II.A Advanced Combustion and Emission Control Research for High-Efficiency Engines

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

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

DOE Technology Development Manager: Kevin Stork

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.

Approach

- Utilize our unique expertise in both spray measurement and x-ray physics to perform x-ray studies of sprays. Such methods allow quantitative measurements in the near-nozzle region of the spray that is inaccessible with other techniques.
- Measurements are performed at Argonne's Advanced Photon Source (APS), a high-intensity x-ray source that allows us to make quantitative spray measurements with precise position and time resolution. Measurements must be relevant to the engine community while also being compatible with the existing facilities at the x-ray source. Currently, this limits us to performing spray measurements in static pressurized vessels at room temperature.
- Our measurements are designed to study the effects of several different injection parameters of interest to the engine community, such as orifice geometry, injection pressure, and ambient gas density. With our powerful measurement technique we can quantify the effect of each of these variables on the structure of the spray.
- Using x-ray absorption, we can measure the instantaneous mass distribution of the fuel with very good position and time resolution. This is a unique and unambiguous observation of the structure of the spray. Measurements such as these provide a very stringent test of existing spray models and are crucial for the development of models with improved accuracy and predictive power.

Accomplishments

- Robert Bosch donated new fuel system components to our group; they 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. 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.
- An important collaboration with General Motors and the Engine Research Center at the University of Wisconsin was continued in 2005. Two weeks of x-ray measurements in FY 2005 were dedicated to this collaboration.

- Utilizing internal ANL funding, in collaboration with another research group at the APS, we completed the first-ever phase-contrast images of fuel sprays, which revealed the cavitation and ligaments in a spray as it emerges from the nozzle. This revealed a promising new avenue for spray research.
- Improvements in x-ray pressure window fabrication and an ongoing testing regimen have shown that our x-ray windows can consistently support ambient pressures up to 70 bar. The tests also suggest that x-ray exposure and pressure exposure have little influence on the strength of the windows.
- We incorporated a number of new safety features into our experiments which were recommended by Argonne's pressure safety committee. These enhancements will allow us to perform future x-ray measurements at ambient pressures above 20 bar.
- FY 2005 continued our group's record of a large volume of high-quality publications. We published five papers and presented our work at seven national and international meetings.

Future Directions

- Increase the relevance of our measurements by studying sprays under conditions closer to those of modern diesel engines. We have made steady progress over the course of the project, continually increasing the ambient pressure and enabling the use of production nozzles. We will continue to pursue the goal of making measurements under conditions that are directly comparable to an operating 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 are producing 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 20 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

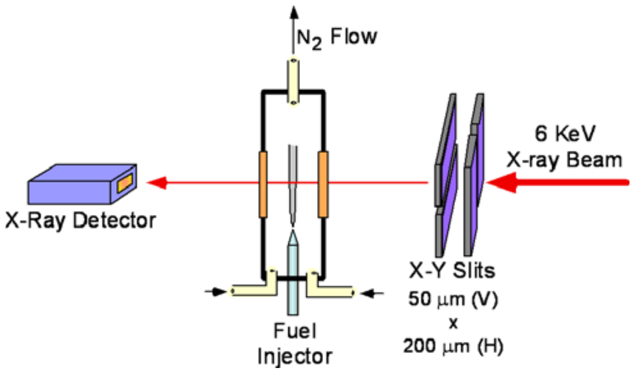

Figure 1. Schematic of the Experimental Setup

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

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

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

Our group's collaboration with Robert Bosch GmbH was greatly expanded in FY 2005. Based on a handshake agreement with Gerd Bittlinger of Bosch Corporate Research, Bosch donated new fuel system 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; it is pictured in Figure 2. Bosch also sent their employee Thomas Riedel to work with our group for four months and take part in several experiments. 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 valve-covering orifice (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. This asymmetry is shown in Figure 3; as the spray leaves the nozzle, the

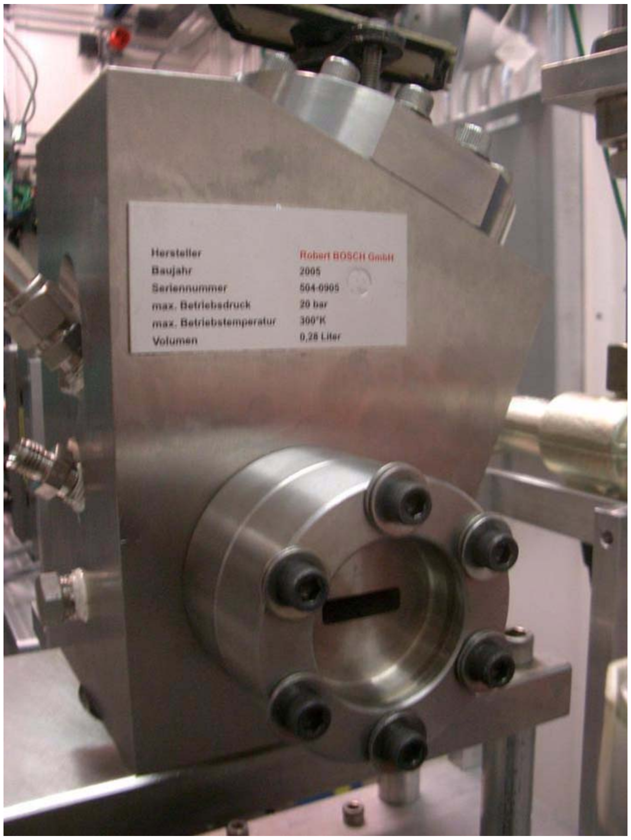

Figure 2. Bosch-Funded Spray Chamber for X-Ray Measurements

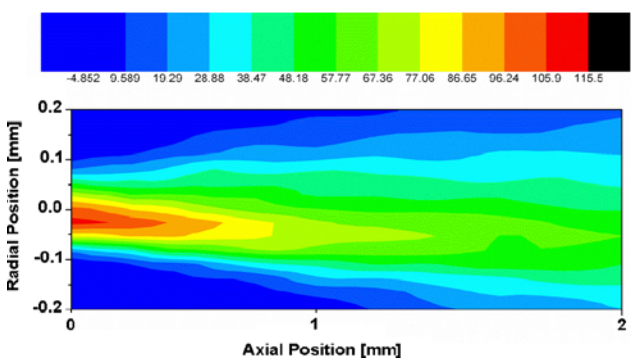

Figure 3. Spray Image Reconstructed from X-Ray Measurements

fuel density is higher at one edge than at the other. 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 ANL and Bosch, spray modeling will be done by Bosch, and a joint paper will be published.

FY 2005 saw the continuation of an important collaboration with General Motors and the Engine Research Center (ERC) at the University of Wisconsin. Two weeks of x-ray measurements in FY 2005 were dedicated to this collaboration. Measurements were performed at ambient pressures up to 17 bar for several different nozzle geometries. The analysis of the results is being performed by students and faculty at 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.

Utilizing internal ANL funding and in collaboration with another research group at Argonne's APS, in FY 2005 we completed the first-ever phase-contrast images of fuel sprays. These images revealed the cavitation and ligament structure of a spray as it emerged from the nozzle. These measurements revealed a promising new avenue for spray research. While the technique cannot provide the quantitative measurements of the fuel distribution like the x-ray radiography technique, it can give an instantaneous view of the boundaries between liquid and gas in the spray as it emerges from the nozzle. Together, the two x-ray techniques provide the best diagnostics for understanding the mechanisms of spray breakup.

In 2005 we made significant advances in an effort to make measurements of sprays under conditions similar to those in a real engine. We began a regimen of testing our x-ray pressure windows to verify quality control and ensure the safety of the experimenters. These tests, along with improvements in x-ray pressure window fabrication, have shown that our x-ray windows can consistently support ambient pressures up to 70 bar. Preliminary results also indicate that x-ray exposure and pressure exposure have little influence on the strength of the windows. These important steps will allow us to make measurements at pressures above 20 bar in the near future.

In order to make measurements at pressures above 20 bar, we incorporated a number of new safety features into our experiments which were recommended by Argonne's pressure safety committee. Pressurization of the spray chamber is now done remotely to protect the experimenters in the event of a window failure. We have also successfully tested energy-dissipating baffles that will minimize damage to equipment in the x-ray laboratory should a window fail while under pressure. These enhancements will allow us to perform future x-ray measurements at pressures above 20 bar.

In addition to technical accomplishments, FY 2005 saw the establishment of a new collaboration with PSA Peugeot-Citroen. PSA will donate fuel system equipment to Argonne in FY 2006, Argonne will perform spray measurements, and PSA will test their spray modeling based on the measurement results. This will lead to a joint publication between Argonne and PSA, and the results will be freely publishable by Argonne. The expanding list of collaborators keeps us connected to the world's experts in the field and focuses our research on the areas in which it will have the most impact.

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.

FY 2005 Publications/Presentations

1. "X-Ray Vision of Fuel Sprays", Jin Wang, Journal of Synchrotron Radiation, 12, pp. 197-207, 2005.
2. "Near-Field Spray Characterization of Multi-Hole Fuel Injector for Direct Injection Gasoline Engines Using Ultrafast X-Tomography", Xin Liu, Seong-Kyun Cheong, Christopher F. Powell, Jin Wang, David L.S. Hung, James R. Winkelman, Mark W. Tate, Alper Ercan, Daniel R. Schuette, Lucas Koerner, Sol M. Gruner, ILASS Americas, 18th Annual Conference on Liquid Atomization and Spray Systems, Irvine, CA, May 2005.
3. "Recent Progress of X-Ray Fuel Spray Characterization at Argonne", Presentation at DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation, Argonne National Laboratory, May, 2005.
4. "Diesel Spray Characterization Using Synchrotron X-Rays", Presentation at DOE AEC-MOU Meeting, USCAR, Southfield, MI, September, 2005.
5. "X-Ray Characterization of Diesel Sprays", Christopher Powell, Alan Kastengren, Thomas Riedel, Seong-Kyun Cheong, Xin Liu, Yujie Wang, Jin Wang, DEER Conference, Chicago, IL, August, 2005.

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, and J. Schaller, SAE 2001-01-0531 (2001).

II.A.2 X-Ray Studies of Heavy-Duty Injector Spray Characteristics

Christopher F. Powell (Primary Contact), Seong-Kyun Cheong, Sreenath Gupta, Essam El-Hannouny, Jin Wang
Argonne National Laboratory
9700 S. Cass Ave.
Argonne, IL 60439

DOE Technology Development Manager: Kevin Stork

Objectives

- Study the mechanisms of spray atomization by making detailed, quantitative measurements in the near-nozzle region of sprays from heavy-duty injectors.
- Provide near-nozzle data that is crucial for the development of accurate spray models.
- Compare the data measured using the x-ray technique with computational models of spray structure to test the validity of the models and support model development.

Approach

- Build a laboratory fuel injection system that is compatible with the x-ray technique based on the design of the existing system at Sandia National Laboratories (SNL).
- Test the fuel system for proper operation using visible light imaging techniques.
- Perform x-ray measurements of the fuel sprays generated from several different injector nozzle geometries at several ambient pressures.

Accomplishments

- The fuel system was constructed and the first x-ray measurements were completed in FY 2003. In these studies, we measured the time-resolved mass distribution of sprays from three different nozzle geometries at atmospheric pressure.
- A series of conventional measurements were performed in FY 2004 on the same three nozzles, including rate-of-injection measurements and visible light imaging.
- Two weeks of x-ray experiments were completed in FY 2004. These experiments studied the effects of elevated ambient pressure and injection pressure on the sprays from two different nozzles. The results of these measurements were published in FY 2005.
- Collaboration was established between the researchers at Argonne and a modeling group at Helsinki University of Technology. Data from the x-ray measurements was shared with Helsinki spray modelers, and a joint publication will be presented at the 2006 SAE World Congress.

Future Directions

- The collaboration with spray modelers from Helsinki University is continuing; they are pursuing further comparisons between their spray models and our measurement results. We continue to provide them with data and technical support in these studies.
- Measurements of the Detroit Diesel Corporation heavy-duty injector have been completed. Further x-ray measurements of sprays from heavy-duty injectors will be part of the Caterpillar Cooperative Research and Development Agreement (CRADA) and will be performed on modern Caterpillar injection systems.

Introduction

The fuel injection system is 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 20 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 utilizes a heavy-duty fuel injector designed and built as a prototype by Detroit Diesel Corporation with specially-fabricated single-hole nozzles. The injector and nozzles are similar to those which have been studied at Sandia National Laboratories over a wide range of conditions using a number of different measurement techniques [1,2,3]. Our approach is to make detailed measurements of the sprays from this injector using the x-ray technique. This allows us to compare the x-ray results with the large body of existing data, and extend the existing knowledge into the near-nozzle region. The x-ray measurements were performed at

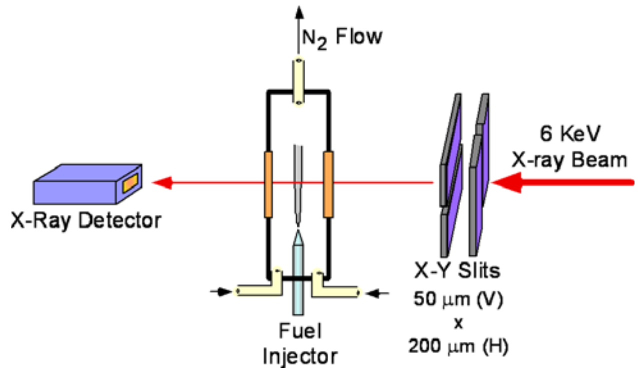

Figure 1. Schematic of the Experimental Setup

the 1BM-C station of the Advanced Photon Source (APS) at Argonne National Laboratory. A schematic of the experimental setup is shown in Figure 1; detailed descriptions of the experimental methods are given in [4] and [5]. The technique is straightforward; it is similar to absorption or extinction techniques commonly used in optical analysis. However, the x-ray technique has a significant advantage over optical techniques in the measurement of sprays: because the measurement is not complicated by the effects of scattering, there is a simple relation between the measured x-ray intensity and the mass of fuel in the path of the x-ray beam. For a monochromatic (narrow wavelength bandwidth) x-ray beam, this relation is given by

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

where I and I_0 are the transmitted and incident intensities, respectively; μ_M is the mass absorption constant; and M is the mass of fuel. The constant μ_M is measured in a standard cell, and the incident and transmitted intensities are measured as a function of time by the x-ray detector. This allows direct determination of the mass of fuel at any position in the spray as a function of time. It is the goal of our work to use the x-ray technique to measure sprays from our heavy-duty fuel injector at different injection pressures, different ambient pressures, and using different nozzle geometries. We will collaborate with spray modelers to incorporate this previously unknown knowledge of 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

A series of x-ray and conventional measurements was performed on sprays from a prototype common rail injector manufactured by Detroit Diesel Corporation. The effects of injection pressure, ambient pressure, and nozzle geometry were explored in these experiments. In FY 2003 we constructed the fuel system and performed a series of x-ray measurements at ambient pressure. In FY 2004 we performed a broader series of measurements designed to study the sprays under a variety of different conditions.

Optical imaging was used to measure the overall spray shape, spray penetration and spray cone angle. These measurements demonstrated the correct performance of the injection system and allowed comparison to similar measurements made in the past at SNL. The nozzle diameter had a strong effect on the spray penetration and angle, as expected from the SNL work. Additional optical imaging was performed using a microscopic lens, allowing a detailed measurement of the spray boundaries and shape.

Another series of conventional spray measurements was made using the Bosch Rate-of-Injection (ROI) meter, shown in Figure 2. This measurement is the industry standard for determining the fuel flow rate and the overall quantity of fuel injected. These measurements showed good agreement with the momentum method used at SNL. Also, the mass flow measured in this way can be compared to the mass measurements made using the x-ray absorption method.

X-ray measurements were performed on three different nozzles under otherwise identical conditions. The first nozzle had an orifice diameter of 180 µm and orifice length to diameter ratio (L/D) equal to four, the second had a diameter of 250 µm and L/D = 4, while the third had a diameter of 250 µm and L/D = 8. The measurements were made at injection pressures of 1000 and 1500 bar, the spray duration was 2.5 ms, and the ambient gas was N_2 at room temperature and pressures of 1 and 10 bar.

The x-ray technique was able to probe the dense region of the spray as close as 0.2 mm (<1.5 nozzle diameters) from the nozzle. Moreover, the x-ray technique provided a quantitative mapping of the mass distribution in two dimensions, which can be used to estimate the volume fraction of the spray as a function of time and space. Several interesting features were observed in the measurements of these nozzles. One such feature is shown in Figure 3, which shows the mass distributions of the spray as measured by the x-ray absorption technique. It can be seen that there are high-density regions of the spray near the leading edge and also near the nozzle. Early in the spray event, these two regions were connected by a core of relatively high density. As time evolved, these two regions separated and the spray became more diffuse. We believe that this illustrates the importance of the dynamics of the spray event. Early in the spray event, the pintle was only partially open and the nozzle was an ineffective atomizer. This led to the high-density leading edge of the spray. Later, the pintle opened further and pressure built throughout the nozzle, leading to more efficient atomization by the injector and the lower density seen in the later images of Figure 3.

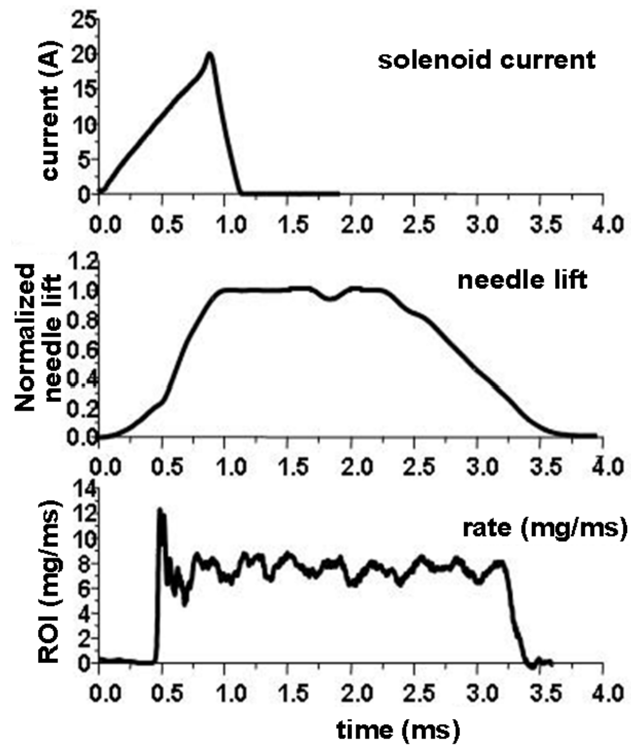

Figure 2. Injection Current, Needle Lift, and Rate-of-Injection These tests verify the correct operation of the injection system.

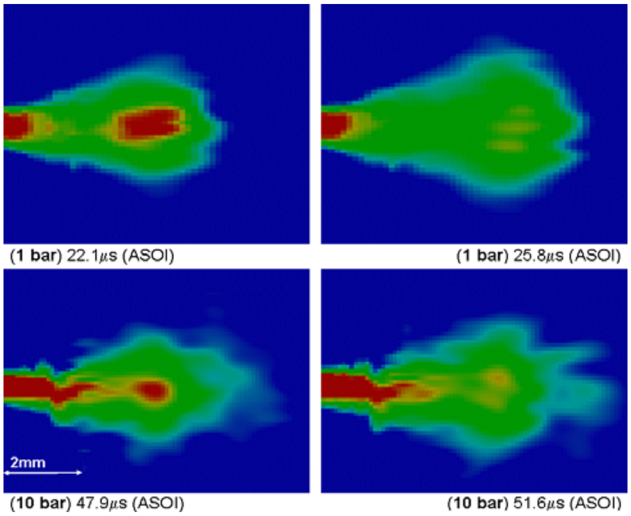

Figure 3. X-ray Images of the Spray at 1 Bar and 10 Bar Ambient Pressure

Measurements such as these illustrate the importance of spray dynamics and point to the need for very careful spray modeling efforts.

One very important accomplishment in FY 2005 was the completion of a joint paper between Argonne and a modeling group at the Helsinki University of Technology. The group from Helsinki has been provided with the results of our measurements and has compared them with calculations using the KH-RT and the CAB droplet breakup models. This paper has been submitted to SAE and will be presented at the 2006 SAE World Congress. This modeling collaboration will increase the impact of our work, since our measurements provide unique information on the structure of sprays that is extremely valuable to modelers.

Conclusions

- Testing has shown that the fuel system which we designed and built is operating as expected and is also compatible with measurements using the x-ray technique.
- 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 may be 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.

FY 2005-2006 Publications/Presentations

1. "Time Resolved X-Ray Measurements of Diesel Sprays at Elevated Back Pressure", Essam M. El-Hannouny, Sreenath Gupta, Christopher F. Powell, Seong-Kyun Cheong, and Jin Wang, ILASS Americas, 18th Annual Conference on Liquid Atomization and Spray Systems, Irvine, CA, May 2005.
2. Presentation at DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation, Argonne National Laboratory, May, 2005.
3. "Near Nozzle Diesel Spray Modeling and X-Ray Measurements", Ville Vuorinen, Eero Antila, Ossi Kaario, Martti Larmi, Essam El-Hannouny, and Sreenath Gupta, Submitted for publication at SAE Congress 2006.

References

1. D. L. Siebers, SAE 980809, (1998).
2. J. D. Naber and D. L. Siebers, SAE 960034, (1996).
3. B. S. Higgins, C. J. Mueller, and D. L. Siebers, SAE 1999-01-0519, (1999).
4. C. F. Powell, Y. Yue, R. Poola, and J. Wang, J. Synchrotron Rad. 7:356-360 (2000).
5. C. F. Powell, Y. Yue, R. Poola, J. Wang, M.-C. Lai, and J. Schaller, SAE 2001-01-0531, (2001).

II.A.3 Low-Temperature Automotive Diesel Combustion

Paul Miles
Sandia National Laboratories, MS9053
P.O. Box 969
Livermore, CA 94551-0969

DOE Technology Development Manager: Kevin Stork

Subcontractor:
University of Wisconsin, Madison, Wisconsin

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.

Approach

- Obtain measurements of flow and thermophysical properties in an optically accessible engine using laser-based measurement techniques.
- Closely coordinate and compare in-cylinder measurements and engine emissions and performance to model predictions.
- Refine and improve models and engine operating strategies.

Accomplishments

- Expanded previous work on late-injection, low-temperature diesel combustion regimes to include higher levels of exhaust gas recirculation (EGR) (i.e., dilution levels) that allow early-injection strategies. Examined engine performance and emissions for a wide variety of system parameters, including injection pressure, swirl ratio, O_2 concentration (EGR rate), and start of injection (SOI).
- Identified "under-mixed" fuel as a dominant source of CO emissions (and combustion inefficiency) for high-dilution operating conditions.
- Clarified the relative importance of complete combustion, heat transfer, and combustion phasing on the fuel conversion efficiency of low-temperature combustion regimes.
- Revised the phenomenological picture of the progression of low-temperature combustion regimes in the equivalence ratio-temperature (ϕ-T) plane to include high-dilution regimes.
- Commenced design work to incorporate a new, GM diesel production engine in the Automotive Low-Temperature Diesel Combustion Laboratory, thereby strengthening ties with GM-funded research at the University of Wisconsin and multi-cylinder testing to take place at Oak Ridge National Laboratory.

Future Directions

- Evaluate the effect of engine boost on low-temperature combustion systems and on the fuel conversion efficiency loss typically observed with high dilution levels.

- Experimentally obtain full-field flow-structure information, including single-cycle realizations of in-cylinder flow structure.
- Compare the results of the above measurements with the results of numerical simulations; evaluate the accuracy of the simulations and the need for more expensive large eddy simulations (LES) to capture the important features of the combustion process on a single-cycle basis.

Introduction

Direct-injection diesel engines have the highest fuel conversion efficiency and the lowest CO_2 emissions of any reciprocating internal combustion engine technology. This efficiency comes at the cost, however, of high NO_x and particulate matter (soot) emissions. Reduction of these emissions through clean in-cylinder combustion processes is imperative if vehicles powered by these engines are to be available at a competitive cost. Low-temperature diesel combustion (LTC) regimes have been shown to dramatically reduce NOx emissions without unduly prejudicing the soot emissions. However, the lowest NOx emissions are often associated with a loss of fuel conversion efficiency, due in many cases to an inability to completely mix the fuel with sufficient oxidant in the available time. The high level of EGR (low O_2 concentration) employed in these systems to achieve low combustion temperatures means that a greater mass of ambient fluid must be mixed with the fuel than is needed for conventional diesel combustion. Enhancing the mixing processes is central to recovering fuel conversion efficiency and extending the operating range of LTC strategies.

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 measurements taken from an optically accessible laboratory test engine which are then closely coordinated with numerical simulation efforts. Detailed flow and thermo-chemical property measurements are made during the fuel preparation and combustion processes, along with more traditional emissions, performance and fuel consumption measurements. The experimental results are compared with the predictions of complex, multi-dimensional computer models. These efforts are mutually complementary. For example, detailed measurements of flow variables permit the evaluation and refinement of the computer models, while the model results can be used to clarify the flow physics—a process that is difficult if only limited measurements are employed.

Results

The optically accessible diesel engine facility is depicted in Figure 1. This facility employs a slotted, extended piston assembly with a quartz combustion chamber that permits the progress of combustion to be visualized from below. In addition, the upper region of the cylinder liner is equipped with quartz windows that allow a lateral view of the combustion process to be obtained. This lateral view capability, in a configuration that maintains the faithful

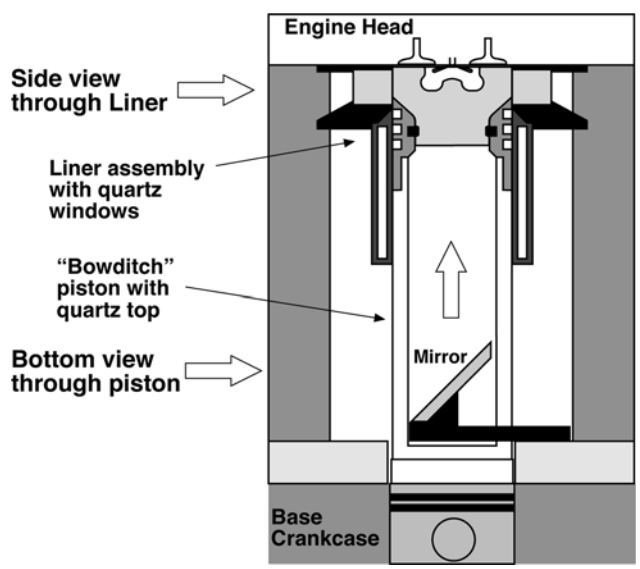

Figure 1. Schematic View of the Optical Engine, Depicting the Quartz Piston Top with a Realistic Combustion Chamber Geometry

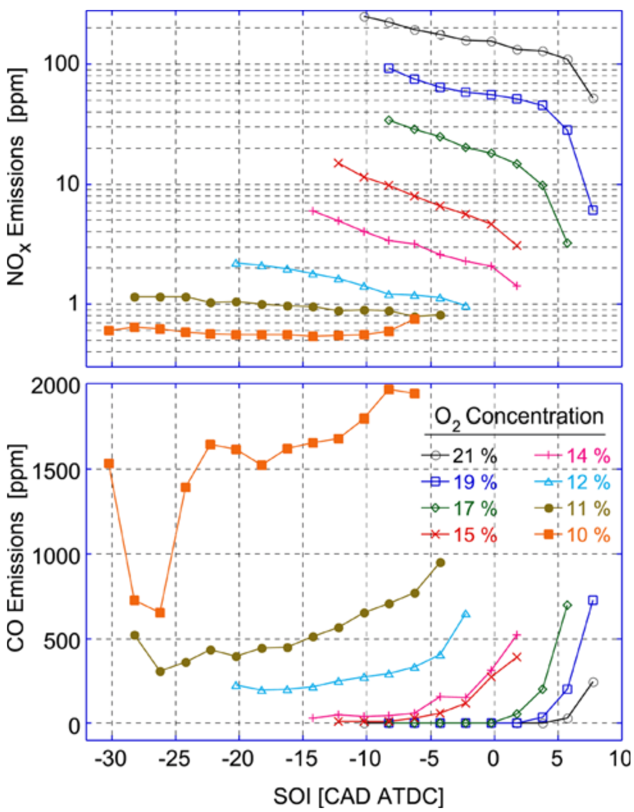

Figure 2. Variation in the emissions of NOx and CO as the dilution level and the injection timing are varied. These data were taken under skip-fired operation, and the corresponding emissions for a continuously fired engine will be 4 times the value shown. Load = 3 bar, 1500 RPM, R_s = 3.77, P_{inj} = 800 bar.

combustion chamber geometry, is a pioneering aspect of this facility that has now been duplicated in several other laboratories. The engine bowl geometry, bore, stroke, and fuel injection equipment are typical of state-of-the-art direct-injection diesel engines for passenger car applications. Variable cylinder swirl levels can be achieved through throttling of one of the intake ports.

A major thrust of the research performed in FY 2005 was directed towards obtaining a more comprehensive view of the emissions, performance, and efficiency behavior of low-temperature combustion systems over a wide range of operating conditions. Accordingly, we have varied both SOI and O_2 concentration over a broad range encompassing the full spectrum of low-temperature diesel combustion regimes. NO_x emissions measured under these conditions are shown in the upper portion of Figure 2. Note that, at moderate O_2 concentrations (greater than 14%), the NOx emissions are highly dependent on injection timing. In previous work [1], we have described how the degree of initial mixing and the phasing of combustion influence the path of the combustion process in the $\phi - T$ plane. It is the variation in this path with SOI that influences the NOx emissions. Soot emissions will similarly be affected.

However, as the mixture becomes more dilute, the NOx emissions become insensitive to injection timing, indicating that both mixing processes and ambient temperature (within the range of adjustment achievable by changing the injection timing) no longer significantly influence the net NOx formation/destruction processes. Fundamentally, the path followed by a fuel element in the $\phi - T$ plane does not pass through the NOx formation regions regardless of the ambient temperature or the degree of initial premixing achieved [2].

In contrast, CO emissions (shown in the lower portion of Figure 2) are very low at moderate O_2 concentrations and, except at the most retarded injection timing, insensitive to SOI. At lower O_2 concentrations, significant variations in CO emissions (and, though not shown, fuel conversion efficiency) are seen as SOI is varied. CO emissions measured at high dilution conditions decrease with increasing ignition delay and with increasing injection pressure; consequently, we believe the dominant source of these emissions is the incomplete combustion of fuel which was not mixed with a sufficient quantity of air before cylinder volume expansion slowed reaction rates excessively. The large variation in CO emissions observed with low O_2 concentrations is thus a measure of the effectiveness of the overall mixing process, which in turn exerts a significant influence on the fuel conversion efficiency.

To better understand how improved mixing processes and more complete combustion can be promoted by the designer, we have also investigated the influence of flow swirl on the emissions of CO and combustion efficiency. Experimentally, CO emissions are observed to increase dramatically with increased swirl. We also observe experimentally that

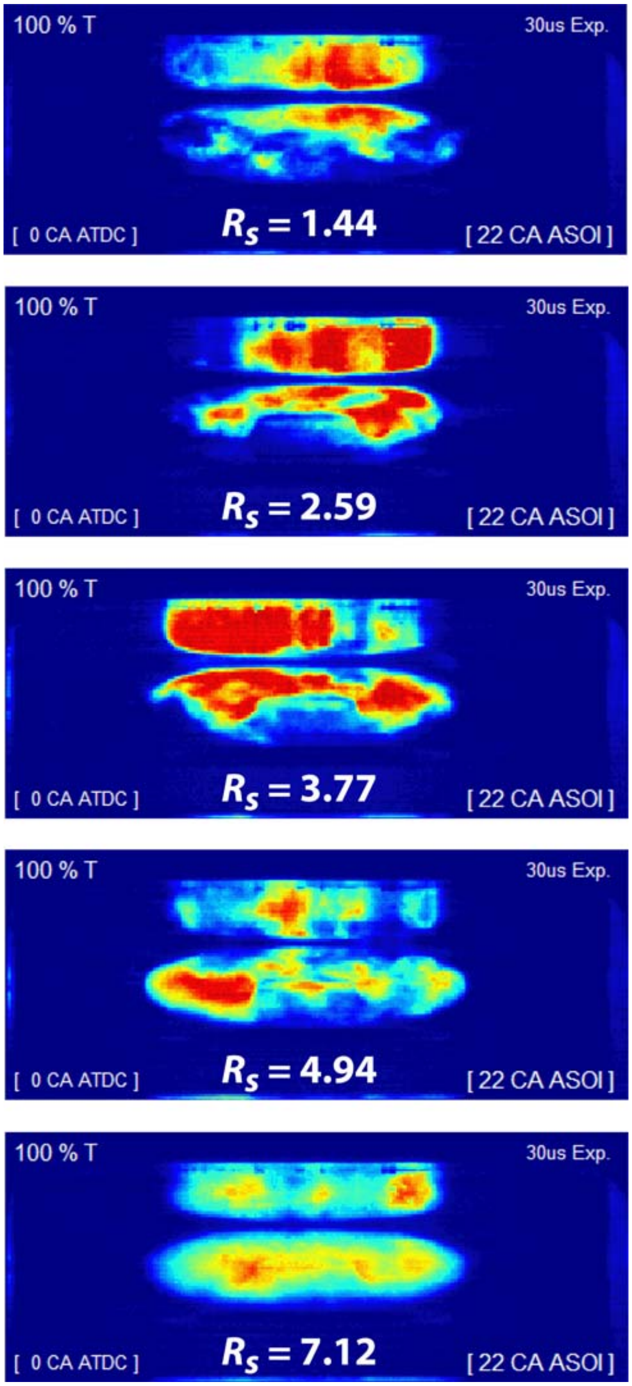

Figure 3. Spatial distribution of soot luminosity observed at various swirl ratios. Load = 3 bar, 1500 RPM, P_{inj} = 800 bar.

luminous emissions from soot originate from deeper in the bowl and are more uniformly dispersed within the bowl (Figure 3). Because soot and partially burned fuel are expected to be spatially co-located within the bowl, this observation suggests that higher

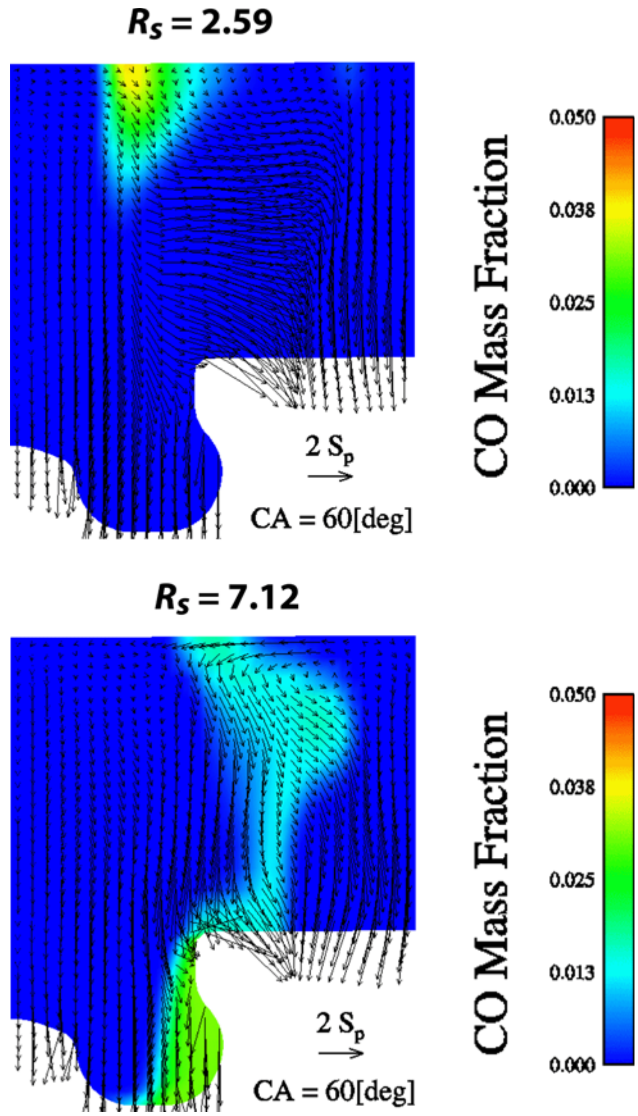

Figure 4. Numerical simulations indicate that the partially burned fuel (marked by CO) is trapped within the bowl at the higher swirl ratios.

levels of CO are likely to be found deep within the bowl for higher swirl ratios. Numerical simulations support this expectation. Not only is the CO predicted to be located deep in the bowl along the outer periphery, but it is found to be co-located with the high-swirl fluid within the bowl. Due to the high centrifugal forces acting on these fluid elements, the CO resists inward displacement and remains trapped within the bowl until well into the expansion stroke. In contrast—as illustrated by Figure 4—at lower swirl ratios the CO exits the bowl and is predominantly located within the squish volume, where it is more readily oxidized.

Conclusions

- At high dilution rates, the insensitivity of NOx and PM emissions to mixing processes and to injection timing is due to the low peak-temperature path of the combustion process in the $\phi - T$ plane.
- CO emissions (and fuel conversion efficiency) are strongly influenced by mixing processes at high dilution rates and stem predominantly from insufficient mixing with ambient fluid.
- A combination of emissions measurements, combustion imaging, and numerical simulation have shown that excessive swirl is detrimental to CO emissions due to trapping of partially burned fuel within the bowl.

FY 2005 Presentations

1. Miles PC, "Clean Diesels in the 21st Century...Don't Hold Your Breath!," Sandia National Laboratories R&D Focus Symposium, January 2005.
2. Choi D, "Comparison of Smokeless Rich Combustion and Late Injection MK-like Diesel Combustion," DOE OFCVT Advanced Engine Combustion Meeting, February 2005.
3. Miles PC, "Automotive Low-Temperature Diesel Combustion Research," DOE OFCVT Advanced Engine Combustion Peer Review, April 2005.
4. Miles PC, "Turbulent Flow Structure in Swirl-Supported, Direct-Injection Diesel Engines: Mean Flow Development, Turbulence Production, and Modeling," Korea Advanced Institute of Science and Technology, May 2005. *Invited Seminar*
5. Miles PC, "Low-Temperature, Highly-Premixed Diesel Combustion Strategies," 2005 KSAE Spring Meeting, Seoul, S. Korea, May 2005. *Keynote Address, also presented as an invited seminar at the Hyundai Motors R&D Center*
6. Miles PC, "The Role of Flow Structures and Mixing on Low-Temperature Diesel Combustion," 9th International Conference on Present and Future Engines for Automobiles, May/June 2005. *Invited Presentation*
7. Miles, PC, "The Role of Flow Structures and Mixing on Low-Temperature Diesel Combustion," Volvo Car Corporation, September 2005. *Invited Seminar*
8. Miles PC, "Full-field Flow Structure Measurements in an HSDI Diesel Engine," DOE OFCVT Advanced Engine Combustion Meeting, September 2005.

FY 2005 Publications

1. Tao F, Liu Y, RempelEwert BH, Foster DE, Reitz RD, Choi D, and Miles PC (2005) "Modeling the Effects of EGR and Injection Pressure on Soot Formation in a High-Speed Direct-Injection (HSDI) Diesel Engine Using a Multi-Step Phenomenological Soot Model," SAE Paper No. 2005-01-0121. Also presented at the 2005 SAE World Congress, April 2005. *Selected for inclusion in 2005 SAE Transactions*
2. Miles PC, Choi D, Kook S, Bergin MJ, Reitz RD (2005) "The Influence of Flow Structures and Mixing on Low-Temperature Diesel Combustion," Fifth Symposium Towards Clean Diesel Engines, June 2005. *Invited Paper and Keynote Lecture*
3. Kook S, Bae C, Miles PC, Choi D, and Pickett LM (2005) "The Influence of Charge Dilution and Injection Timing on Low-Temperature Diesel Combustion and Emissions," SAE Paper No. 2005-01-3837. Also presented at the 2005 SAE Fall Powertrain and Fluid Systems Conference, October 2005. *Selected for inclusion in 2005 SAE Transactions*
4. Choi D, Miles PC, Yun H, Reitz RD (2005) "A Parametric Study of Low-Temperature, Late-Injection Combustion in an HSDI Diesel Engine," *To be published in JSME Intl. Journal, Series B, November 2005*
5. Kook S, Bae C, Miles PC, Choi D, Bergin M, and 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," *Paper submitted to 2006 SAE World Congress*
6. Miles PC (2004) "Low-Temperature Automotive Diesel Combustion," DOE OFCVT Annual Report, 2004.

References

1. Miles PC, Choi D, Pickett LM, Singh IP, Henein N, RempelEwert BH, Yun H, Reitz RD (2004) "Rate-Limiting Processes in Late-Injection, Low-Temperature Diesel Combustion Regimes," Paper presented at Thermo- and Fluid-Dynamic Processes in Diesel Engines: THIESEL 2004. September 8-10, Valencia.
2. Kook S, Bae C, Miles PC, Choi D, and Pickett LM (2005) "The Influence of Charge Dilution and Injection Timing on Low-Temperature Diesel Combustion and Emissions," SAE Paper No. 2005-01-3837.

II.A.4 Characterization of Early-Injection, Low-Temperature Heavy-Duty Diesel Combustion Using Multiple Optical Diagnostics

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

DOE Technology Development Manager: Kevin Stork

Objectives

- The overall objective of this project is to advance the understanding of the spray, combustion, and emissions formation processes of low-temperature combustion (LTC) 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 2005 included:
  - Apply multiple laser/optical diagnostics to study spray, ignition, combustion, and pollutant formation processes for an early-injection LTC operating condition.
  - Begin to extend Sandia's conceptual model of conventional diesel combustion to many promising multi-mode LTC operating conditions, such as pilot/post/split injections, Modulated Kinetics (MK-type) combustion, Uniform Bulky Combustion System (UniBUS) combustion, and others.
  - Initiate computer modeling collaboration to improve predictive capabilities and enhance understanding of multiple LTC operating conditions. Also, model the influence of soot radiative cooling on nitrogen oxides (NOx) formation (previous year's experimental work).

Approach

- Operate a heavy-duty optical engine at an early-injection, LTC condition using conventional diesel engine hardware and a common-rail injector.
  - Reduce flame temperature with simulated exhaust gas recirculation (N_2 dilution), to 12.7% intake oxygen, by volume.
  - Advance fuel injection timing to increase pre-combustion mixing, until in-cylinder soot nearly ceases to form, to create a low-sooting condition on the "edge" of soot formation.
  - Set the longest possible fuel injection duration that does not cause damage to optical materials (maximum heat release rate of approximately 500 J/deg).
- Apply multiple optical/imaging diagnostics to reveal the in-cylinder processes that are responsible for the performance and emissions of LTC conditions.

Accomplishments

- Studied spray, combustion, and pollutant formation for a typical early-injection, LTC operating condition.
  - Use of multiple, simultaneous imaging diagnostics provided new understanding of in-cylinder processes.
- Expanded Sandia's conceptual model of diesel combustion to include early-injection, LTC operating conditions.
  - Included significant differences in spray penetration, liquid vaporization, spatial location of soot formation and combustion reactions.

- Initiated computer modeling collaboration with University of Wisconsin.
  - Will involve simulation of multiple LTC strategies.
  - 6-month student visit to Sandia to collect data for computer model validation.
- Examined relationship between soot radiation and NOx formation at pilot-injection conditions.
  - Radiative cooling from hot soot and compression heating of burned gases contribute to increased exhaust NOx with premixed burning.

Future Directions

- Apply optical diagnostics/analyze data for other LTC multiple/early/late injection schemes.
  - Late injection/MK-type combustion
  - UniBUS/split-main injection schemes
- Collaborate with University of Wisconsin to improve computer modeling of LTC strategies.
- Develop new diagnostic capabilities to study sources of unburned fuel for LTC schemes.
  - New post-doc, Thierry Lachaux, will lead this effort.
- Continue to expand the conceptual model of diesel combustion for LTC strategies.

Introduction

Recently, alternative mixing and combustion strategies for compression-ignition engines have been explored to satisfy future pollutant emissions targets. Compared to conventional diesel combustion, these new operational strategies generally employ increased pre-combustion fuel-air mixing and/or aggressive exhaust gas recirculation (EGR). One way to increase pre-combustion fuel-air mixing is by injecting the fuel early, well before top dead center (TDC) [1,2]. To achieve significant NOx reductions without EGR, fuel injection timing must be very early to provide enough time to create lean mixtures with sufficient dilution to reduce combustion temperatures. Unfortunately, depending on the injection timing and intake conditions, penetration of the liquid fuel with conventional hardware can be excessive, and liquid fuel may impinge on and wet cylinder walls and/or pistons surfaces, leading to poor mixing and associated emissions and oil dilution problems [2]. Also, for very early injection, ignition becomes decoupled from the timing of the injection event, leading to the same combustion phasing control problems experienced in homogeneous charge compression ignition (HCCI) engines. As an alternative, EGR may be introduced into the intake stream to provide the necessary dilution to reduce combustion temperatures and NOx formation. With EGR dilution, the premixing requirements are less demanding, so early-injection EGR-diluted operating conditions can tolerate injection closer to the combustion event, improving controllability and lessening liquid fuel impingement problems. While the closer proximity of fuel injection to the combustion event affords a measure of combustion-phasing control, EGR-diluted early-injection strategies can still suffer from carbon monoxide (CO) and unburned hydrocarbon (UHC) emissions problems, as well as load range limitations [1]. Better knowledge of the in-cylinder processes that affect emissions and limit the load range for such alternative diesel fuel injection schedules would aid the development of these strategies.

The focus of the FY 2005 effort on this project was to use multiple laser and imaging diagnostics to create a knowledge base for typical low-sooting, low-NOx, early-injection EGR-diluted diesel combustion conditions. This investigation, and all of the work on this project, is conducted in cooperation with our industrial partners (including Cummins, Caterpillar, Detroit Diesel, Daimler-Chrysler, 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 diesel 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, though it is not used in the current study. Rather, images are acquired through a window inserted in the cylinder head in place of one of the exhaust valves, which provides a view of the "squish" region above the piston. A portion of the piston bowl rim was cut out to allow one of the eight jets to penetrate all the way to the cylinder wall without striking the piston, providing a more fundamental "free-jet" structure for study. Windows inserted in the cylinder wall provide cross-optical access for the laser diagnostics. The engine was operated at a simulated EGR-diluted, low-load condition, with an inlet oxygen concentration of 12.7% and a load of about 4 bar indicated mean effective pressure. The fuel injection starts at about -22° after top dead center (ATDC).

In the current study, a suite of optical laser/imaging diagnostics are used: 1) laser elastic scatter to measure liquid fuel penetration, 2) ultraviolet (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 (PLIF) of hydroxyl radicals (OH) to study the flame structure and/or hot ignition/combustion, 5) imaging of natural broadband soot luminosity, and 6) planar laser-induced incandescence (PLII) of soot. These diagnostics are applied in various simultaneous pairings to study the instantaneous in-cylinder interactions between the measured phenomena. Space limitations do not allow these diagnostics to be fully described here, but the complete details may be found in previous publications [3,4].

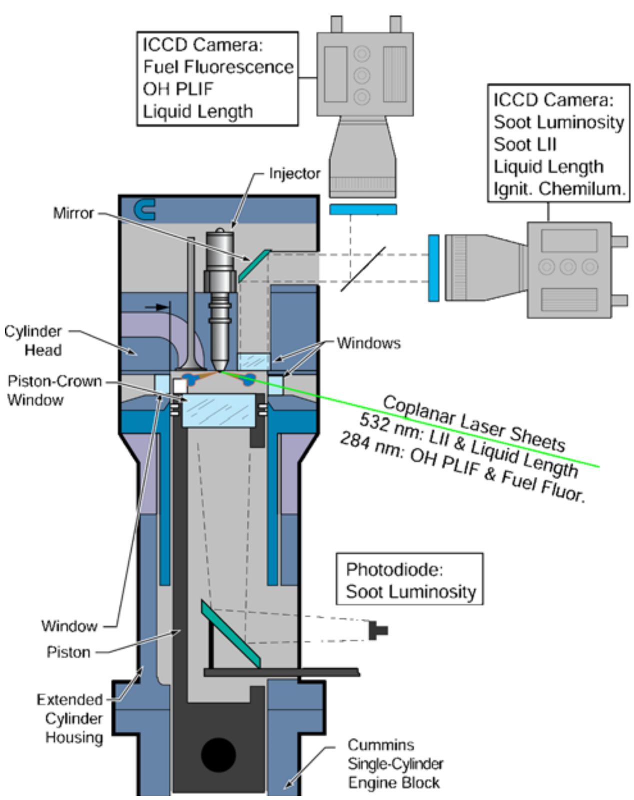

Figure 1. Schematic Diagram Showing Optical Engine and Laser/Imaging Diagnostics

Results

Shown in Figure 2 is a combined image of laser elastic scattering, which indicates liquid fuel penetration (in blue), along with simultaneous UV fuel fluorescence, which shows the perimeter of the vapor-fuel penetration (in green). The perspective of the camera is from above the piston, looking down through the window in place of one of the exhaust valves (see Figure 1 for reference). Only a portion of the complete combustion chamber is viewable through aperture provided by the window, as indicated by the white circle in Figure 2. The fuel injector is outside of the field of view, approximately 25 mm to the left of the edge of the round window (see scale in Figure 2). The large-radius arc represents the edge of the cylinder, and the smaller-radius dashed curve represents the edge of the

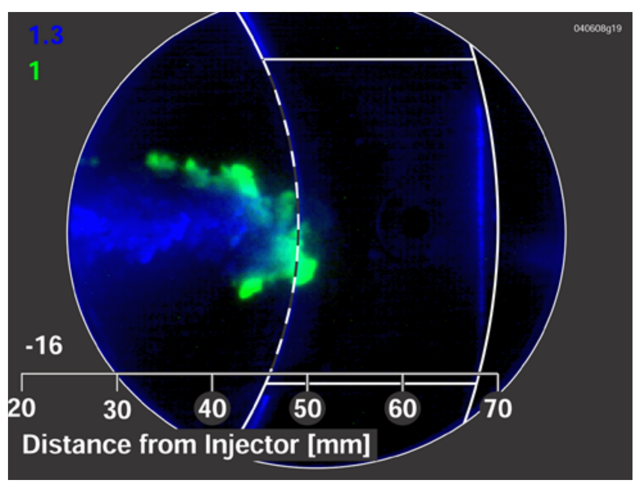

Figure 2. Elastic Scattering from Liquid Fuel (Blue) and Vapor Fuel Perimeter (Green), as Viewed Through the Cylinder Head Window

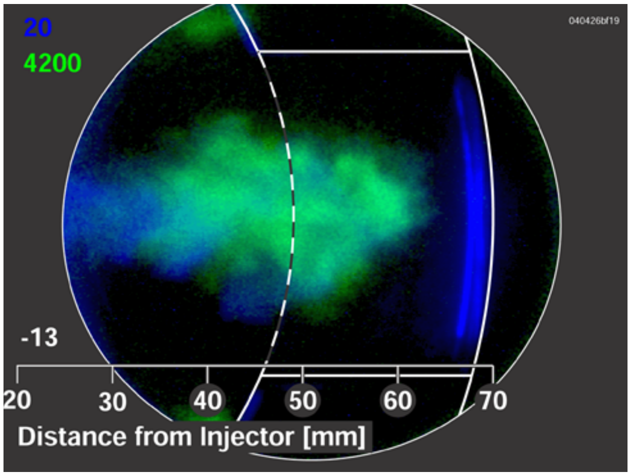

Figure 3. Elastic Scattering from Liquid Fuel (Blue) and Ignition Chemiluminescence (Green)

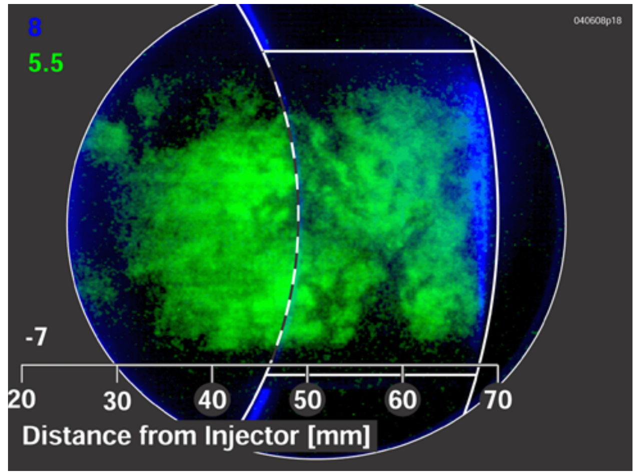

Figure 4. Elastic Scattering from Liquid Fuel (Blue) and OH PLIF (Green)

portion of the piston bowl that has been cut out, as described in the previous section. The image in Figure 2 was acquired at -16° ATDC, 6 crank angle degrees (CAD) after the start of injection. At that time, the tip of the jet has penetrated nearly to the position where the bowl rim would normally be (dashed curve). The liquid fuel (blue) penetrates up to 50 mm before vaporizing, which is approximately twice the penetration observed for conventional diesel conditions. Therefore, if a portion of the piston bowl rim had not been cut out, some liquid fuel likely would have impinged on the piston for this operating condition. Impingement of liquid fuel on in-cylinder surfaces is known to have a negative impact on UHC and soot emissions, and this condition is borderline for such effects.

A few CAD later, weak chemiluminescence, which is indicative of the first-stage ignition reactions, is observed in the downstream region of the jet, as shown in green in Figure 3. During the first-stage ignition, a small amount of chemical energy is liberated, raising temperatures to an estimated 900-1000 K [5]. The liquid fuel identified in Figure 2 rapidly vaporizes concurrent with the low-temperature ignition, and it is likely that the temperature rise associated with ignition contributes to the vaporization of the fuel.

Shortly after the first stage of ignition is complete, the second stage of ignition commences, with a rapid combustion of the premixed fuel and air. Shown in Figure 4 is a PLIF image of OH, which is produced primarily in near-stoichiometric regions.

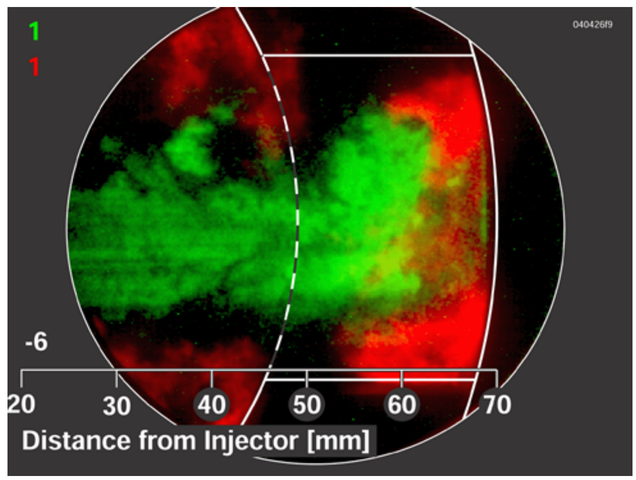

Figure 5. OH PLIF (Green) and Natural Luminosity of Soot (Red)

The presence of OH throughout the jet cross-section indicates that much of the jet is mixed to near-stoichiometric conditions, which should inhibit soot formation (see below). This is in contrast to conventional diesel combustion, for which second-stage ignition is generally fuel-rich, and OH resides primarily in a thin diffusion flame on the outer envelope of the jet [3]. Although in-cylinder NO was not directly measured, OH is an indirect indicator of regions that are favorable for NO formation. Thus, NO is expected to be formed throughout the jet cross-section, which is in contrast to conventional diesel combustion, for which NO forms in a thin envelope surrounding the jet [6].

Finally, Figure 5 shows a combined image of OH PLIF (in green) with an image of soot luminosity (in red). In this image, the regions containing OH and soot are generally spatially separate. As described above, OH is indicative of regions that are near-stoichiometric, where soot cannot form. Soot is known to form in rich regions, which are generally located near the head of the jet for this condition, especially in the roll-up region of the head vortex. This is in contrast to conventional diesel combustion conditions, for which soot is observed much farther upstream and throughout the rich cross-section of the jet [3].

Conclusions

The in-cylinder spray, combustion, and pollutant-formation processes for early-injection, LTC conditions are significantly different than for conventional diesel engine conditions. Sandia's conceptual model for diesel combustion has been extended to describe these observations. A pictorial summary of the main in-cylinder features of the extended model is shown in Figure 6, and the features are summarized below.

- Compared to conventional diesel combustion, the liquid fuel penetrates about twice as far into the combustion chamber before vaporizing, potentially wetting in-cylinder surfaces.

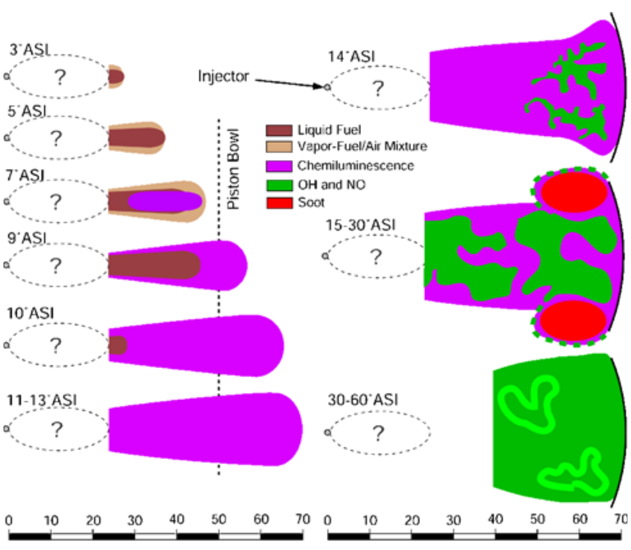

Figure 6. Schematic Representation of the Features in the Jet Cross-Section of the Extension of the Conceptual Model for Diesel Combustion to Early-Injection, Low-Temperature Conditions

- A distinct cool flame event overlaps the liquid fuel spray and likely contributes to rapid fuel vaporization.
- Rather than residing in a thin sheet on the periphery of the diesel jet, OH is found throughout the jet cross-section, indicating more complete fuel-air mixing and leaner mixtures in the jet interior.
- While LTC conditions produce much less NO than conventional diesel combustion, the spatial distribution of NO formation must also be very different. Rather than being formed near a thin diffusion flame on the jet periphery, NO is likely formed throughout the jet cross-section, in the same relatively hot, oxygen-available environments where OH exists.
- Rather than being formed upstream and throughout the jet cross-section, soot is formed much farther downstream, primarily in the fuel-rich head vortex, where mixing is slowest.

FY 2005 Publications/Presentations

1. "Multiple Simultaneous Diagnostic Imaging of Early-Injection Low-Temperature Combustion in a Heavy-Duty Diesel Engine," M. P. B. Musculus, Submitted to 2006 SAE International Congress and Exposition.
2. "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. P. B. Musculus, Submitted to 2006 SAE International Congress and Exposition.
3. "In-Cylinder Imaging of Conventional and Advanced, Low-Temperature Diesel Combustion," M. P. B. Musculus, 2005 Diesel Engine Emission Reduction Conference.
4. "Diagnostic Considerations for Optical Laser-Extinction Measurements of Soot in High-Pressure Transient Combustion Environments," M. Musculus and L. Pickett, Combustion and Flame; v. 141, no. 4, p. 371-391, June 2005.
5. "Measurements of the Influence of Soot Radiation on In-Cylinder Temperatures and Exhaust NOx in a Heavy-Duty Diesel Engine," M. Musculus, SAE Paper 2005-01-0925, accepted for publication in SAE Transactions.

6. "On the Correlation between NOx Emissions and the Diesel Premixed Burn," M. Musculus, SAE Paper 2004-01-1401, accepted for publication in SAE Transactions in 2005.
7. "Two-Stage Lagrangian Modeling of Soot Precursor Formation at Diesel Engine Operating Conditions," J. Caton, L. Pickett, M. Musculus, and A. Lutz, Fourth Joint Meeting of the US States Sections of the Combustion Institute, March 2005.
8. "Effects of Diesel Fuel Combustion-Modifier Additives on In-Cylinder Soot Formation in a Heavy-Duty DI Diesel Engine," M. Musculus and J. Dietz, SAND report 2005-0189.
9. "Measurements of the Influence of Soot Radiation on In-Cylinder Temperatures and Exhaust NOx in a Heavy-Duty Diesel Engine," Presented at 2005 SAE International Congress and Exposition.
10. "Potential for In-Cylinder NOx Reduction by Pilot Injection," Presented at Advanced Engine Combustion Working Group Meeting, January 2005.

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. Takeda, Y., Keiichi, N., and Keiichi N., "Emission Characteristics of Premixed Lean Diesel Combustion with Extremely Early Staged Fuel Injection," SAE Paper 961163, SAE Transactions, 105, No. 4, pp. 938-947, 1996.
3. Dec, J. E., "A Conceptual Model of D.I. Diesel Combustion Based on Laser-Sheet Imaging," SAE Paper 970873, SAE Transactions, 106, No. 3, pp. 1319-1348, 1997.
4. Musculus, M. P. B., "Multiple Simultaneous Optical Diagnostic Imaging of Early-Injection Low-Temperature Combustion in a Heavy-Duty Diesel Engine," submitted to SAE International Congress and Exposition, April 2006.
5. Westbrook, C. K., "Chemical Kinetics of Hydrocarbon Ignition in Practical Combustion Systems," Proc. of the Combust. Inst., 28, pp. 1563-1577, 2000.
6. Dec, J. E. and Canaan, R. E., "PLIF Imaging of NO Formation in a DI Diesel Engine," SAE Paper 980147, SAE Transactions, 107, No. 3, pp. 176-204, 1998.

II.A.5 Using Non-Traditional Diesel Fuels and Optical Diagnostics to Understand and Optimize In-Cylinder Processes

Charles J. Mueller (Primary Contact), Ansis Upatnieks[1], Glen C. Martin
Sandia National Laboratories
7011 East Ave., MS 9053
Livermore, CA 94550-9517

DOE Technology Development Manager: Kevin Stork

Objectives

- Determine whether fuel changes can enable an efficient, 2010-emissions-compliant combustion strategy that is not limited by difficulties with controlling ignition timing (at all loads) and with excessive pressure-rise rates (at high loads). Avoiding such difficulties has been challenging with homogeneous charge compression ignition (HCCI), the prevailing strategy to date.
- Introduce a parameter that accurately quantifies the proximity of a reactant mixture to its stoichiometric condition when fuel molecules contain oxidizer elements or when oxidizer molecules contain fuel elements. Such a parameter is important for understanding mixture stoichiometry effects on low-temperature combustion processes by quantifying mixture stoichiometry once reactions have begun; it is also important when oxygenated fuels are used.

Approach

- Upgrade experimental facility to enable the simulation of high exhaust gas recirculation (EGR) rates. Select a highly oxygenated fuel with a short ignition delay for testing. Conduct engine experiments with oxygenated fuel at high EGR rates to determine whether high-efficiency, emissions-compliant operation is achievable when employing a mixing-controlled combustion strategy.
- Develop a clear understanding of why conventional parameters for the quantification of mixture stoichiometry can be inaccurate when fuel molecules contain oxidizer elements or when oxidizer molecules contain fuel elements. Derive a parameter that properly quantifies mixture stoichiometry under these conditions. Show the relationship between the new parameter and existing parameters such as the equivalence ratio. Quantify the errors involved when the equivalence ratio is used outside of its range of validity.

Accomplishments

- Both objectives were achieved.
- Fuel changes were used to enable a high-efficiency (>44% indicated efficiency), 2010-emissions-compliant (<0.2 g/hp-hr NOx, <0.05 filter smoke number) combustion strategy where ignition timing is simply controlled by injection timing, and peak pressure-rise rates are lower than for conventional diesel combustion. Insight into the important in-cylinder processes was gained through the application of optical diagnostics. This accomplishment directly supports DOE objectives of identifying and enhancing the understanding of high-efficiency, clean combustion modes. The strategy could be an attractive alternative to HCCI, or it could be used at low- and high-load conditions with HCCI at moderate loads.
- A parameter was derived that accurately quantifies mixture stoichiometry after reactions have begun or when oxygenated fuels are used. This accomplishment directly supports the DOE objective of developing

[1]Currently employed at General Motors Research and Development Center in Warren, Michigan.

the fundamental science base required to understand and optimize high-efficiency, clean combustion modes.

Future Directions

- Determine the extent to which the high-efficiency, clean combustion alternative to HCCI identified in FY 2005 research activities can be achieved with more-traditional fuels such as #2 diesel, biodiesel, and Fischer-Tropsch paraffins.
- Continue investigations into the reasons for higher NOx emissions when biodiesel is used in conventional diesel combustion systems.
- Demonstrate the first successful application of two-photon laser-induced fluorescence detection of NO within an operating engine.

Introduction

Emissions regulations coming into force in 2010 for heavy-duty on-highway engines, combined with increasing concerns over the stability of imported petroleum supplies, are driving the development of cleaner, more efficient engine technologies. One promising approach to meeting these challenges without costly exhaust aftertreatment systems is low-temperature combustion (LTC). In LTC, 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 and/or decreasing in-cylinder temperatures below those required for soot formation. The fundamentals of LTC are not yet well understood, however, and this has been a barrier to it being successfully employed in production engines. For example, implementation of HCCI (the prevailing LTC strategy to date) has been slow due to challenges with controlling ignition timing and limiting peak pressure-rise rates at high loads. It is known that fuel properties, fuel/oxidizer mixture preparation, and exhaust gas recirculation (EGR) level are important, but it is not yet known how to use these parameters to optimally employ LTC in engine applications.

Work in our laboratory has been focused on providing experimental and theoretical results to support the development of a fundamental science base of fuel and mixture-preparation effects on LTC to 1) employ LTC operating strategies with improved performance characteristics, 2) determine the extent to which fuel changes can facilitate operation in LTC regimes, and 3) provide theoretical tools necessary to better understand the effects of mixture stoichiometry on LTC processes.

Approach

The approach to developing the science base of fuel and mixture-preparation effects on LTC includes both experimental and theoretical components. The experimental work has been 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 theoretical work has concentrated on understanding mixture stoichiometry under non-trivial conditions, such as once reactions have begun or when oxygenated fuels are used, so that this important LTC control parameter can be properly quantified and its effects understood.

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. 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, makes the SCORE a versatile instrument for studying the

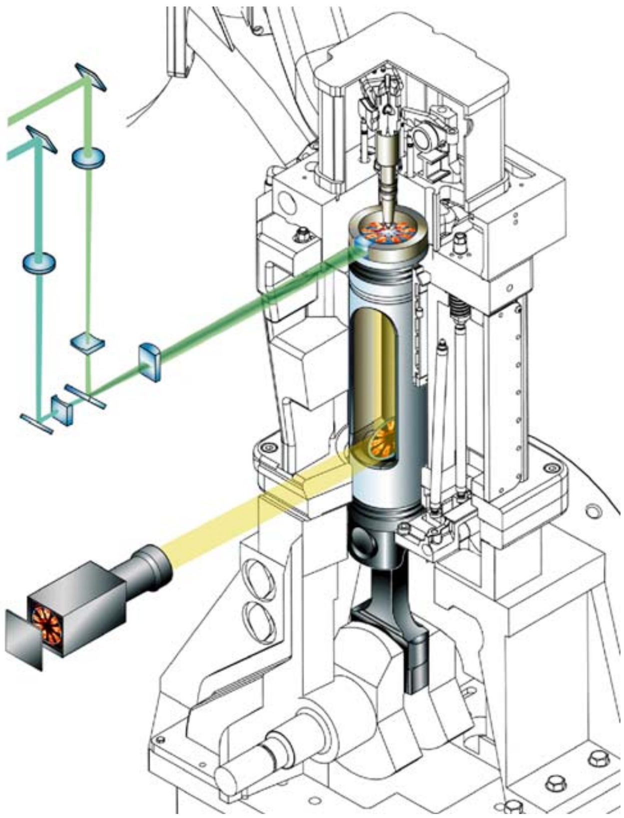

Figure 1. Schematic of Sandia Compression-Ignition Optical Research Engine (SCORE)

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

details of fuel effects on in-cylinder processes and corresponding impacts on emissions. Optical-engine data also complement measurements from multi-cylinder production engines tested over standard driving cycles, and can be used to verify the accuracy of computational fluid dynamics models.

Results

Experimental study of new LTC strategy – As described above, a primary objective of FY 2005 activities was to study mixing-controlled reaction under high-EGR conditions as a means to achieve high-efficiency, clean combustion while avoiding the control problems and excessive pressure-rise rates that can occur with HCCI. We have called this strategy dilute clean diesel combustion (DCDC). DCDC can be viewed as traditional diese combustion that has been shifted into the LTC regime by the use of high EGR levels, and in this way it is similar to "smokeless rich combustion" [2,3], but DCDC also uses a "clean" fuel to suppress PM emissions. The control problems of HCCI are avoided because with DCDC, as with traditional diesel operation, combustion phasing is controlled by fuel-injection timing. Figure 2 shows results from DCDC experiments that were run at steady-state conditions using neat diethylene glycol diethyl ether (DGE), a short-ignition-delay, oxygenated fuel. Emissions are plotted as a function of the mole fraction of oxygen in the intake charge. NOx emissions are below the 2010 limit for intake oxygen mole fractions less than approximately 14%, and smoke emissions are well below 0.05 filter smoke number (FSN) over the range of oxygen concentrations in the study. High fuel-conversion efficiency (defined as the product of thermal efficiency and combustion efficiency [4]) is maintained at intake oxygen concentrations as low as

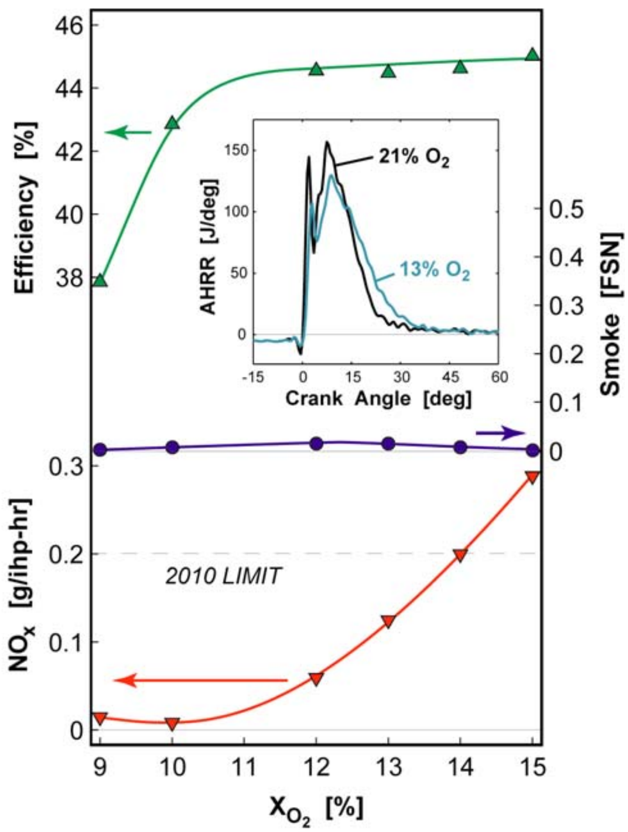

Figure 2. Engine-out NOx and smoke emissions, indicated fuel-conversion efficiency, and apparent heat-release rate data (inset) for DCDC operation. Data obtained at 1200 rpm and an engine load of 7.0 bar indicated mean effective pressure, for intake temperature and pressure of 25°C and 2.23 bar (abs.), respectively. EGR was simulated with nitrogen gas.

approximately 11%, indicating that there is a substantial window for desirable DCDC operation. The inset shows that heat-release rates are even lower under DCDC conditions than for traditional diesel combustion, which should lead to quieter engine operation. Longer flame lift-off lengths and more diffuse combustion are observed as dilution level increases (see Figure 3). The total natural luminosity signal intensity drops by two orders of magnitude as the intake oxygen concentration is lowered from 21% to 9%, indicating significant decreases in soot volume fraction and/or temperature under DCDC operation. Results have been acquired at up to 18 bar indicated mean effective pressure, which represents 3/4-load operation. See Refs. [5,6] for further details about DCDC operation.

Theoretical study of quantification of mixture stoichiometry – A parameter called the oxygen equivalence ratio, denoted ϕ_Ω, was derived to accurately quantify mixture stoichiometry in situations where fuel molecules contain oxidizer elements or oxidizer molecules contain fuel elements. The oxygen equivalence ratio is defined as the amount of oxygen (moles or mass) required to convert all fuel elements to saturated stoichiometric products (SSPs), divided by the amount of oxygen present in the given mixture. The oxygen equivalence ratio can be expressed mathematically as:

$$\phi_\Omega = \frac{2n_C + \frac{1}{2}n_H}{n_O}$$

where n_C, n_H, and n_O are the numbers of carbon, hydrogen, and oxygen atoms, respectively. An SSP is defined as a product species with no net charge, each of whose constituent atoms has a saturated (i.e., filled or closed-shell) valence orbital. Atoms that are initially bound in SSPs in the reactants are neglected in the calculation of the oxygen equivalence ratio. The oxygen equivalence ratio is a valid measure of mixture stoichiometry in any mixture for which the SSPs are CO_2, H_2O, N_2, and/or noble gases. See Ref. [7] for details about the oxygen equivalence ratio.

Conclusions

- Fuel changes were found to enable a high-efficiency (>44% indicated fuel-conversion efficiency), 2010-emissions-compliant (<0.2 g/hp-hr NOx, <0.05 filter smoke number) combustion strategy where ignition timing is simply controlled by injection timing, and peak pressure-rise rates are lower than for conventional diesel combustion. Insight into the important in-cylinder processes was gained through the application of optical diagnostics. This accomplishment directly supports DOE objectives of identifying and enhancing the understanding of fuel effects on high-efficiency, clean combustion modes.
- A parameter was derived that accurately quantifies mixture stoichiometry after reactions have begun or when oxygenated fuels are used.

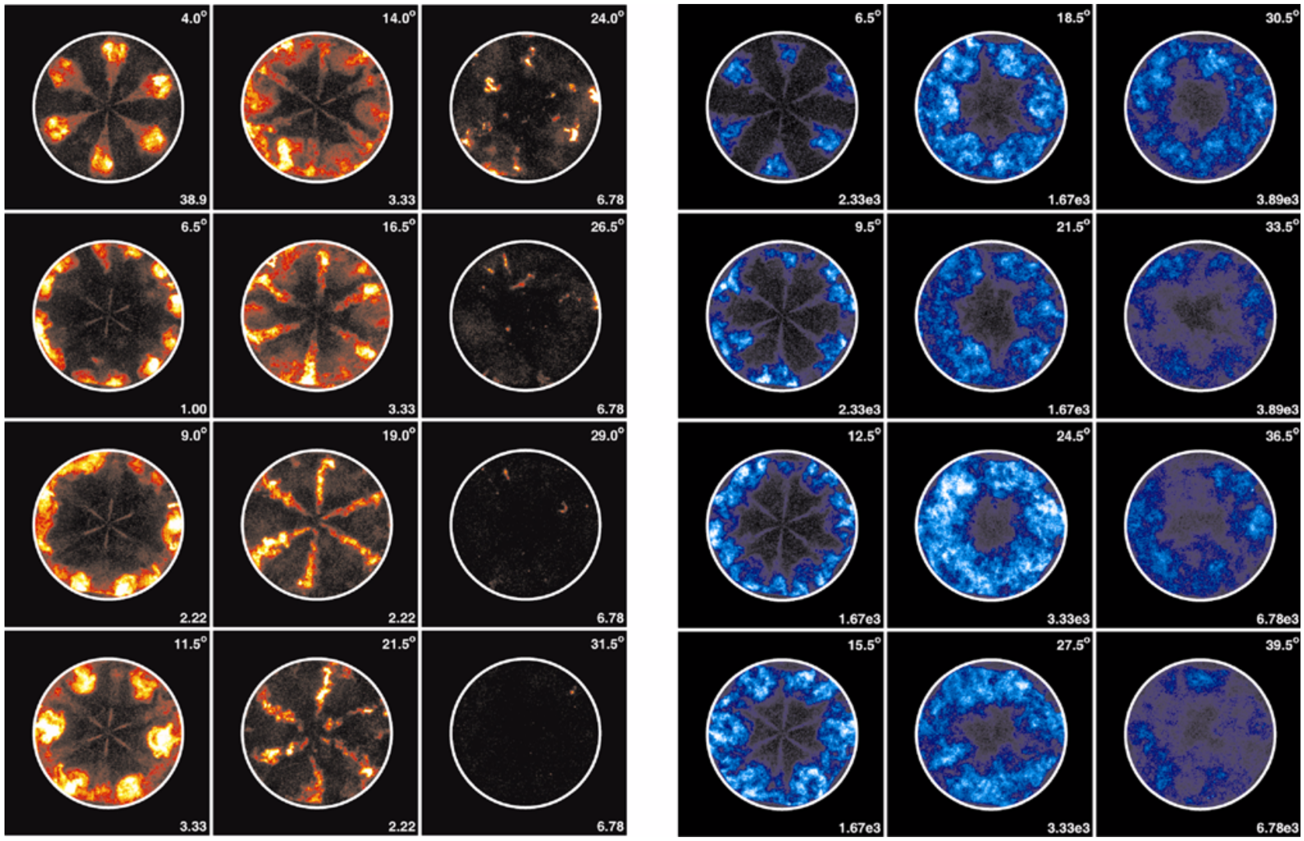

Figure 3. Natural luminosity images for combustion at (left) 21% oxygen (i.e., undiluted) and (right) 9% oxygen at same speed, load, and intake conditions as Figure 2. Numbers in upper- and lower-right corners of each image indicate crank angle at which image was acquired and camera gain, respectively. Higher camera gain = fainter luminosity signal. Images of undiluted combustion (left) show high signal levels due to soot incandescence; images for dilute case (right) show more diffuse combustion and are typically 1000 times dimmer, indicating that hot soot is no longer present.

This accomplishment directly supports the DOE objective of developing the fundamental science base of fuel and mixture-preparation effects required to understand and optimize high-efficiency, clean combustion modes.

Special Recognitions & Awards

1. Society of Automotive Engineers ***Arch T. Colwell Merit Award***, for paper entitled “Effects of Oxygenates on Soot Processes in DI Diesel Engines: Experiments and Numerical Simulations,” *SAE Technical Paper 2003-01-1791*. This was one of 11 papers honored in 2004 for being most innovative and original out of approximately 2,500 papers published during the preceding year.
2. Society of Automotive Engineers ***Lloyd L. Withrow Distinguished Speaker Award***. This was one of 8 such awards presented in 2005 to recognize individuals who have received SAE’s Oral Presentation Award more than twice.

FY 2005 Publications

1. 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*.
2. 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*.
3. 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*.

4. 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 Transactions*, Vol. 113, Sect. 3, 2004.
5. Buchholz, B.A., Mueller, C.J., Upatnieks, A., Martin, G.C., Pitz, W.J., and Westbrook, C.K., "Using Carbon-14 Isotope Tracing to Investigate Molecular Structure Effects of the Oxygenate Dibutyl Maleate on Soot Emissions from a DI Diesel Engine," *SAE Transactions*, Vol. 113, Sect. 4, 2004.
6. Buchholz, B.A., Mueller, C.J., Martin, G.C., Cheng, A.S., Dibble, R.W., and Frantz, B.R., "Tracing Fuel Component Carbon in the Emissions from Diesel Engines," *Nuc. Inst. and Meth. Phys. B*, Vol. 223-224, pp. 837-841, 2004.
7. Mueller, C.J., "In-Cylinder Processes under Early Direct-Injection Diesel HCCI Conditions," *Proc. of DOE Advanced Engine Combustion, Emission Control, and Fuels Program Review*, Argonne National Laboratory, Argonne, IL, 2004.
8. Martin, G.C., Mueller, C.J., and Lee, C.F., "Two-Photon Laser-Induced Fluorescence of Nitric Oxide in a Diesel Engine," submitted for presentation at SAE World Congress, 2006.
9. Martin, G.C., Mueller, C.J., and Lee, C.F., "Two-Photon NO LIF Measurements in a Diesel Engine," submitted to *Applied Optics*, 2005.
10. Cheng, A.S., Upatnieks, A., and Mueller, C.J., "Investigation of the Impact of Biodiesel Fueling on NOx Emissions Using an Optical DI Diesel Engine," submitted to *International Journal of Engine Research*, 2005.

FY 2005 Presentations

1. Mueller, C.J., "Dilute Clean Diesel Combustion Achieves Low Emissions and High Efficiency While Avoiding Control Problems of HCCI," *Caterpillar 10/4 Tech Team Meeting*, Mossville, IL (September 27, 2005).
2. Mueller, C.J., "Dilute Clean Diesel Combustion Achieves Low Emissions and High Efficiency While Avoiding Control Problems of HCCI," *Advanced Engine Combustion Working Group Meeting*, Detroit, MI (September 13, 2005).
3. Mueller, C.J., "Dilute Clean Diesel Combustion Achieves Low Emissions and High Efficiency While Avoiding Control Problems of HCCI," *11th Annual Diesel Engine Emissions Reduction (DEER) Conference*, Chicago, IL (August 22, 2005).
4. Mueller, C.J., "Emerging Trends in Engine Combustion," invited plenary address at *Oil-Sands Chemistry and Engine Emissions Workshop*, Edmonton, Canada (June 6, 2005).
5. Mueller, C.J., "Optical-Engine Studies of Fuel Effects on Low-Temperature Combustion Processes: Sandia Diagnostics and Activities," *Caterpillar/ExxonMobil/Sandia HECC Project Teleconference* (May 19, 2005).
6. Upatnieks, A., "The Influence of Charge-Gas Dilution and Temperature on DI Diesel Combustion Processes Using a Short-Ignition-Delay, Oxygenated Fuel," *SAE Spring 2005 Fuels and Lubricants Meeting*, Rio de Janeiro, Brazil (May 11, 2005).
7. Mueller, C.J., "Engine Combustion Research at the CRF," *Sandia Energy PDS Meeting*, Livermore, CA (May 4, 2005).
8. Upatnieks, A., "Clean, Controlled DI Diesel Combustion Using Dilute, Cool Charge Gas and a Short-Ignition-Delay, Oxygenated Fuel," *SAE 2006 World Congress*, Detroit, MI (April 11, 2005).
9. Mueller, C.J., "Optical-Engine Studies of Fuel Effects on Low-Temperature and CIDI Combustion Processes," *DOE Fuels Technology R&D Program Review*, Golden, CO (March 8, 2005).
10. Mueller, C.J., "The Quantification of Mixture Stoichiometry When Fuel Molecules Contain Oxidizer Elements or Oxidizer Molecules Contain Fuel Elements," *HCCI University Working Group Meeting*, Livermore, CA (February 3, 2005).
11. Mueller, C.J., "An Investigation into Causes of Increased NOx Emissions with Biodiesel Fueling," *Advanced Engine Combustion Working Group Meeting*, Livermore, CA (February 1, 2005).
12. Upatnieks, A., "Dilute Clean Diesel Combustion Using a Short-Ignition-Delay, Oxygenated Fuel," *Advanced Engine Combustion Working Group Meeting*, Livermore, CA (February 1, 2005).

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. Akihama, K., Takatori, Y., Inagaki, K., Sasaki, S., and Dean, A.M., "Mechanism of the Smokeless Rich Diesel Combustion by Reducing Temperature," SAE Paper 2001-01-0655, *SAE Trans.*, Vol. 110, Sect. 3, 2001.

3. Pickett, L.M. and Siebers, D.L., "Non-Sooting, Low Flame Temperature Mixing-Controlled DI Diesel Combustion," SAE Paper 2004-01-1399, *SAE Trans.*, Vol. 113, Sect. 4, 2004.
4. Heywood, J.B., Internal Combustion Engine Fundamentals, McGraw-Hill, New York, 1988, p. 52.
5. 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.
6. 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.
7. 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.

II.A.6 Soot Formation under High-EGR, LTC Conditions

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

DOE Technology Development Manager: Kevin Stork

Objectives

- Investigate soot formation dependencies on equivalence ratios and temperature for diesel fuel sprays.
- Determine how the use of extensive exhaust gas recirculation (EGR) (causing reduction in ambient oxygen levels to 10-15%) affects soot formation by performing quantitative *in-situ* measurements of soot.
- Identify factors that affect the low-temperature limit for soot formation.

Approach

- Utilize advanced optical diagnostics coupled with a unique optically accessible diesel combustion simulation facility (DCSF) to conduct these investigations.
- Systematically adjust EGR level (ambient gas oxygen concentration) over an extensive range, including conditions where NOx formation is low enough to meet 2010 emissions.
- Perform quantitative soot and combustion measurements within reacting diesel fuel sprays at well-controlled conditions.

Accomplishments

- Demonstrated that the low-temperature limit for soot formation depends upon mixing parameters, rather than only temperature and equivalence ratio.
- Completed a quantitative database showing the effect of EGR on soot in reacting diesel fuel jets. Results show that soot volume fraction decreases with decreasing ambient oxygen concentration, but the total soot in the jet cross-section increases and then decreases to zero as the ambient oxygen concentration decreases from 21% to 8%. The trend is caused by competition between soot formation rates and increasing residence time for soot formation.

Future Directions

- Determine how combustion of pre-injection fuel affects combustion and soot formation of a second main-injection.
- Investigate the effect of intake air pressure boost and EGR cooling on soot formation at high-EGR, low-temperature combustion (LTC) conditions.
- Perform direct measurements of mixing (equivalence ratio) in diesel fuel jets.

Introduction

This year we have investigated soot formation at low-temperature diesel combustion conditions using extensive EGR. It has been shown that 2010 NOx emission regulations for heavy-duty diesel engines can be met when flame temperatures are lowered by using EGR levels causing a reduction in ambient oxygen levels to approximately 12-15%. However, particulate matter (PM) emissions generally rise, especially at higher engine load. Other studies have shown that PM emissions begin to decrease when the

EGR level is increased further (8-13% ambient oxygen) [1]. A detailed understanding of soot formation at these conditions could therefore lead to a simultaneous reduction in soot and NOx emissions. Accordingly, this year we have performed quantitative measurements of the soot formed *in-situ* in reacting diesel fuel sprays while the EGR level was systematically varied.

Approach

The research was performed in the DCSF using a common-rail diesel fuel injector. Figure 1 shows a picture of the DCSF in operation. The experimental ambient and injector conditions are carefully controlled in this facility, thereby facilitating investigation of the effects of fundamental parameters on diesel combustion. The DCSF also has full optical access, allowing advanced soot and combustion measurements to be performed. Quantitative measurements of in-situ soot in n-heptane and #2 diesel fuel jets were made by using laser extinction and planar laser-induced incandescence (PLII) [2].

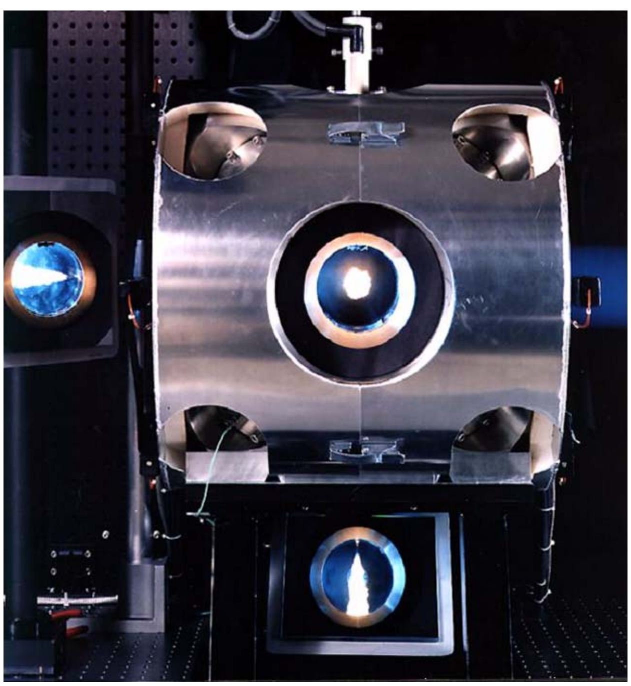

Figure 1. Photograph of the DCSF in operation, demonstrating the optical access to the diesel spray. The bright spot in the center of the front window is a burning diesel spray penetrating toward the viewer. Mirrors at 45° next to the bottom and left-side windows show side views of the burning spray.

Results

Composite-average PLII images for n-heptane with the same ambient temperature and density and the same injector conditions are shown in Figure 2. The ambient oxygen concentration is shown on the upper left corner and the camera gain relative to the 21% oxygen condition is shown on the lower left corner of each image. The lift-off location obtained from OH chemiluminescence images is also shown on the PLII images as a reference. The image shown for each EGR condition was obtained by averaging images obtained from multiple fuel injection events. The average soot field map for the different ambient oxygen concentrations is represented in the PLII images. For the 8% O_2 condition, there is no PLII signal, suggesting the absence of any soot formation even though the camera gain was set to its maximum at this condition. The increasing camera gain

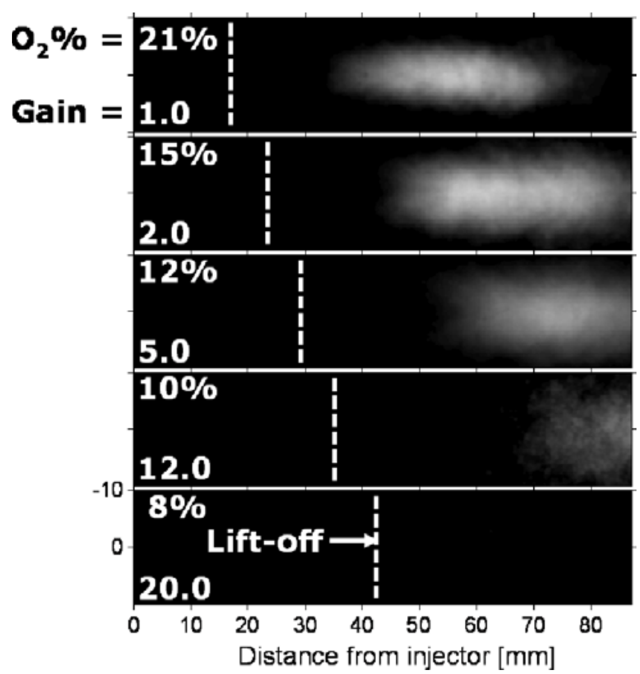

Figure 2. Composite-average PLII images for n-heptane at different EGR conditions. The lift-off location derived from the OH chemiluminescence images is shown as a vertical dashed line. Camera gain is at the lower left. 1000 K ambient temperature, 14.8 kg/m^3 ambient density, 1500 bar orifice pressure drop, 100 μm nozzle.

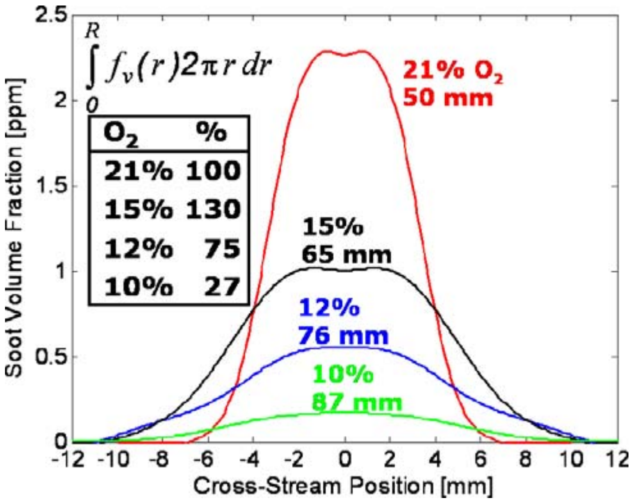

Figure 3. Radial soot volume fraction (f_v) profiles for n-heptane at different EGR conditions. The axial location where the measurements were made is also shown on the figure. The total soot estimated in the jet cross-section is shown in the legend.

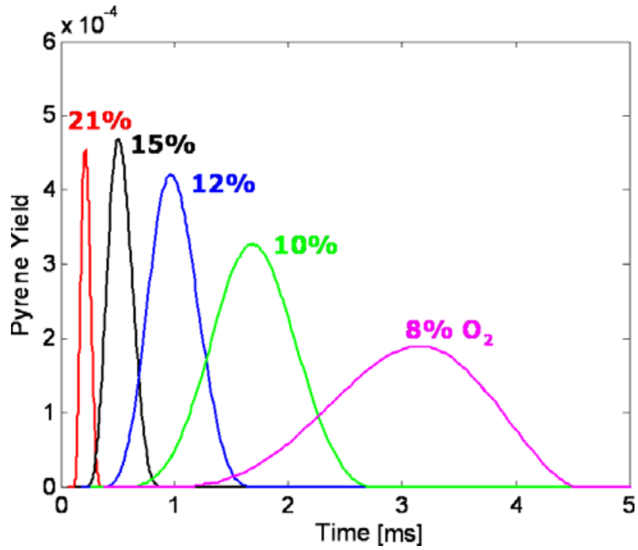

Figure 4. The pyrene yield prediction from the TSL model for n-heptane at an ambient temperature of 1000 K and different ambient oxygen concentrations.

indicates that the soot volume fraction (f_v) decreases with decreasing ambient oxygen concentration. The regions of soot formation are effectively "stretched out" to longer axial and radial distances from the injector with increasing EGR, according to the dilution in ambient oxygen.

Although the soot volume fraction decreases with increasing EGR, at the same time, the width of the sooting region is longer, and it is unknown if the total soot increases or decreases. Radial extinction measurements were therefore performed near the peak location in the axial soot profiles to measure the total soot in the jet cross-section. These measurements were used to obtain the soot volume fraction radial profiles. Once the radial soot profiles are known, the integral $\int f_v(r)2\pi r dr$ will be proportional to the total soot in the jet cross-section. Figure 3 shows soot volume fraction distributions. The integral over the jet cross-section is given in the legend. The total soot in the jet cross-section increases initially, reaches a maximum at 15% oxygen, and then decreases to zero as the oxygen concentration decreases to 8%.

For interpretation, we have exercised the two-stage Lagrangian (TSL) reacting-jet model for n-heptane combustion [3]. The TSL model employs a diffusion flame reactor and homogenous core reactor with entrainment rates determined by empirical correlations. Detailed chemical kinetics is used for predictions of n-heptane oxidation and soot precursor formation up to seven-ring polycyclic aromatic hydrocarbons (PAHs). Figure 4 shows TSL predictions of pyrene yield, a four-ring PAH assumed to closely represent soot. The pyrene yield of the core reactor is plotted as a function of time. For each oxygen concentration, the pyrene yield increases, reaches a maximum, and then decreases, corresponding to a time when regions of the fuel jet are dominated by formation or oxidation of soot precursors, respectively. The duration of soot precursor formation increases with decreasing oxygen. However, the time required to mix with ambient oxygen to promote soot precursor oxidation also increases. This increased time is related to the increasing $(A/F)_{st}$ with decreasing oxygen concentration, requiring more ambient mass to be mixed into the jet to complete combustion. The time needed to accomplish this mixing increases, and the net result is that the residence time for soot formation also increases. The entrainment rate of ambient oxygen therefore has a strong effect on the soot history.

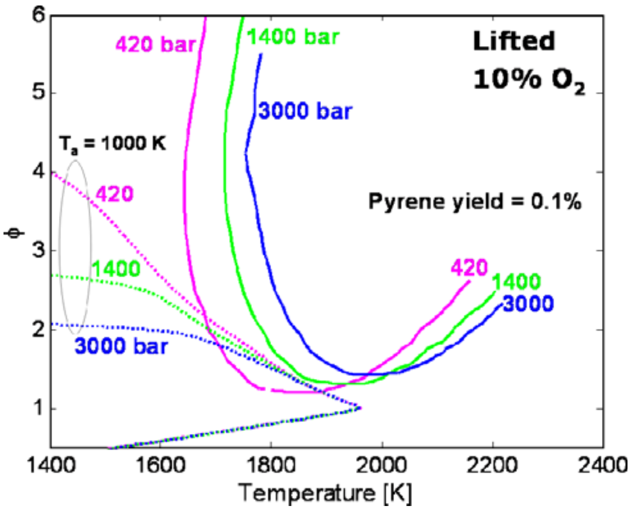

Figure 5. Comparison of 0.1% pyrene yield contours for different injection pressures. Dotted lines are ϕ-T curves for an ambient gas temperature of 1000 K.

For high ambient oxygen concentrations, the high combustion temperatures promote fast soot formation, but the rapid oxygen entrainment quickly impedes soot formation and consumes soot formed upstream. For low oxygen concentrations, the soot formation rate is low because of the low combustion temperature, but the low oxygen entrainment rate means that there is more residence time for soot formation. The variation in ambient oxygen concentration shows how these competing processes affect the total soot. The longer residence time compensates for the slower soot formation rate at 15% oxygen, but further reductions in ambient oxygen concentration eventually lower the total soot formed. The TSL predictions and experimental soot measurements are consistent with engine-out PM measurements in that soot increases, decreases, and then goes to zero with increasing EGR [1]. However, engine-out PM measurements offer little information about the *in-situ* soot formation processes when using EGR.

Other factors that affect the limits of soot formation have been explored at very high EGR levels. Figure 5 shows TSL predictions of the equivalence ratio-temperature limit of soot formation (solid line) for three different injection pressures and an ambient oxygen concentration of 10% [3]. The dashed line is the ϕ-T path for a fuel jet at an ambient temperature of 1000 K. Note that the 1400-bar and 3000-bar paths do not intersect the ϕ-T boundary of soot formation, while the 420-bar path intersects the soot formation region. Verified experimentally, the results show that the ϕ-T boundary of soot formation depends on factors other than ϕ and T. These findings are significant because it has become common to represent soot formation limits in terms of only ϕ and T.

Conclusions

- An extensive, quantitative database showing the effect of EGR on soot in reacting diesel fuel jets has been completed. The database, from 21% to 8% ambient oxygen, is unique in the world and critical to engine combustion because little is know about PM emissions in the 10-13% ambient oxygen range required for low-NOx production. The research shows that soot volume fraction decreases with decreasing ambient oxygen concentration, but the total soot in the jet cross-section increases and then decreases to zero as the oxygen concentration decreases from 21% to 8%. The trend is caused by competition between soot formation rates and increasing residence time for soot formation.
- We have also demonstrated that the low-temperature limit for soot formation depends upon mixing parameters, rather than only temperature and equivalence ratio. For example, at the same T and ϕ, our experiments show that fuel jets with fast mixing rates, produced by high injection pressure, have no soot formation while low-injection-pressure fuel jets do form soot.

Awards

1. 2003 SAE Russell S. Springer Award for best technical paper by a lead-author 36 years of age or younger. (Paper 2003-01-3080). One award given each year out of approximately 2700 SAE papers.
2. 2003 SAE Arch T. Colwell Merit Award for outstanding technical paper. 11 awards given out of 2700 papers. (For paper 2003-01-1791 by Mueller, Pitz, Pickett, Martin, Siebers, and Westbrook.)

FY 2005 Presentations

1. Pickett, L.M., "Soot Formation at Low Flame Temperature Diesel Operating Conditions," 9th International Conference on Present and Future Engines for Automobiles, San Antonio, TX, June 2005.
2. Pickett, L.M., "Soot Formation at Low Flame Temperature Diesel Operating Conditions," Engine Research Center Seminar Series, Madison, WI, November 2004.
3. Pickett, L.M., "Soot Formation at High-EGR, LTC Conditions," DOE Advanced Combustion Engine Annual Review, Chicago, IL, April 2005.
4. Pickett, L.M., López, J.J., "Jet-Wall Interaction Effects on Diesel Combustion and Soot Formation," SAE World Congress, Detroit, MI, April 2005.
5. López, J.J., and Pickett, L.M., "Jet/Wall Interaction Effects on Soot Formation in a Diesel Fuel Jet," COMODIA 2004, Yokohama, Japan, August 2-5.
6. Pickett, L.M., "Low Flame Temperature Limits for Mixing-Controlled Diesel Combustion," 30th International Symposium on Combustion, Chicago, IL, July 2004.

FY 2005 Publications

1. 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," submitted to International Journal of Engine Research, 2005.
2. Pickett, L.M., and Siebers, D.L. "Soot Formation in Diesel Fuel Jets near the Lift-off Length," accepted to International Journal of Engine Research, 2005.
3. 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.
4. Idicheria, C.A., and Pickett, L.M. "Soot Formation in Diesel Combustion under High EGR Conditions," SAE Paper 2005-01-3834, 2005.
5. 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.
6. Pickett, L.M., and López, J.J. "Jet-Wall Interaction Effects on Diesel Combustion and Soot Formation," SAE World Congress, 2005-01-0921.
7. Caton, J.A., Pickett, L.M., Musculus, M.P.B., Lutz, A.E. "Two-Stage Lagrangian Modeling of Soot Precursor Formation at Diesel Engine Operating Conditions," 4th Joint Meeting of the US States Sections of the Combustion Institute, Philadelphia, PA, March 21-23, 2005.
8. Musculus, M.P.B., and Pickett, L.M. "Diagnostic Considerations for Optical Laser-Extinction Measurements of Soot in High-Pressure Transient Combustion Environments," Combustion and Flame 141(4):371-391, 2005.
9. Pickett, L.M. "Low Flame Temperature Limits for Mixing-Controlled Diesel Combustion," Proceedings of the Combustion Institute, 30:2727-2735, 2005.
10. López, J.J., and Pickett, L.M. "Jet/Wall Interaction Effects on Soot Formation in a Diesel Fuel Jet," COMODIA 2004, Yokohama, Japan, August 2-5.
11. Siebers, D.L., and Pickett, L.M. "Aspects of Soot Formation in Diesel Fuel Jets," THIESEL 2004 Conference on Thermo- and Fluid-Dynamic Processes in Diesel Engines, Valencia, Spain, 2004.
12. Miles, P.C., Choi, D., Pickett, L.M., Singh, I.P., Henein, N., RempelEwert, B.A., Yun, H., and Reitz, R.D. "Rate-Limiting Processes in Late-Injection, Low-Temperature Diesel Combustion Regimes," THIESEL 2004 Conference on Thermo- and Fluid-Dynamic Processes in Diesel Engines, Valencia, Spain, 2004.

References

1. Akihama, K., Takatori, Y., Inagaki, K., Sasaki, S., Dean, A.M. "Mechanism of Smokeless Rich Diesel Combustion by Reducing Temperature," SAE Paper 2001-01-0655, 2001.
2. Idicheria, C.A., and Pickett, L.M. "Soot Formation in Diesel Combustion under High-EGR Conditions," SAE Paper 2005-01-3834, 2005.
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," submitted to International Journal of Engine Research, 2005.

II.A.7 Achieving High-Efficiency Clean Combustion (HECC) in Diesel Engines

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

DOE Technology Development Manager: Kevin Stork

Objectives

- Investigate methods of expanding the HECC speed/load operation envelope in a light-duty multi-cylinder diesel engine.
- Explore potential to transition between normal and HECC operation as well as navigate through HECC space.
- Improve the understanding of HECC operation through detailed thermodynamic analysis.

Approach

- Explore methods and strategies for managing HECC operation in a multi-cylinder engine.
- Analyze HECC from a thermodynamic efficiency point of view.
- Characterize exhaust chemistry to enhance understanding of the combustion process and implications for aftertreatment systems.

Accomplishments

- Upgraded control system (as recommended by review panel) and used for all FY 2005 experiments.
- Demonstrated HECC operation for extended range of speed-load conditions.
- Investigated transition from conventional to HECC operation and navigation through HECC space with no significant excursions in efficiency or emissions.
- Initiated detailed thermodynamic analysis of HECC operation.
- Investigated exhaust chemistry focusing on the implications of the formation of particulate matter (PM) and PM precursor compounds for low-temperature combustion (LTC) and HECC combustion modes.

Future Directions

- Initiate acquisition and installation of new engine platform. Sandia National Laboratories and the University of Wisconsin are installing single-cylinder engines with the same geometry as the new Oak Ridge National Laboratory (ORNL) engine platform.
- Estimate potential Federal Test Procedure (FTP) emissions and efficiency benefits of advanced combustion strategies through modal experiments and/or simulations.
- Identify and characterize injection strategies and injector characteristics (e.g., orifice diameter, number of holes, etc.) for expanding the speed/load operating range and improving transitions between normal and HECC modes as well as within HECC modes.

Introduction

Researchers at ORNL have been exploring the potential of new combustion regimes that exhibit simultaneous low NOx and PM emissions. An improved understanding of these combustion modes is critical for lowering the performance requirements for post-combustion emissions controls and meeting future U.S. emissions and efficiency goals. Through proper combustion management, ORNL has achieved significant reductions in NOx and PM emissions without the decrease in efficiency typically associated with operating in these regimes. This type of operation is commonly referred to as high-efficiency clean combustion (HECC) and was demonstrated at ORNL on a multi-cylinder engine using only production-like hardware. This achievement is dramatically different from other approaches to HECC which may require expensive hardware modifications or require the acceptance of significant fuel consumption penalties.

Approach

The overall objective of this activity is to improve the understanding of and the ability to achieve and transition to HECC operation for a range of real-world speed/load conditions with only production-like parameters and controls. A combination of thermodynamic and detailed exhaust chemistry information will be used to dramatically improve the understanding of HECC regimes, which is expected to result in even cleaner and more efficient operation of diesel engines. The thermodynamic and exhaust chemistry information will also be shared with industry and/or other national laboratories for the development and validation of improved combustion models and catalysts.

A Mercedes 1.7-L common rail diesel engine is the experimental platform for this study. This engine is equipped with a rapid-prototype, full-pass engine controller capable of actuating the exhaust gas recirculation (EGR) valve, intake throttle, and fuel injection parameters (timing, duration, fuel rail pressure, and number of injections). HECC operation was achieved on this engine under road-load conditions using a combination of high EGR and injection parameters. Specifically, EGR was used to achieve a low-NOx, low-PM condition (aka low-temperature combustion, LTC), and injection parameters were used to adjust combustion phasing to recover efficiency. The effect of transition path from the original equipment manufacturer (OEM) condition to HECC operation using this approach was also investigated using the advanced controller.

Results

Extensive experiments have been performed to develop strategies for achieving HECC operation in a light-duty diesel engine. HECC was achieved for a significant portion of the speed-load map, as shown in Figure 1. Figure 1 also shows the five steady-state conditions which have been used by others (weighting factors indicated by the size of the symbols) to estimate light-duty FTP engine-out emissions. Note that the three highest weighted conditions, which contribute 88% of the total FTP estimation, are achievable with HECC combustion modes and production-like hardware. Emission rates for HECC as compared to conventional combustion are summarized for the first three mode points in Table 1. Significant reductions were realized for NOx and PM emissions with the same or improved efficiency as compared to the conventional conditions. As has been seen previously and reported elsewhere, HECC operation is typically accompanied by an increase in CO and HC emissions. Preliminary results suggest that achieving HECC operation in Mode 4 is possible with a low-pressure EGR system, which would result in 98.7% of the total FTP estimation being achievable with minimal modifications to the engine system.

The experimental data used to construct Figure 1 is shown in more detail in Figure 2 in terms of NOx emission rate as a function of intake O_2 concentration for speeds ranging from 900 to 3000

Table 1. Change in Emission Rates from OEM to HECC Conditions for the Three Most Heavily Weighted Mode Points

	Change in Emission Rate			
Mode	**NOx**	**PM**	**CO**	**HC**
1	80% ↓	99% ↓	187% ↑	23% ↑
2	90% ↓	57% ↓	156% ↑	40% ↑
3	78% ↓	67% ↓	59% ↑	40% ↑

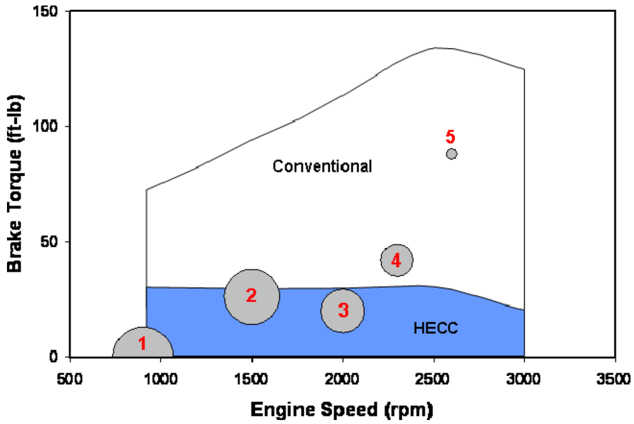

Figure 1. HECC operation was achieved for the most frequently visited range of the speed-load map for light-duty applications.

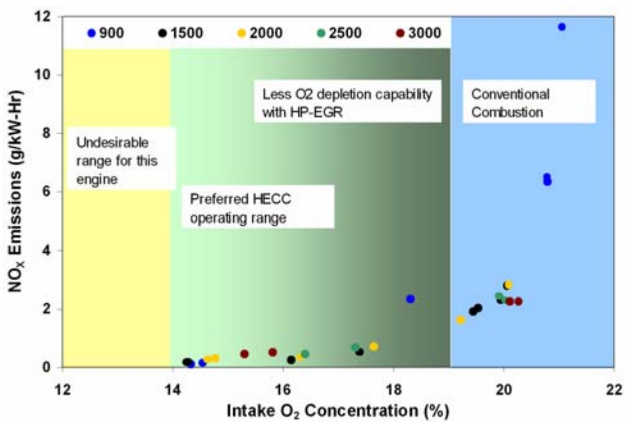

Figure 2. Significant reductions were observed in NOx emissions as a function of intake O_2 concentration.

rpm. Data shown in the "Conventional Combustion" section correspond to conventional diesel combustion modes. Data shown in the middle section correspond to high EGR (low intake O_2) levels where injection parameters were manipulated to maintain efficiency while achieving low emissions (i.e., HECC operation). The preferred intake O_2 level which results in the most significant reductions in NOx and PM is in the range 14-16%. However, for the OEM EGR system, we were not able to achieve these O_2 levels for all conditions and found that significant emissions benefits were still achievable at higher O_2 levels as indicated in the 16-18% O_2 range in Figure 2. The region corresponding to O_2 concentrations less than 14% shown in Figure 2 corresponds to an undesirable O_2

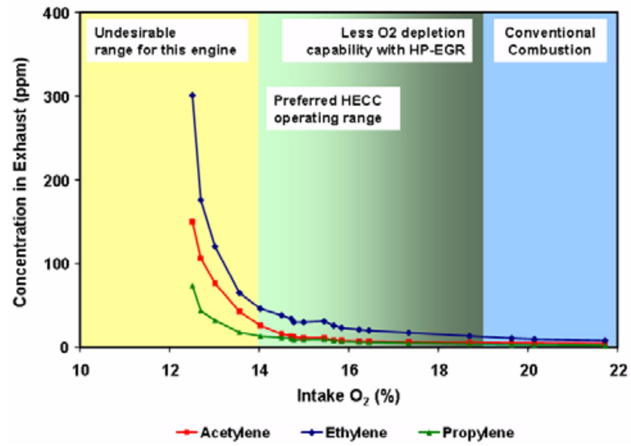

Figure 3. PM precursors were observed to increase exponentially at very low O_2 concentrations. Engine conditions are 1500 rpm and 2.6 bar BMEP.

range for this engine where low PM and high efficiency were not simultaneously achievable.

Experiments were also performed to isolate and investigate the effect of intake O_2 concentration on gas-phase PM precursors. In these experiments, all parameters with the exception of EGR rate (i.e., intake O_2 concentration) were held constant. Acetylene, ethylene, and the propargyl radical have been identified as key gas-phase species leading to the formation and growth of polynuclear aromatic hydrocarbon (PAH) species that subsequently nucleate to form soot. The concentrations of acetylene, ethylene, and propylene are shown in Figure 3 as a function of intake O_2 concentration. Since the propargyl radical is not likely to survive the combustion process to exit the combustion chamber, propylene is shown as an indicator of propargyl-related species. The species shown in Figure 3 are relatively low for O_2 concentrations higher than 14%. For intake O_2 concentrations less than 14%, we see an exponential increase in the PM precursor species. This increase is problematic in achieving HECC operation due to the recirculation of these species which may lead to increased PM emissions. The use of an EGR oxidation catalyst would reduce or eliminate the re-introduction of these problematic species to the combustion process and may improve the possibility of achieving HECC operation at the lower O_2 concentrations.

Due to the concise nature of this report, we were not able to discuss all of the research performed during this activity in FY 2005. Please see the publications/presentations listed below for more information.

Conclusions

The conclusions listed below are based on observations from all of the research performed for this activity in FY 2005.

- HECC was achieved for a range of speed-load conditions including 3 of 5 mode points which have been used by others to estimate engine-out FTP emissions.
- HECC operation below intake O_2 concentrations of 14% is difficult to achieve due to increased PM precursor formation and higher HC emissions.
- Seamless transitions were demonstrated between conventional and HECC operation as well as within the HECC regime.
- More detailed thermodynamic analysis provides insight into efficiency improvements and opportunities.

FY 2005 Publications/Presentations

1. 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).
2. C. S. Sluder, R. M. Wagner, S. A. Lewis, J. M. Storey, "PM and Precursor Species in HECC Combustion Modes", presented to Advanced Engine Combustion Working Group (Detroit, MI USA; September 2005).
3. R. M. Wagner, C. Scott Sluder, S. A. Lewis, and J. M. Storey, "Combustion Mode Switching for Improved Emissions and Efficiency in a Diesel Engine", Fourth Joint Meeting of the U.S. Sections of the Combustion Institute (Philadelphia, PA USA; March 2005).
4. R. M. Wagner, C. Scott Sluder, "High Efficiency Clean Combustion in a Multi-Cylinder Diesel Engine", presented to Advanced Engine Combustion Working Group (Livermore, CA USA; February 2005).
5. C. S. Sluder, R. M. Wagner, S. A. Lewis, and J. M. Storey, "High Efficiency Clean Combustion in a Direct Injection Diesel Engine", 2004 AFRC/JFRC Joint International Combustion Symposium (Maui, HI USA; October 2004).

II.A.8 Large Eddy Simulation Applied to Hydrogen and Low-Temperature Engine Combustion Research

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

DOE Technology Development Manager: Kevin Stork

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 by performing companion simulations.
- Focus initially on an optical hydrogen-fueled engine experiment, and then systematically extend focus to low-temperature combustion (LTC) applications.

Approach

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

Accomplishments

- Unified modeling framework in place, preliminary staging studies completed, and simulation of the optical hydrogen-fueled engine in progress.
  - General purpose time-varying engine grid constructed with metrics mapped for piston and valve movement to match experimental conditions.
  - Hierarchy of studies synchronized with experimental activities with current emphasis on premixed and direct-injection operation.
- Systematic model validation being conducted in collaboration with the DOE Basic Energy Sciences program (International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames www.ca.sandia.gov/tnf).
- Acquisition of dedicated high-performance computational resources in progress, including expansion of our on-site "Computational Combustion and Chemistry Laboratory" and gaining access to DOE "Leadership Class" supercomputers.

Future Directions

- Continue to perform systematic set of high-fidelity LES calculations focused on the optical hydrogen-fueled engine.
  - Move to direct-injection cases at conditions identical to experiment.
  - Perform comparisons between measured and modeled results.
  - Perform hydrogen injector pattern optimization studies.
- Begin to extract information complementary to the experimental dataset, which cannot be measured in a physical engine, to gain quantitative physical insights and improve predictive models.
- Systematically extend the approach to other optical engine experiments underway at the Sandia Combustion Research Facility (i.e., HCCI and LTC).

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. Together, 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.

The investment in time and resources provides two significant benefits. After systematic validation of key processes, quantitative data can be extracted from the simulations that are not otherwise available. These data will provide 1) a complete detailed description of intricately coupled processes not measurable by experimental diagnostics, and 2) information required to better understand the merits and utility of various engineering-based "KIVA-like" models that provide the fast turn-around times required by industry designers. Significant improvements can then be derived to provide enhanced accuracy and confidence in these models. The combination of detailed experiments and high-fidelity LES provides a unique and unparalleled capability to study in-cylinder combustion and transport processes in a manner that presents new opportunities to understand the central physics of flow-flame interactions and develop predictive models for turbulent combustion in internal combustion (IC) engines.

Approach

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 is 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 2005 have been focused on completing the time-varying grid of the Sandia Combustion Research Facility hydrogen-fueled IC-engine (H_2-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 has 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 coupled system of models is directly coupled to the dynamic modeling procedure and facilitates direct treatment of turbulence-chemistry interactions and multiple-scalar mixing processes without the use of tuned model constants.

The baseline grid of the Sandia Combustion Research Facility (CRF) H_2-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 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 valve topology is shown in the cutaway view at 225 crank angle degrees (CAD). The black lines highlight a typical generalized multiblock decomposition (129 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 2.1 million cells. Subsequent calculations will approach on the order of 10 million cells. In addition to advanced software, performing the detailed calculations requires significant computational resources. To facilitate routine application of LES for this purpose, the Sandia Combustion Research Facility is currently engaged

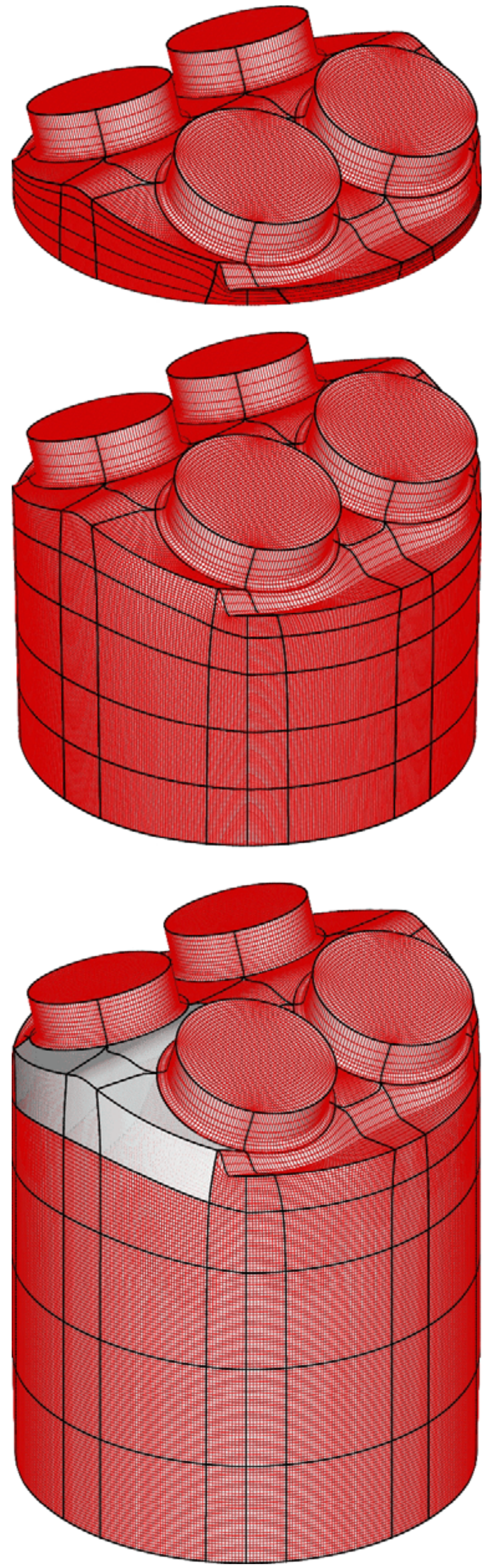

Figure 1. Generalized Time-Varying Multiblock Grid at 0, 90, and 225 CAD Used for LES of the CRF H_2-ICE Engine (ports removed from images)

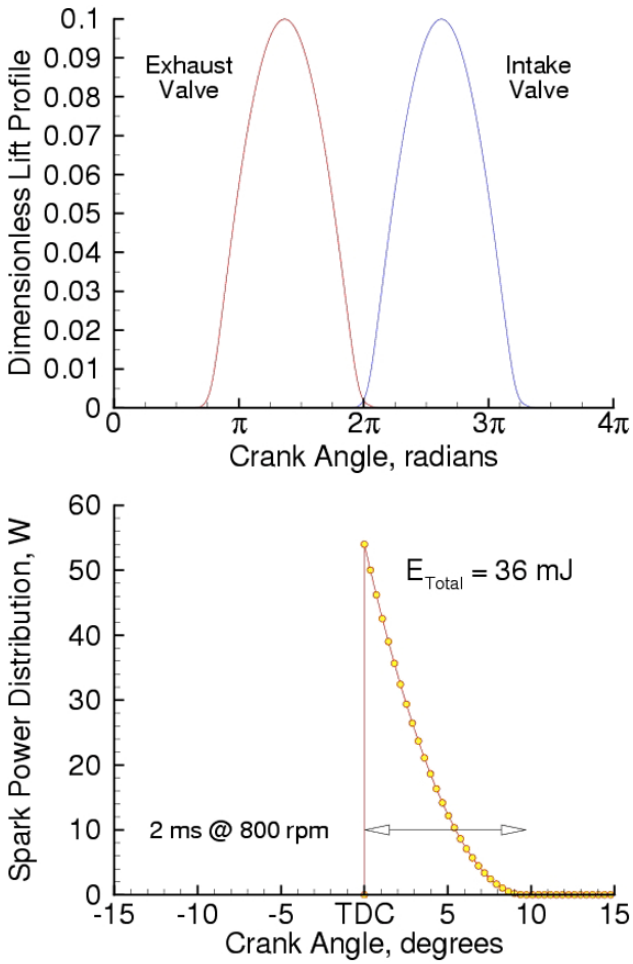

Figure 2. Valve and Spark Timing Profiles

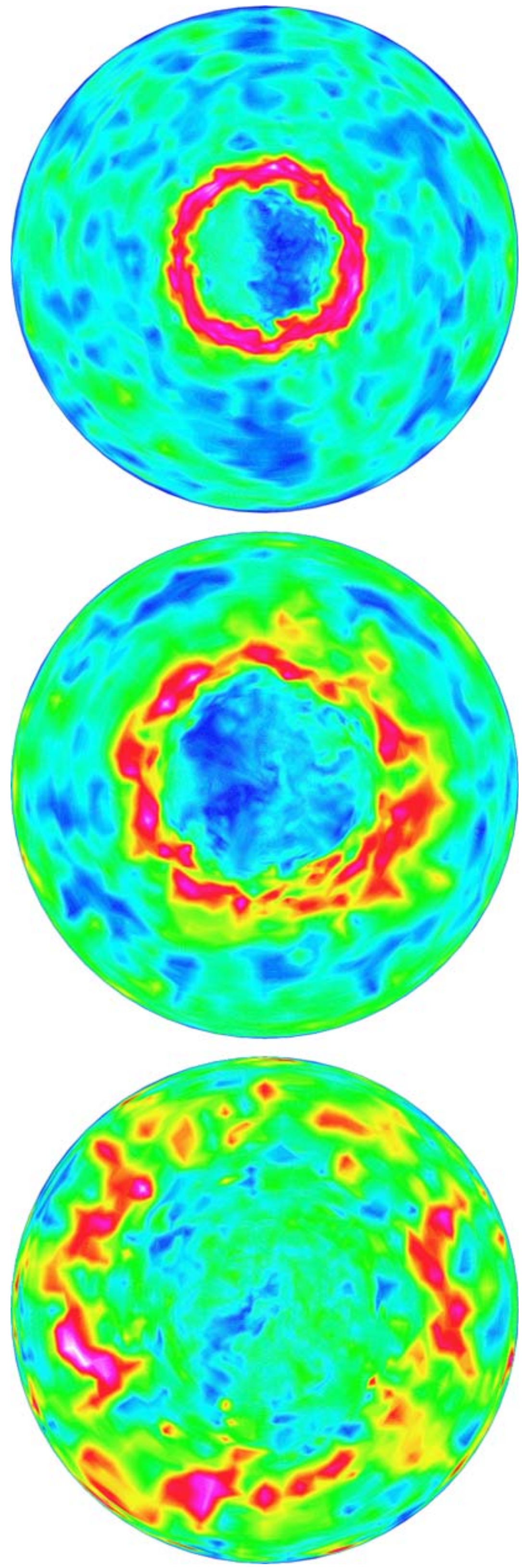

Figure 3. Instantaneous H_2O Mass Fraction Distribution at 4, 8, and 12 CAD, Respectively, after Spark

in a pilot project aimed at establishing dedicated computational 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 highly scalable, massively-parallel, computational capacities. The base systems provide 284 and 128 AMD Opteron™ (Model 246, 2.0 GHz) processors, respectively, with InfiniBand interconnect switches and approximately 20 terabytes of RAID 5 disk storage. These dedicated resources enable both implementation of production-level simulations and porting of larger simulations to high-end "capability-computing" DOE supercomputer facilities for larger grand-challenge applications.

As one example of the collaborative 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 3 shows representative numerical results from the LES that show the instantaneous H_2O mass fraction 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 2 is used as a measure of the instantaneous flame front, similar to 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 mass fraction 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-emission H_2-ICEs. Through interdisciplinary leveraging with other projects, we will continually perform assessments of the base model and select chemical kinetics mechanisms to 1) verify that the chemical mechanisms selected for the 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 2005 Publications/Presentations

1. J. C. Oefelein. Large Eddy Simulation for Turbulent Combustion and Propulsion (Invited). Submitted to *Progress in Aerospace Sciences*, June 2005.
2. J. C. Oefelein. Mixing and Combustion of Cryogenic LOX-H_2 Shear-Coaxial Jet Flames at Supercritical Pressure (Invited). *Combustion Science and Technology*, accepted May 2005.
3. J. C. Oefelein, R. W. Schefer and R. S. Barlow. Toward Validation of LES for Turbulent Combustion (Invited). *AIAA J*, accepted May 2005.
4. J. C. Oefelein. Thermophysical Characteristics of Shear-Coaxial LOX–H_2 Flames at Supercritical Pressure. *Proc. Combust. Inst.*, 30, 2929–2937, 2005.
5. J. C. Oefelein. Large Eddy Simulation of Liquid Rocket Injection and Combustion Processes (Invited). *Proceedings of the Computational and Engineering Science Conference*, Washington DC, April 26-27 2005.
6. J. C. Oefelein and R. S. Barlow. Large Eddy Simulation of Turbulent Combustion: The Role of High-Performance Computing and Advanced Experimental Diagnostics. *Proceedings of the Computational and Engineering Science Conference*, Washington DC, April 26-27 2005.
7. J. C. Segura, J. K. Eaton and J. C. Oefelein. LES of Two-Way Coupled Particle-Laden Turbulent Channel Flow. *Proceedings of the 57th Annual Meeting of the Division of Fluid Dynamics*, American Physical Society, Seattle WA, November 21-23 2004.

8. J. C. Segura, J. K. Eaton and J. C. Oefelein. Predictive Capabilities of Particle-Laden Large Eddy Simulation. *Report No. TSD-156*, Mechanical Engineering Department, Stanford University, October 2004.
9. H. H. Chiu and J. C. Oefelein. Chapter 6: Modeling Liquid-Propellant Spray Combustion Processes (Invited). *Liquid Rocket Thrust Chambers, Aspects of Modeling, Analysis and Design*, Progress in Astronautics and Aeronautics. American Institute of Aeronautics and Astronautics, New York, 2004.

II.A.9 Detailed Modeling of HCCI and PCCI Combustion and Multi-Cylinder HCCI Engine Control

Salvador Aceves (Primary Contact), Daniel Flowers, Francisco Espinosa-Loza, Robert Dibble, Randy Hessel, Aristotelis Babajimopoulos
Lawrence Livermore National Laboratory
7000 East Ave. L-644
Livermore, CA 94550

DOE Technology Development Manager: Kevin Stork

Subcontractors:
University of California Berkeley, Berkeley, CA
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.

Approach

- Develop and use fluid mechanics-chemical kinetics models for analysis of HCCI and PCCI combustion and for evaluation of possible control strategies.
- Conduct experiments on a 4-cylinder Volkswagen TDI engine and on a single-cylinder Caterpillar 3401 engine to evaluate control strategies, develop combustion sensors, and validate HCCI fundamentals.

Accomplishments

- Delivered a computationally efficient analysis procedure for detailed and accurate analysis of HCCI and PCCI combustion based on KIVA and multi-zone CHEMKIN (KIVA3V-MZ).
- Validated KIVA3V-MZ against experimental homogeneous charge engine data and against numerical data for partially stratified operation.
- Parallelized the code for even better computational efficiency. The parallel version of the code has been titled KIVA3V-MZ-MPI.

Future Directions

- *Validate KIVA3V-MZ-MPI against experimental data under partially stratified conditions*. We are working with engine researchers at Sandia Livermore (John Dec and Dick Steeper) to conduct validations of our code at PCCI conditions.
- *Use KIVA3V-MZ-MPI as a predictive tool for engine geometry and fuel injection optimization.* A well-validated KIVA3V-MZ-MPI code should be applicable for improving and optimizing engine characteristics in an HCCI or PCCI engine.

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 it 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. The authors have previously shown multi-zone models to be accurate to capture geometry-dependent processes in homogeneous charge compression ignition (HCCI) engines [1]. It would be extremely useful if the same procedure could be extended for partially stratified operating conditions.

Approach

We have developed a version of KIVA-3V fully coupled with a multi-zone chemical kinetics model (KIVA3V-MZ). Computational efficiency is achieved by utilizing a relatively small number of chemical kinetics zones (~100) compared to the much greater number of nodes typically used in a CFD simulation (~100,000). The multi-zone model communicates with KIVA-3V at each computational time step, as in the ideal fully integrated case. The composition of the cells, however, is mapped back and forth between KIVA-3V and the multi-zone model, introducing significant computational time savings. The methodology uses a novel re-mapping technique that can account for both temperature and composition non-uniformities in the cylinder. Further speed-up is achieved through code parallelization. The parallel version of the code is titled KIVA3V-MZ-MPI.

Results

We have analyzed a geometry and experimental conditions previously used by Dec and Sjoberg [2]. While they analyzed only homogeneous (HCCI) conditions, we have also analyzed idealized operating conditions in which different degrees of stratification are set at intake valve closing. To achieve stratified mixtures, we impose distributions of equivalence ratio linearly from the centerline of the combustion chamber to the cylinder liner. Three different fuel-air distributions are used: "uniform," "shallow," and "steep," as used in previous work by the authors [3]. The uniform distribution is the same as the homogeneous fuel-air distribution used in the experiments [2]. For the shallow distribution, the local equivalence ratio at the centerline of the combustion chamber is double the overall equivalence ratio, and the local equivalence ratio is one-half the overall equivalence ratio at the cylinder wall. The steep distribution results in a local equivalence ratio three times the average equivalence ratio at the centerline of the combustion chamber and zero at the cylinder wall. Again, these equivalence ratio distributions are imposed at intake valve closing; thus, mixing affects the fuel-air distribution throughout the compression stroke as the mixture moves towards ignition.

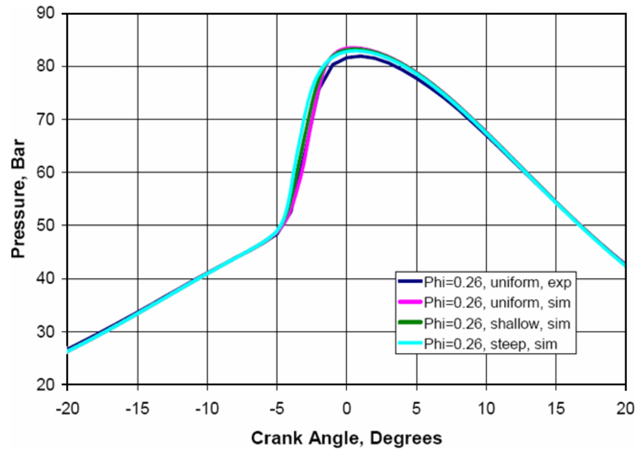

Figure 1. Pressure versus crank angle for three fuel-air distributions – homogeneous, shallow, and steep – with overall equivalence ratio of 0.26. Experimental (exp) results shown for homogeneous case, simulated (sim) results for all three distributions.

Figures 1 and 2 show numerical pressure traces and rates of heat release versus crank angle for the highest equivalence ratio being analyzed (0.26). The figures also show an experimental pressure trace [2]. The figures show that stratification slightly advances ignition timing and promotes slightly faster combustion. The steep distribution has faster combustion than the shallow distribution, which is

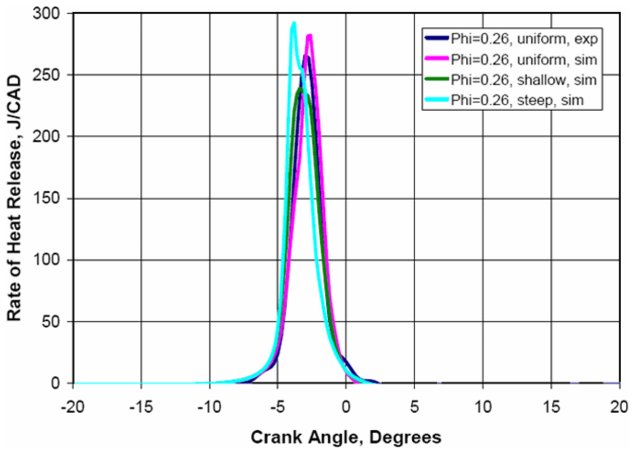

Figure 2. Rate of heat release versus crank angle for three fuel-air distributions – homogeneous, shallow, and steep – with overall equivalence ratio of 0.26. Experimental (exp) results shown for homogeneous case, simulated (sim) results for all three distributions.

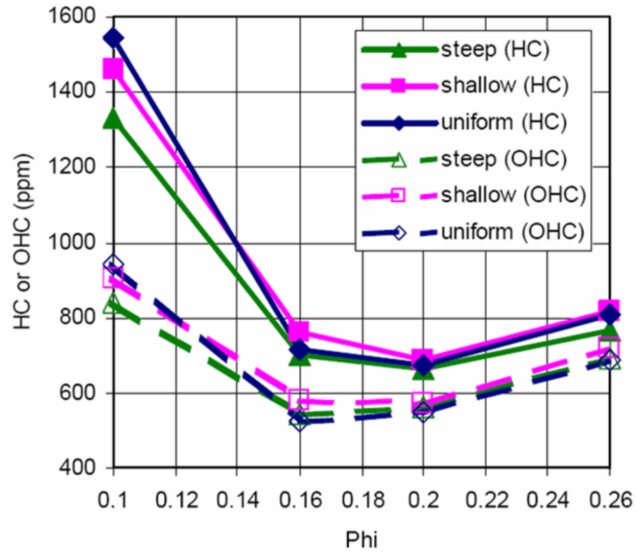

Figure 3. Comparison of hydrocarbon (HC) emissions and oxygenated hydrocarbon (OHC) emissions versus overall equivalence ratio for the three different equivalence ratio distributions.

faster than the uniform distribution. The imposed stratification tends to concentrate higher equivalence ratio mixture in the higher temperature regions of the combustion chamber. This combination of higher equivalence ratio and higher temperature appears to result in accelerating the ignition chemistry and promotes earlier ignition and shorter burn duration.

One intended benefit of stratifying the charge is to reduce the emissions, especially hydrocarbon and carbon monoxide emissions, which tend to be high in HCCI engine combustion. Figure 3 shows total hydrocarbon (HC) and oxygenated hydrocarbon (OHC) emissions versus overall equivalence ratio for the different initial fuel-air distributions. The results are mixed as far as reduction of HC and OHC emissions are concerned. At the lowest equivalence ratio, 0.10, the stratified cases result in lower HC and OHC emissions than the uniform distribution. However, at higher equivalence ratios, the shallow distribution results in higher HC and OHC emissions. The steep distribution results in lower HC and OHC emissions, especially at 0.26 equivalence ratio.

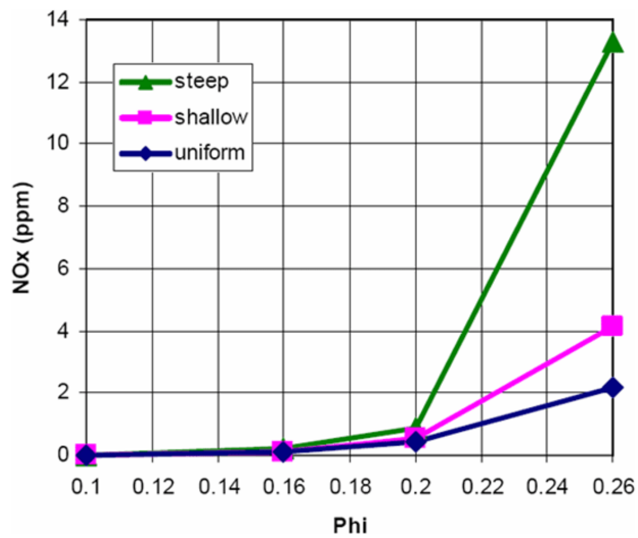

Figure 4. Comparison of oxides of nitrogen emissions versus overall equivalence ratio for the three different equivalence ratio distributions.

NOx emissions versus equivalence ratio are shown in Figure 4 for the uniform, shallow, and steep initial fuel-air distributions. While NOx emissions are very low in all cases, the impact of stratification is to increase the NOx emissions, especially at the highest equivalence ratio. At 0.26 overall equivalence ratio, the shallow distribution results in doubling of the NOx emissions relative to the uniform case, while the steep distribution results in more than a six-fold increase relative to the uniform distribution.

This analysis presents artificially created fuel-air distributions, albeit with features that are representative of seemingly desirable stratification strategies: fuel kept out of crevices and boundary layer of the combustion chamber. It may be beneficial to investigate further optimization of fuel-air distribution in the combustion chamber, such as distributing fuel so that maximum equivalence ratio occurs in intermediate temperature regions of the combustion chamber. In addition, stratification combined with optimization of combustion parameters such as ignition timing can also play a role in improving performance and reducing emissions.

Conclusions

- We have developed a computationally efficient method for analysis of HCCI and PCCI engines.
- Our method reduced the computational time by 90% relative to solving chemistry in every cell when applied to a low-resolution grid (10,000 elements). Considerably higher reductions in computational time can be expected if higher-resolution grids are used.
- The model was validated against experimental HCCI data and numerical PCCI data. Ongoing work is dedicated to validating the model against experimental PCCI data.
- Overall, the proposed methodology offers a computationally efficient alternative to the CFD approach with detailed chemistry in every cell, while maintaining good agreement with the detailed solution. The fully coupled KIVA-3V-MZ-MPI can provide a useful tool for the fundamental understanding of PCCI combustion, the effects of temperature and composition stratification on ignition and burn duration, and the sources of emissions.

Special Recognitions & Awards/Patents Issued

1. Salvador M. Aceves invited to deliver a seminar at the SAE 2005 seminar on HCCI, September 2005, Lund, Sweden.
2. Controlling and Operating Homogeneous Charge Compression Ignition (HCCI) Engines, Daniel L. Flowers, United States Patent 6,923,167, August 2, 2005

FY 2005 Publications/Presentations

1. Analysis of Homogeneous Charge Compression Ignition (HCCI) Engines for Cogeneration Applications, Salvador M. Aceves, Joel Martinez-Frias, Gordon M. Reistad, Proceedings of the ASME Advanced Energy Systems Division, 2004, Accepted for Publication, Journal of Energy Resources Technology.
2. 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.
3. 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.
4. 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.
5. 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, Vol. 6, pp. 465-474, 2005.
6. 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 paper 2005-01-2135.
7. 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 paper 2005-01-2149.
8. Using Carbon-14 Isotope Tracing to Investigate Molecular Structure Effects of the Oxygenate Dibutyl Maleate on Soot Emissions from a DI Diesel Engine, B. A. Buchholz, C. J. Mueller, A. Upatnieks, G. C. Martin, W. J., Pitz, and C. K. Westbrook, SAE Paper No. 2004-01-1849.

9. Investigation of HCCI Combustion of Diethyl Ether and Ethanol Mixtures Using Carbon 14 Tracing and Numerical Simulations, J. Hunter Mack, Daniel L. Flowers, Bruce A. Buchholz, Robert W. Dibble, Proceedings of the Combustion Institute, Vol. 30, 2004.
10. Measuring the Effect of Fuel Structure and Blend Distribution on Diesel Emissions Using Isotope Tracing, B. A. Buchholz, R. W. Dibble, C. J. Mueller, A. S. Cheng, Proceedings of the Western States Section of the Combustion Institute, Davis, CA, March 2004.
11. Tracing Fuel Component Carbon in the Emissions from Diesel Engines, B. A. Buchholz, C. J. Mueller, G. C. Martin, A. S. Cheng, R. W. Dibble, B. R. Frantz, Nucl. Instrum. Methods Phys. Res. Sect. B, Vol. 223-4, 837-841, 2004.
12. 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.
13. 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.
14. Spatial Analysis of Emissions Sources for HCCI Combustion at Low Loads Using a Multi-Zone Model, Salvador M. Aceves, Daniel L. Flowers, Francisco Espinosa-Loza, Joel Martinez-Frias, John E. Dec, Magnus Sjöberg, Robert W. Dibble and Randy P. Hessel, SAE Paper 2004-01-1910, SAE Transactions, Journal of Fuels and Lubricants, 2004.
15. 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.
16. Thermal Management for 6-Cylinder HCCI Engine: Low Cost, High Efficiency, Ultra-Low NOx Power Generation, Joel Martinez-Frias, Daniel Flowers, Salvador M. Aceves, Francisco Espinosa-Loza, Robert Dibble, Paper ICEF2004-930, Proceedings of the 2004 Fall Technical Conference, ASME Internal Combustion Engine Division, October 2004.
17. The Use of Hydrogen Combustion for Power Generation, D. Walther, C. Fernandez-Pello, and R. Dibble, S. Aceves and D. Flowers, Paper AIAA-2005-5753, 3rd International Energy Conversion Engineering Conference and Exhibit, San Francisco, California, Aug. 15-18, 2005.

References

1. Aceves, S. M., Flowers, D. L., Westbrook, C. K., Pitz, W., Smith, J.R., Dibble, R. W. Christensen, M., and Johansson, B., 2000, "A Multi-Zone Model for Prediction of HCCI Combustion and Emissions," SAE paper 2000-01-0327.
2. Dec, J. E. and Sjöberg, M., 2003, "A Parametric Study of HCCI Combustion - the Sources of Emissions at Low Loads and the Effects of GDI Fuel Injection," SAE Paper 2003-01-0752.
3. Aceves, S. M., Flowers, D. L., Espinosa-Loza, F., Babajimopoulos, A. and Assanis, D. N., 2005, "Analysis of Premixed Charge Compression Ignition Combustion with a Sequential Fluid Mechanics-Multizone Chemical Kinetics Model," SAE Paper 2005-01-0115.

II.A.10 In-Cylinder Combustion Visualization in a Non-Optical Engine

Stephen Ciatti (Primary Contact), Scott Miers
Argonne National Laboratory
9700 S. Cass Ave.
Building 362
Argonne, IL 60439

DOE Technology Development Manager: Kevin Stork

Objectives

- Evaluate the performance of emissions-reducing technologies, such as exhaust gas recirculation (EGR), bio-derived fuels and advanced injection systems, by utilizing endoscope imaging.
- Demonstrate the potential of endoscope imaging to provide combustion information at high speed, high load engine operation.
- Complement the data and engine operating conditions utilized by the Combustion Research Facility (CRF) at Sandia National Laboratories to provide a more complete view of advanced engine combustion.

Approach

- Install the endoscope system in an automotive type diesel engine (Mercedes A-class 1.7 liter currently; GM Diesel Euro 4 engine for FY 2006).
- Operate the engine using various conditions, such as different levels of EGR, different injector nozzles, different fuels. Endoscope imaging in this case provided calculated 2-D images of combustion temperature and soot volume fraction as a function of time.
- Utilize endoscope imaging along with other engine diagnostics such as thermophoretic sampling for particulate matter (PM), gaseous emissions measurements, and cylinder pressure measurements.
- Synthesize all of the measurements to provide a more complete evaluation of the fluid mechanics and chemistry mechanisms involved in advanced combustion.

Accomplishments

- Achieved successful installation of the endoscope system into a Mercedes 1.7 liter engine.
- 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. This type of detailed information is not available from traditional, 0-D measurements.
- Bio-derived Fischer-Tropsch type diesel fuel (SunDiesel) was utilized in this experiment. It was shown that this type of fuel has superior PM oxidation compared to traditional diesel fuel, resulting in lower engine-out PM emissions. This is despite the very short ignition delay resulting from its high cetane number and high fuel volatility, which tend to increase soot production.

Future Directions

- Install the endoscope system in the GM Diesel engine.
- Utilize the capability of the GM Diesel engine to operate in low-temperature combustion regimes such as homogenous charge compression ignition (HCCI) and perform combustion imaging under those conditions.
- Conduct experiments that vary important parameters, such as EGR level, multiple injections, fuel type, and other conditions.
- Evaluate the capability of this engine to meet Tier 2, Bin 5 emissions standards with minimal 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. Most low-temperature combustion type engines suffer from power density losses compared to traditional engines, so the ability to operate the engine under all conditions becomes very important.

Approach

The endoscope imaging system was installed in an automotive style engine, a Mercedes 1.7 liter turbocharged, direct injected diesel engine that meets Euro II emissions standards. This engine was available and provided the lowest-cost opportunity to explore the capabilities of endoscope combustion imaging. The engine was controlled by an external system called Rapid Prototyping Engine Control System made by Southwest Research Institute. This provided the opportunity to vary and control almost all engine operating parameters. The endoscope system provided the ability to view up to 4 of the 6 injector spray plumes in the engine and to extract temperature and soot volume fraction information by using 2-color optical pyrometry.

The engine was operated at several road load type conditions – 2500 RPM 50% load (cruise point) and 3500 RPM 75% load (hard acceleration). Parameters that were varied include EGR (from 0% to roughly 20%), fuels (pump diesel and SunDiesel) and injector nozzles (highly finished and roughly finished). Several test matrices were conducted to insure repeatability of the data, and the endoscope data was acquired in conjunction with traditional measurements to insure proper operation of the engine.

Results

The results obtained in these experiments are explained and shown in the following. An example of a combustion image acquired via endoscope imaging is shown in Figure 1. Figures 2 and 3 show the calculated temperature and soot volume fraction

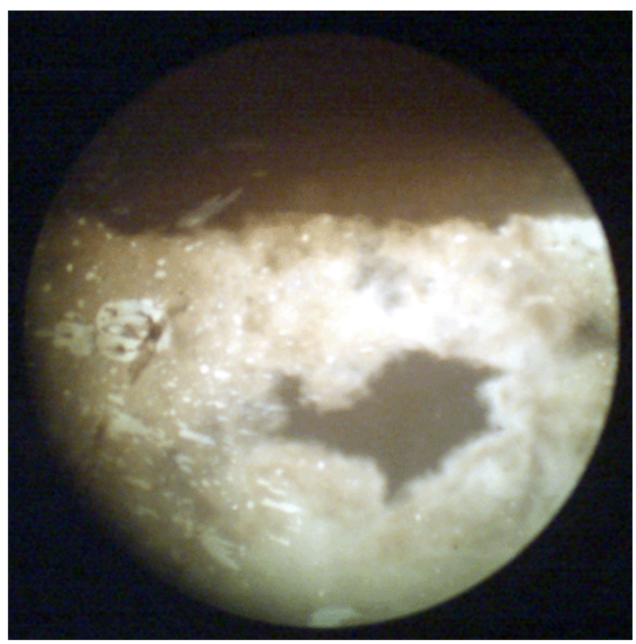

Figure 1. Sample Combustion Image Taken from Endoscope

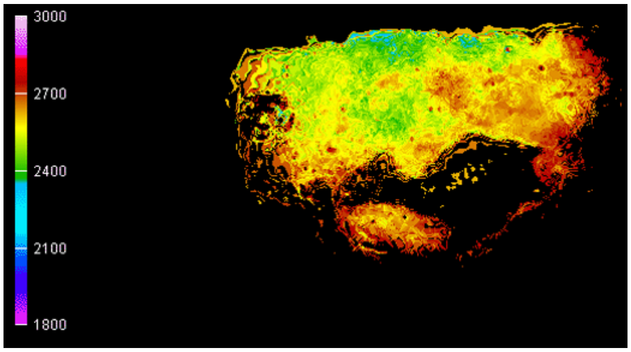

Figure 2. Thermal Image Derived from Combustion Image (Scale at left is deg K)

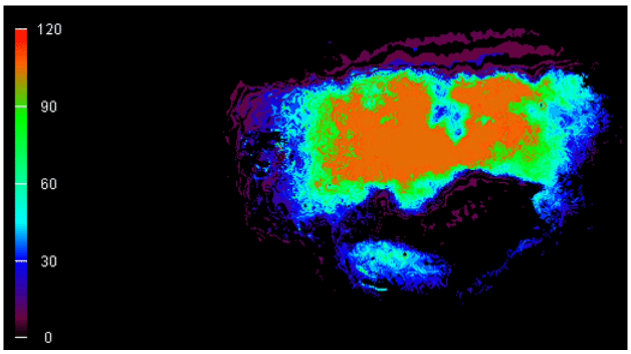

Figure 3. Relative Soot Volume Fraction Image Derived from Combustion Image (Scale at left is arbitrary units)

images acquired from the raw image in Figure 1. Each raw image was acquired using a 10 micro-second exposure time and the lowest amplification gain setting available on the camera. The images were acquired every 0.5 degrees of crankshaft rotation (roughly every 33 micro-seconds). Each image was taken during one combustion cycle – i.e., for the collection of images in a movie, each image represents a different, successive combustion event.

First, the SunDiesel comparison tests with conventional diesel fuel were conducted. For the SunDiesel, there was a lower amount of late-cycle (30-40 CA deg ATDC) soot luminosity as compared to conventional diesel. SunDiesel has significantly lower levels of sulfur and aromatic content, which are both soot formation precursors. The data clearly show that soot oxidation is enhanced using the neat SunDiesel fuel compared to conventional diesel.

A similar study was conducted using various levels of EGR. The engine was operated at 2500 RPM, 50% load and 0%, 10% and 19% EGR (max available) conditions. As EGR increased, the soot radiation temperature levels decreased, leading to a reduction in NOx production. However, soot volume fraction increased as EGR increased. The endoscope imaging and heat release analysis confirm the increase in overall combustion duration due to the decreased rate of chemical reaction. This decreased rate of chemical reaction is caused by the reduction of available oxygen due to the EGR dilution of the intake air stream.

Finally, a study was conducted using different nozzle tips in the same engine. These nozzle tips were specially manufactured to provide nearly identical flow rates but drastically different flow characteristics. Using the endoscope imaging technique, it was shown that the highly finished nozzles produced roughly a 10% reduction in late-cycle soot compared to the roughly finished nozzles. The superior fuel atomization and preparation in the highly finished nozzle provided significant influence over these results.

Conclusions

- Endoscope imaging provides 2-D information that captures much more detail about engine combustion than 0-D techniques can provide.
- Real, multi-cylinder engines can be 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 measurement, emissions measurement, and others.
- Detailed temperature and soot volume fraction measurements can be calculated from endoscope images, providing insight into the mechanisms behind engine combustion changes.

FY 2005 Publications/Presentations

1. ASME paper ICEF2005-1327, “Influence of EGR on the Soot/NOx Tradeoff for a Light Duty Diesel Engine”, S. A. Ciatti, S. A. Miers, H. K. Ng, September 2005
2. SAE paper 2005-01-3670, “Emissions, Performance and In-Cylinder Combustion Analysis in a Light-Duty Diesel Engine Operating on a Fischer-Tropsch,

Biomass-to-Liquid Fuel", S. A. Miers, S. A. Ciatti, H. K. Ng

3. Presentation to Department of Energy Secretary Samuel Bodman, "In-Cylinder Combustion Analysis to Improve Engine Efficiency and Reduce Emissions", S. A. Ciatti, Argonne National Laboratory, May 2005

II.A.19 Free Piston Engine Research

Peter Van Blarigan
Sandia National Laboratories
7011 East Ave.
Livermore, CA 94550

DOE Technology Development Manager: Kevin Stork

Objectives

- Model the stability of electrically coupled opposed free pistons in a single-cylinder free-piston engine
- Utilize computational fluid dynamics (CFD) modeling to design the inlet/exhaust parameters for opposed piston uniflow scavenging

Approach

- Utilize Mathematica-based model incorporating all significant dynamic parameters to assess the stability of the opposed piston coupling under unsymmetrical piston friction loads
- Develop a KIVA model of piston motion and port geometry – optimize based on scavenging and trapping efficiency

Accomplishments

- Stability of the electromagnetic coupling between opposed motion pistons has been verified in the single-phase and three-phase electrical machines investigated
- Preliminary scavenging port design has been developed to give various trapping/scavenging efficiency combinations

Future Directions

- Refine scavenging system to include port fuel injection
- Optimize electrical configuration for existing linear alternators used in an opposed piston, electrically coupled configuration
- Begin research prototype design integration based on opposed piston configuration

---

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 (IC) 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 program goal is to combine the developed components into a research prototype for demonstration of performance.

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.

Results

Scavenging Investigation

A KIVA mesh of the uniflow opposed cylinder configuration is shown in Figure 1. The figure gives an idea of the aspect ratio of the cylinder and the relative size of the intake and exhaust ports. The uniflow configuration is attractive for the large cylinder length to bore ratios utilized here, allowing a desirable compromise between trapping efficiency and scavenging efficiency. The opposed piston geometry has two principal advantages over the single piston geometry. First, perfect balance of the device is achieved, requiring no isolation or mitigating methods to be employed for transportation applications. Second, the two pistons control the exhaust and intake port opening and closing, eliminating the need for remotely actuated exhaust valves as have been shown in the earlier single piston design. This is a powerful cost-saving modification, particularly as lower-power devices are required when hybrid drivetrains become more refined.

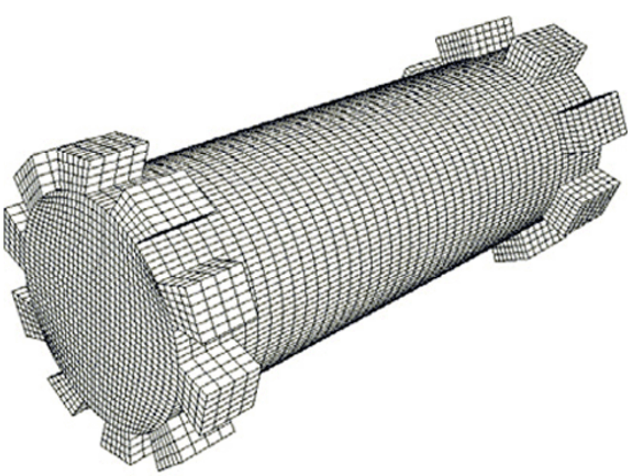

Figure 1. Uniflow Mesh Showing Inlet (Left) and Exhaust Port Configuration

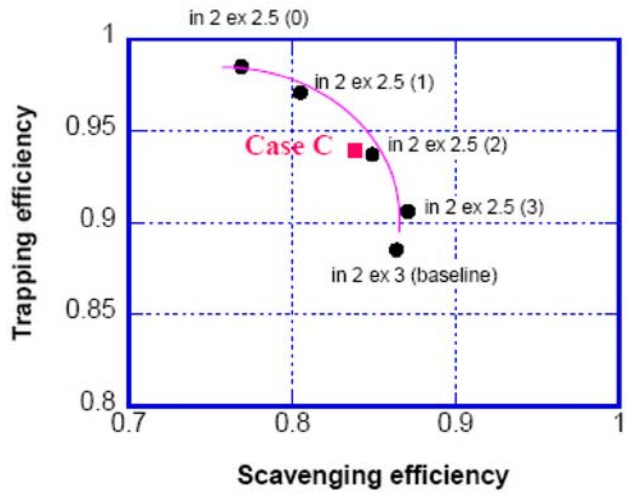

Figure 2. Performance of the Scavenging System

The results of the study this year are presented in Figure 2. Trapping efficiency versus scavenging efficiency is plotted for several variants of port geometry and port timing. It can be seen that reasonable scavenging efficiency can be achieved at high trapping efficiency, the desired goal. With the addition of port fuel injection, a shift toward higher scavenging efficiency can be realized by allowing early flushing gas to not contain fuel, thus achieving high results for both parameters.

Piston Stability

The modeling effort undertaken this year has more positively quantified the extent of piston motion synchronization and compared a three-phase geometry with the single-phase geometry investigated to date.

The Mathematica-based model incorporates all of the forces necessary to fairly judge performance, including friction, gas pressures, combustion, magnetic induction, etc. In addition, an energy balance is calculated to assure that all of the terms (exhaust, ohmic heating, power out, combustion energy, etc.) are conserved. Interestingly, after initial startup, the model may take thousands of cycles to reach (or not reach) a stable operating point.

The problem is complicated by the need to also optimize the parameters for power generation so as to make maximum utilization of the linear generating capacity. In addition to assessing stability, the model is proving useful for predicting electrical circuit parameters for such optimization. For example, for maximum power generation, the capacitance value in series with the electrical load is different for the piston power stroke compared to the return stroke.

As a basis for understanding the results to date, the electrical phase relationship between the two pistons must be referenced. Essentially, when the electrical phase shift between the two pistons reaches 90 degrees, the pistons will "slip a tooth" and further operation of the generator is not possible. Thus, the goal is to not approach this operating limit under various friction magnitudes and variability between the pistons.

Table 1. Stability of Various Friction Cases for Opposed Piston Design

Phase of alternator	Energy Input	Oscillation Frequency	Power Output	Relative Phase Variation	Friction Each Piston
Single Phase	1.4 kJ	49 Hz	33 kW	+/- 20 degrees	0.1, 0.2 N s/m viscous
Single Phase	1.4 kJ	49 Hz	33 kW	+/- 1 degree	1.0, 2.0 N s/m viscous
Single Phase	1.4 kJ	49 Hz	33 kW	+/- 13 degrees	20.0, 22.0 N dry friction
Three Phase	1.5 kJ	45 Hz	35 kw	+/- 60 degrees	0.1, 0.2 N s/m viscous
Three Phase	1.5 kJ	45 Hz	35 kw	+/- 55 degrees	1.0, 2.0 N s/m viscous
Three Phase	1.5 kJ	45 Hz	35 kw	+/- 30 degrees	5.0, 6.0 N s/m viscous
Three Phase	1.5 kJ	45 Hz	35 kw	+/- 60 degrees	20.0/ 22.0 N dry friction

Table 1 shows results of the model for both single-phase and three-phase configurations of the linear alternator. The current configuration of the alternators supplied by Magnequench International, Inc. is single-phase. However, the units could be reconfigured as three-phase devices by replacing the permanent magnets with new magnets of lengths varied to achieve the three-phase configuration. There are advantages to the three-phase geometry in ease of starting, lower cogging force, etc. that warrant investigation.

The results presented in Table 1 show that the single-phase geometry has higher stability than the three-phase case. It is interesting to note that higher friction does not immediately translate into lower stability, as can be seen for the second case single-phase predictions. While the three-phase results have considerably greater relative variation, there appears to be a limit which still remains in the stable regime.

The coupling concept is robust enough that we believe the advantages of the opposed piston design warrant proceeding in this direction for our research prototype design.

Conclusions

- The two-stroke cycle scavenging and inherent coupling stability of electromagnetically synchronized pistons has been assessed.
- The scavenging parameters need to be further refined, but the design window appears adequate for achieving the desired results.
- Piston stability modeling has shown good synchronization for both three-phase and single-phase configurations. The synchronizing forces appear capable of maintaining position (no slipped tooth positions) over a wide range of friction variations and magnitudes between the two pistons.

II.A.20 In-Cylinder Hydrogen Combustion Visualization in a Non-Optical Engine

Stephen Ciatti (Primary Contact) and Thomas Wallner
Argonne National Laboratory
9700 S. Cass Ave.
Building 362
Argonne, IL 60439

DOE Technology Development Manager: Kevin Stork

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.
- 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.

Approach

- Install the endoscope system in a single-cylinder, automotive style engine (Ford Motor Company engine with 0.5 liter displacement).
- Operate the engine using PFI for FY 2005 – providing a performance baseline for the engine and verifying the operation of the safety systems and hydrogen fuel system.
- Utilize endoscope imaging along with other engine diagnostics such as gaseous emissions measurements and cylinder pressure measurements.
- Synthesize all of the measurements to provide a more complete evaluation of the fluid mechanics and chemistry mechanisms involved in hydrogen combustion.

Accomplishments

- Achieved successful installation of endoscope system into the Ford single-cylinder engine.
- 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.

Future Directions

- More fully utilize the endoscope system in the Ford single-cylinder engine.
- Operate the hydrogen engine using direct injection (DI) to assess injector and engine performance.
- 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 enable use of 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 to the access windows, resulting in emissions measurements that are usually not representative of actual engines. To maintain optical quality, the access windows 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 pressures, emissions, 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 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, if hydrogen combustion anomalies such as knock and pre-ignition can be overcome.

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.

Figure 1. Field of View of Endoscope in Hydrogen Engine Combustion Chamber

The engine was operated at several conditions – 1500 RPM 50% load, 3000 RPM 75% load and 4500 RPM 50% load. The primary variable for baselining the engine was spark timing (moving from the knock limit to the pre-ignition limit). Several test matrices were conducted to insure repeatability of the data, and the endoscope data was acquired in conjunction with traditional measurements to insure proper operation of the engine.

Results

The results obtained in these experiments are shown in the accompanying figures. An example of the field of view inside the hydrogen engine combustion chamber is shown in Figure 1. Figures 2 and 3 show the ultraviolet images obtained at the time of spark discharge and during peak OH* intensity. Each image was acquired using a 20 micro-second exposure time and a mid-level amplification gain setting available on the camera. The images were acquired every 0.5 degrees of crankshaft rotation. Each image was taken during

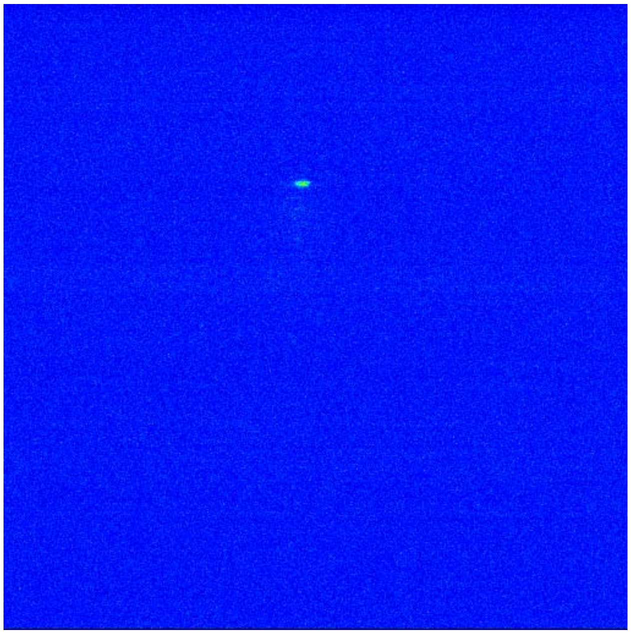

Figure 2. Ultraviolet Image of Spark Discharge

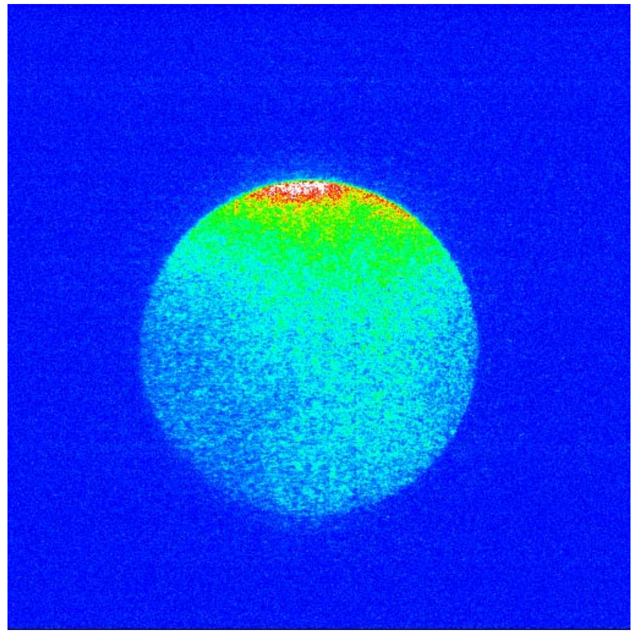

Figure 3. Ultraviolet Image of Peak OH* Chemiluminescence Intensity during Combustion

one combustion cycle – i.e., for the collection of images in a movie, each image represents a different combustion event.

The first study performed was to find the knock and pre-ignition limits for this engine based upon fuel/air ratio (F/A) and spark timing. It was found that the range of available spark timing to avoid combustion anomalies became narrow when the F/A ratios approached stoichiometric. For this particular engine configuration, stoichiometric operation was only possible if the engine was throttled, but other studies (using different engines) have not experienced this limitation.

Finally, once the engine and test cell were operating properly, images were taken using the UV equipment available – including an intensified charge coupled device camera, UV transmittent endoscope and special UV transmittent lenses. OH* chemiluminescence emits photons at roughly 310 nm wavelength, which is below the visible spectrum.

Conclusions

- Endoscope imaging provides 2-D information that captures much more detail about engine combustion than 0-D techniques can provide.
- Real, multi-cylinder engines can be 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 chemiluminescence measurements can be linked to pressure and heat release information, providing insight into the mechanisms behind engine combustion changes.

FY 2005 Publications/Presentations

1. ASME paper ICEF2005-1398, "Study of Combustion Anomalies of H_2ICE with External Mixture Formation", S. A. Ciatti, T. Wallner, H. K. Ng, W. F. Stockhausen, B. Boyer.

II.A.21 Preliminary Evaluation of Mixture Formation and Combustion in a Hydrogen Engine using OH Chemiluminescence

Christopher White
Sandia National Laboratories (SNL)
P.O. Box 969, MS 9053
Livermore, CA 94551

DOE Technology Development Manager: Kevin Stork

Objectives

- Develop the science base needed by engine companies to develop fuel-efficient, low-emissions, hydrogen-fueled internal combustion engines (H_2ICEs) and promote DOE's long-term goal of transitioning to a hydrogen economy.
- Initial focus is to systematically investigate hydrogen-air mixing processes for engine operation with hydrogen injected directly in-cylinder.
- Provide complementary and validation data for the numerical experiments modeling Sandia's H_2ICE being conducted at the Combustion Research Facility (CRF) at SNL.

Approach

- Built a world class optical engine laboratory to investigate fundamental in-cylinder engine phenomena.
- Use the relatively simple imaging technique of OH chemiluminescence as a first step in a systematic approach to study in-cylinder hydrogen-air mixing processes.
- Perform experiments with well-defined initial and boundary conditions that can be used for model and grid validation of the large eddy simulation (LES) numerical simulations.

Accomplishments

- Restored and upgraded an existing optical engine laboratory to operate with hydrogen as a fuel. Notable capabilities include:
  - automotive-sized single-cylinder engine with extensive optical access,
  - port-fuel-injection (PFI) or direct-injection (DI) hydrogen fueling,
  - advanced laser-based diagnostics.
- Operated the engine with hydrogen for the first time and performed systematic experiments to determine operating conditions that are suitable for an optical engine and relevant to industry.
- Preliminary OH chemiluminescence experiments have begun to assess the effects of injection variables on engine operation and mixture formation.

Future Directions

- Continue the OH chemiluminescence studies to measure flame propagation characteristics and cycle-to-cycle variability and to assess mixture formation in an H_2ICE for premixed and direct-injection hydrogen fueling.
- Begin experimental setup to implement the planar laser induced fluorescence (PLIF) technique that will be used to provide a spatially resolved quantitative measure of in-cylinder equivalence ratio.
- Begin to develop experimental-numerical experiments that provide fundamental physical insights that can not be determined from experiments or simulations alone.

Introduction

H_2ICE development efforts are focused to achieve DOE's near-term goals for an advanced spark-ignited hydrogen engine. These goals include efficiencies approaching that of a high-efficiency diesel engine, power density exceeding PFI-gasoline engines, and emissions that are effectively zero. Direct-injection (DI) H_2ICE is one of the most attractive advanced H_2ICE options because of its high power density (approximately 115% the power density of the equivalent engine fueled with PFI-gasoline) and the multiple degrees of freedom available for controlling emissions and optimizing efficiency. The technical challenge with DI-H_2ICE operation is that in-cylinder injection requires hydrogen-air mixing in a very short time (approximately 4 ms at 5000 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 Advanced Hydrogen Engine Laboratory at the CRF has been established to address these technical challenges. The initial work will focus on performing systematic experiments to investigate in-cylinder hydrogen-air mixing processes.

Approach

An existing spark-ignited direct-injection (SIDI) optical engine laboratory was modified to operate with hydrogen as a fuel. The automotive-sized single-cylinder engine provides extensive optical access for application of advanced laser-based optical diagnostics to study in-cylinder hydrogen-air mixing, combustion, and emissions processes. The initial work is focused on the investigation of in-cylinder mixture formation processes in a DI-H_2ICE. As the first step in a systematic experimental approach, OH chemiluminescence imaging is used to evaluate in-cylinder mixture formation and to assess various injection strategies. The experiments include measurements for engine operation with premixed and DI hydrogen fueling. The premixed measurements establish a baseline comparison for DI operation. The value of these measurements is to establish a foundation for the study of in-cylinder hydrogen-air mixing processes using advanced laser-based diagnostics that are more robust, but experimentally more difficult.

Results

Laboratory modifications included upgrades to the gas handling and safety system, installation of two hydrogen fuel lines, machining of the engine head to accept the hydrogen injector, and installation of a high-powered neodymium-doped yttrium aluminum garnet master optical parametric oscillator (Nd:YAG MOPO) system and intensified CCD camera. Additionally, critical measurement instruments have been calibrated and tested. The result is a state-of-the-art optical engine facility that will be used to investigate fundamental in-cylinder engine processes in a DI-H_2ICE. Figure 1 shows

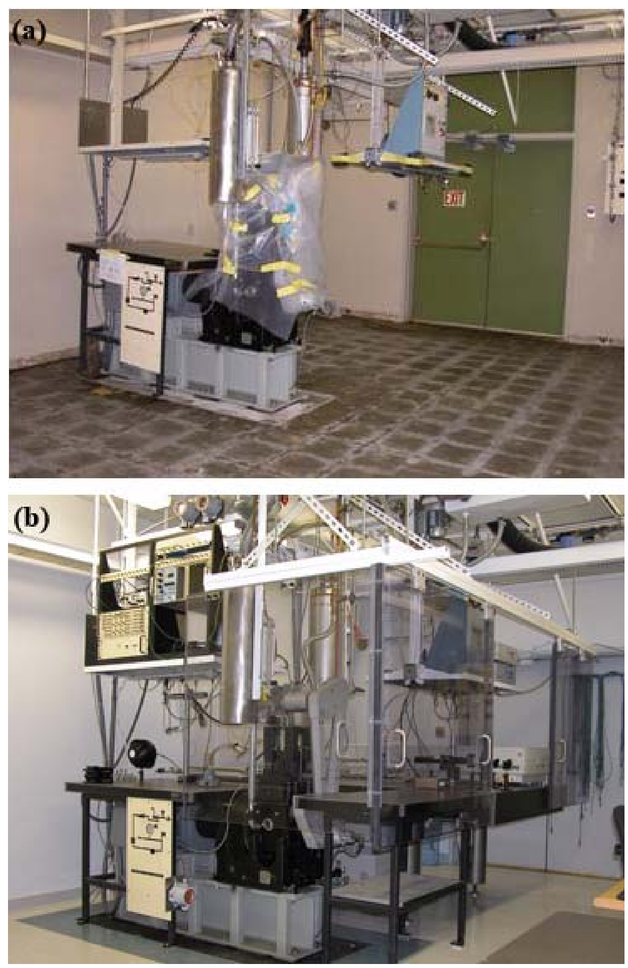

Figure 1. Photographs of engine laboratory (a) during modifications and (b) in its present configuration.

pictures of the laboratory during the modifications and in its present configuration.

OH* chemiluminescence studies have begun to assess the effects of injection variables on mixture formation and 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. For case (i), a premixed fuel-air mixture is considered. This injection strategy emulates engine operation similar to that of a PFI-H_2ICE. For case (ii), direct injection of hydrogen into the cylinder is timed in a manner that coincides with intake valve closure. This provides the maximum in-cylinder mixing times possible for DI-H_2ICE operation. For case (iii), the direct injection of hydrogen ends at approximately 20 crank angle degrees (CAD) before spark. In addition, to qualitatively assess the effect of injection pressure on in-cylinder mixing, for case (ii) and case (iii) two injection pressures of 20 and 100 bar are investigated. For each injection strategy, OH* chemiluminescence images are acquired at some 8-12 CAD over the duration of combustion, and 10-20 images are acquired per CAD. Engine speed is 800 rpm, intake manifold pressure is 50 kPa, and the global equivalence ratio is kept constant at approximately 0.6.

Ensemble-averaged OH* chemiluminescence images for an injection pressure of 20 bar acquired at 9 CAD after spark for cases (i) and (ii) and 19 CAD after spark for case (iii) are shown in Figure 2. The later acquisition time for case (iii) is due to the delay in the peak heat release rate for late injection compared to early injection. The symmetric OH* chemiluminescence intensities observed in Figure 2(a) are indicative of a homogeneous distribution of H_2 within the cylinder. The flame speed is estimated at 16 ± 2 m·s^{-1} by calculating the distance the front travels between two crank angle degrees. Figure 2(b) shows some asymmetry, but the radial flame development suggests a near-homogeneous distribution of H_2 within the cylinder. In contrast, Figure 2(c) illustrates the strong mixture inhomogeneities formed with late direct injection. Furthermore, the high intensities located near the injector (injector is located 90° counter clockwise from the top of the image) suggest poor jet penetration at these conditions.

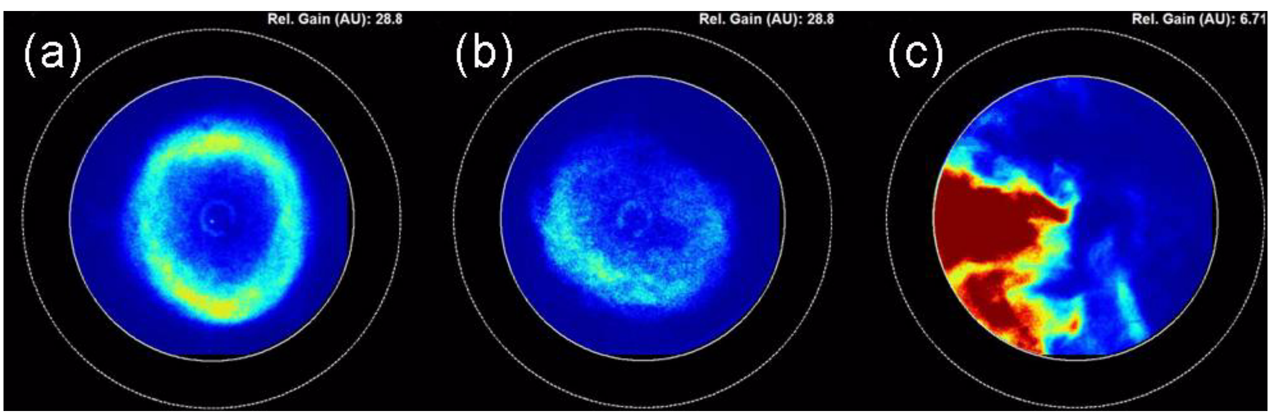

Figure 2. Ensemble-averaged OH* chemiluminescence images acquired for three injection strategies for an injection pressure of 20 bar and a global equivalence ratio of 0.6: (a) premixed at 9 CAD after spark, (b) early direct injection at 9 CAD after spark and (c) late direct injection at 19 CAD after spark. OH* intensities increase linearly from blue to green to red, and the relative gains are 28.8, 28.8 and 6.71 for (a), (b) and (c), respectively. The images were acquired through a quartz window in the piston (i.e., r-θ plane). The inner and outer circles correspond to the diameters of the quartz window and cylinder bore, respectively. The spark is located approximately in the center of the image, and the injector is located 90° counter clockwise from the top of the image.

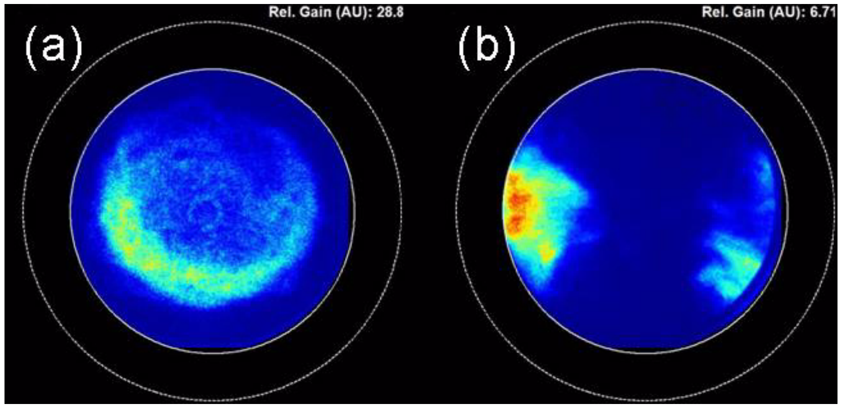

Figure 3. Ensemble-averaged OH* chemiluminescence images acquired for two injection strategies for an injection pressure of 100 bar and a global equivalence ratio of 0.6: (a) early direct injection at 9 CAD after spark and (b) late direct injection at 17 CAD after spark. The relative gains are 28.8 and 6.71 for (a) and (b), respectively.

The experiments for cases (ii) and (iii) are repeated for an injection pressure of 100 bar. With an increase in the injection pressure, theory states that jet penetration should increase by the square root of the pressure ratio, which in the present case is square root 5. Consequently, the expectation is that in-cylinder mixing should improve. Ensemble-averaged OH* chemiluminescence images for an injection pressure of 100 bar acquired at 9 CAD after spark for case (ii) and 17 CAD after spark for case (iii) are shown in Figure 3. The similarities between Figure 3(a) and Figure 2(b) suggest that for early direct injection, the increase in injection pressure has little effect. For late direct injection, Figure 3(b) shows the expected increase in jet penetration with increased injection pressure; however, strong mixture inhomogeneities remain. This result is illustrative of the complex interaction between the injected H_2 and in-cylinder fluid motion. Understanding these interactions will be a primary research focus of the H_2ICE laboratory over the next fiscal year.

Conclusions

OH chemiluminescence images acquired in an optically accessible engine show similar flame characteristics and in-cylinder mixture formation between premixed and early direct injection operation. With late injection, mixture inhomogeneities increase for both the low and high hydrogen injection pressures investigated. The locally rich region near the injector for the low injection pressure is indicative of poor jet penetration, while the large-scale, locally rich structures observed in the high pressure study suggests that a large-scale, in-cylinder flow is set up by the injection process. Consequently, the dynamics of the large-scale structures likely dominate the mixing process. Future work will focus on understanding the complex interaction between the injected H_2 and in-cylinder fluid motion.

FY 2005 Publications/Presentations

1. C. M. White, R. R. Steeper and A. E. Lutz. The hydrogen-fueled internal combustion engine: A technical review. In press *Int. J Hydrogen Energy.*
2. Y. Dubief, C. M. White, V. E. Terrapon, E. S. G. Shaqfeh, P. Moin and S. K. Lele. On the coherent drag-reducing and turbulence enhancing behaviour of polymers in wall flows. *J. Fluid Mech*. 514, 271-280. **Non-Sandia related publication.**
3. C. M. White and J. Oefelein. Sandia Hydrogen Engine Program: An Update of Progress and Plans. Advanced Engine Combustion Working Group Meeting, Sandia National Laboratories, CA, February 2005.
4. C. M. White. Advanced Hydrogen-Fueled Internal Combustion Engines. International Energy Agency, Strategic Committee, Sarasota, FL, February 2005.
5. C. M. White. Sandia Hydrogen Engine Program: An Update of Progress and Plans. Ford Research Center, Dearborn, MI, April 2005.
6. C. M. White. The Proposed H_2ICE Collaborative Task: An Update of Progress and Plans. International Energy Agency, Task Leaders Meeting, Zurich, Switzerland, September 2005.