency based on the second-law thermodynamic availability at various operating conditions and optimization of valve timing was achieved as well. The engine efficiency map generated by the engine simulation was then fed into a simplified vehicle model to predict fuel consumption of a refuse truck on a simple collection cycle. Design and analysis work supporting the concept of retrofitting an existing HVA system with the modifications that are required to run the HVA system with APA functionality was completed. An APA engine with HVA system will be implemented to validate the fuel economy improvement.

Results

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

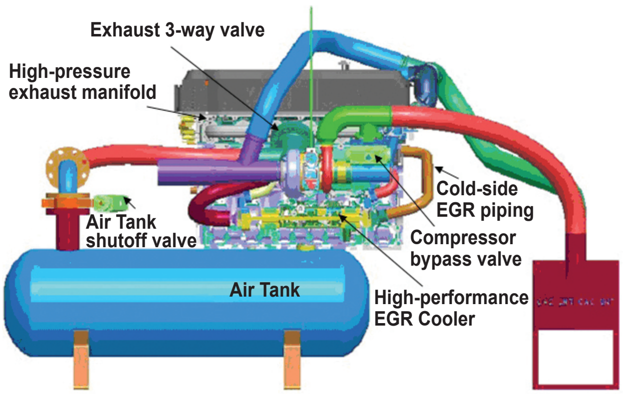

FIGURE 1. APA Air Handling System General View (Exhaust side)

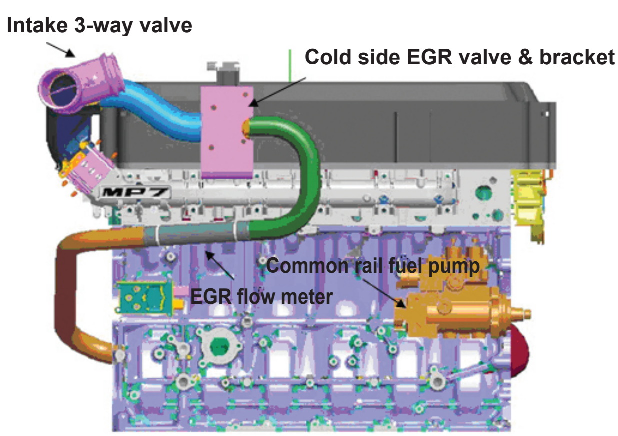

FIGURE 2. APA Air Handling System General View (Intake side)

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

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

TABLE 1. Estimated Efficiency Improvement From Vehicle Simulation

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

Vehicle Simulation with ADVISOR

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

Conclusions

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

References

1. Schechter, M. "Regenerative Compression Braking-A Low Cost Alternative to Electric Hybrids", SAE Technical Paper 2000-01-1025.

2. Tai, C. et al., "Using Camless Valvetrain for Air Hybrid Optimization", SAE Technical Paper 2003-01-0038.

FY 2006 Publications/Presentations

Publications

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

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

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

Presentations

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

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