

## II.A Combustion and Related In-Cylinder Processes

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

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#### Objectives

- Study the mechanisms of spray atomization by making detailed, quantitative measurements in the near-nozzle region of sprays from light-duty diesel injectors.
- Perform these measurements under conditions as close as possible to those of modern diesel engines.
- 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 studies 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, 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

- Performed and published a series of measurements studying the effects of nozzle geometry on the structure of sprays. These measurements demonstrated for the first time that the x-ray technique can be useful for resolving subtle differences in the sprays based on the internal structure of the nozzle.
- Performed our first measurements at ambient pressures of 15 and 20 bar. This greatly expands our maximum achievable pressure and allows us to operate under ambient density conditions similar to those of a light-duty diesel engine under low-load conditions.
- Acquired a pressure vessel that allows measurements of multi-hole nozzles, and performed our first study of multi-hole valve-covering orifice (VCO) nozzles. This enables us to study nozzles identical to those used in real engines.

- Established a large number of new collaborations with both industrial and academic partners. These collaborations increase the relevance of our work and expand its impact by involving experts in the field from around the world.
- Continued our group's record of a large volume of high-quality publications. We published two peer-reviewed papers and four contributions to conference proceedings, and we presented our results at eight national and international meetings. The quality of this work has been recognized by our peers; one publication was awarded "Best Paper" at the American Society of Mechanical Engineers/International Council on Combustion Engines (ASME/CIMAC) conference, and one presentation received an SAE "Excellence in Oral Presentation" award.

## 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 Advanced Combustion Technologies 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.

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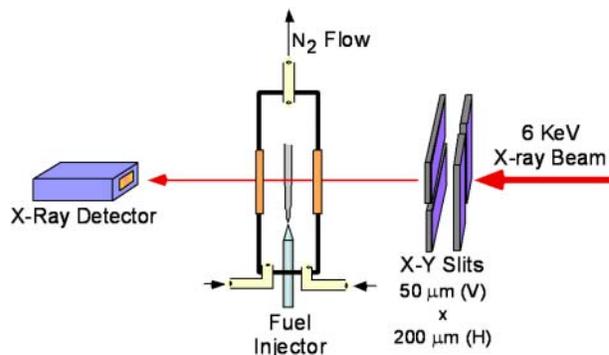
## Introduction

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 laser diagnostics over the last 20 years, scattering of light from the large number of droplets surrounding the spray prevents penetration of the 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 to date only

been compared with data acquired in the region relatively far from the nozzle. It is unknown how well these models apply in the crucial near-nozzle region. The limitations of visible light in the near-nozzle region of the spray have led us to develop the x-ray absorption technique for the study of fuel sprays. X-rays are highly penetrative, and measurements are not complicated by the effects of scattering. The technique is non-intrusive, quantitative, highly time-resolved, and allows us to make detailed measurements of the spray, even in the dense droplet region very near the nozzle.

## Approach

This project studies the sprays from commercially available light-duty diesel fuel injectors. Our approach is to make detailed measurements of the sprays from these injectors using x-ray absorption. This will allow us to make detailed measurements of the fuel distribution in these sprays, extending the existing knowledge into the near-nozzle region. The x-ray measurements

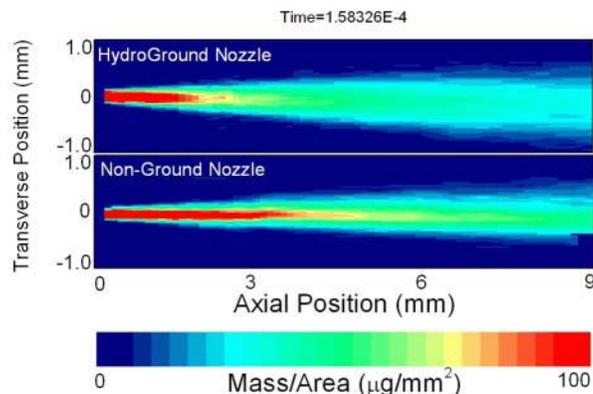


**Figure 1.** Schematic of the Experimental Setup

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

$$\frac{I}{I_0} = \exp(-\mu_M M)$$

where  $I$  and  $I_0$  are the transmitted and incident intensities, respectively;  $\mu_M$  is the mass absorption constant; and  $M$  is the mass of fuel. The constant  $\mu_M$  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



**Figure 2.** The Effects of Nozzle Geometry on the Structure of Sprays

fuel injection systems designed to improve efficiency and reduce pollutants.

## Results

A series of x-ray measurements was performed on sprays from a common rail injector manufactured by Robert Bosch Corp. The effects of injection pressure, ambient pressure, and nozzle geometry were explored in these experiments. In previous years, the maximum ambient pressure attainable was 10 bar, and we were limited to performing experiments on single-hole research nozzles. In FY 2004, we were able to expand the scope of our measurements to include multi-hole nozzles and higher ambient pressures. We also established several new collaborations that greatly expand the impact of our work.

In Figure 2, the mass distributions are shown for two sprays from nozzles with different internal geometries; the measurement conditions are otherwise identical. The differences in structure between the sprays are clearly evident; the nozzle without hydrogrinding shows a narrower spray with a denser core extending farther from the nozzle. Such distinct features have never been measured previously in the near-nozzle region; they can provide a stringent test for models attempting to predict the flow of fuel through the nozzle. Researchers at the University of Massachusetts, Amherst have used the geometry of our nozzles to predict the fuel flow and its effect on the fuel distribution outside the nozzle [3]. These results demonstrated the applicability of our measurements

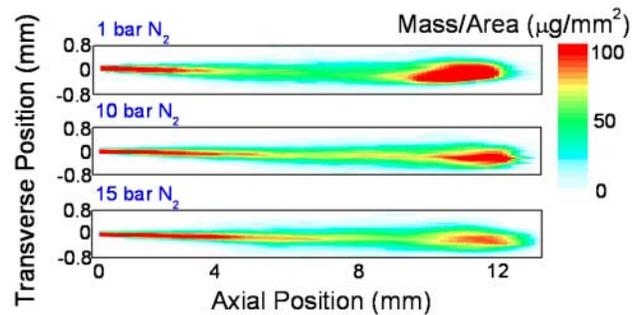


**Figure 3.** X-Ray Spray Chamber for the Study of Multi-Hole Nozzles

and showed the need for improved position resolution in our measurement technique.

FY 2004 marked the beginning of a long-term collaboration between Argonne, the Engine Research Center at the University of Wisconsin, and General Motors. This partnership proposed and received approval from Advanced Photon Source management for a three-year program of fuel spray studies. This partnership guarantees our group nine weeks of x-ray beam access per year for the next three years. This important achievement prevents us from having to go through the quarterly proposal/approval cycle, enabling long-term planning for a fixed number of experiments. This partnership also constructed a pressure vessel designed to allow the testing of multi-hole nozzles. The vessel was funded by General Motors and built by the Engine Research Center with guidance from Argonne. The vessel is pictured in Figure 3. Our first experiment using this vessel studying multi-hole VCO nozzles was completed in FY 2004, and we have three weeks of beam time planned for this collaboration in FY 2005.

Figure 4 shows the mass distributions of sprays from the same injector at ambient pressures of 1, 10, and 15 bar at an equivalent penetration of 13 mm from the nozzle. The figure shows the effect that the increasing ambient pressure has on the mass distribution of the spray. As the pressure increases, the spray core shows less expansion perpendicular to the spray axis. This phenomenon has been observed



**Figure 4.** The Effects of Ambient Pressure on the Mass Distribution of the Spray

several times in x-ray experiments but runs contrary to the well-established expansion of the overall spray cone angle with increasing ambient pressure. This apparent contradiction was resolved in a recent publication in collaboration with modelers at Michigan Technological University, which showed that the discrepancy arises because of the fundamental differences between the x-ray and visible light measurements [4,5]. While the x-ray technique measures the fuel distribution of the spray core, visible light techniques are particularly sensitive to individual droplets at the periphery of the spray. Since current spray models have been developed primarily based on the results of visible light measurements, they may accurately simulate the outer regions of the spray while having little predictive power in the core region of the spray which contains the vast majority of the fuel. The quantitative data provided by the x-ray measurements can aid the development of models with the power to accurately simulate the entire spray over a broad range of conditions.

In addition to technical accomplishments, FY 2004 saw the establishment of a number of new collaborations with outside researchers. In addition to those mentioned above, new collaborations were established with Visteon Corp., Helsinki University of Technology, and Caterpillar. We also continued to work with several existing partners, including DaimlerChrysler, Robert Bosch, University of Colorado, and Wayne State University. This increasing 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 may be a very useful diagnostic tool to fuel system manufacturers when designing and testing new injection systems.
- Significant differences were discovered in spray penetration and fuel distribution as a function of ambient gas pressure.
- 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.

## **Special Honors**

1. Chris Powell, et. al, were awarded “Best Paper” for “Comparison of X-Ray Based Fuel Spray Measurements with Computer Simulation Using the CAB Model” presented at the ASME/CIMAC Congress 2004, Kyoto, Japan, June 2004.
2. Received an SAE “Excellence in Oral Presentation” award.

## **FY 2004 Publications/Presentations**

1. “X-Ray Absorption Measurements of Diesel Sprays and the Effects of Nozzle Geometry,” C. F. Powell, S. A. Ciatti, S. -K. Cheong, J. Liu, J. Wang, Society of Automotive Engineers, Paper 2004-01-2011.
2. “Dynamics of Diesel Fuel Sprays Studied by Ultra-Fast X-Radiography,” S. -K. Cheong, J. Liu, J. Wang, C. F. Powell, S. A. Ciatti, Society of Automotive Engineers, Paper 2004-01-2026.

3. “Analysis of X-Ray-Based Computer Simulations of Diesel Fuel Sprays,” F. X. Tanner, K. A. Feigl, S. A. Ciatti, C. F. Powell, S. -K. Cheong, J. Liu, J. Wang., 17th Annual Conference on Liquid Atomization and Spray Systems, May 2004.
4. “Comparison of X-Ray Based Fuel Spray Measurements with Computer Simulation Using the CAB Model,” S. A. Ciatti, C. F. Powell, S. -K. Cheong, J. Y. Liu, J. Wang, F. X. Tanner, CIMAC/ ASME Congress 2004; Kyoto, Japan; June 2004.
5. Presentation at DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation, Argonne National Laboratory, May 2004.
6. “X-Ray Characterization of Diesel Sprays and the Effects of Nozzle Geometry,” C. F. Powell, S.-K. Cheong, S. A. Ciatti, J. Liu, J. Wang, DEER Conference, San Diego, CA, August 2004.

## **References**

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2. C. F. Powell, Y. Yue, R. Poola, J. Wang, M.-C. Lai, J. Schaller, SAE 2001-01-0531, (2001).
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4. “Analysis of X-Ray-Based Computer Simulations of Diesel Fuel Sprays,” F. X. Tanner, K. A. Feigl, S. A. Ciatti, C. F. Powell, S. -K. Cheong, J. Liu, J. Wang., 17th Annual Conference on Liquid Atomization and Spray Systems, May 2004.
5. “Comparison of X-Ray Based Fuel Spray Measurements with Computer Simulation Using the CAB Model,” S. A. Ciatti, C. F. Powell, S. -K. Cheong, J. Y. Liu, J. Wang, F. X. Tanner, CIMAC/ ASME Congress 2004; Kyoto, Japan; June 2004.

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

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### 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 existing data measured using conventional techniques at Sandia National Laboratory.

### 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.
- 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 was 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.
- A collaboration was established between the researchers at Argonne and a modeling group at Helsinki University of Technology.

### Future Directions

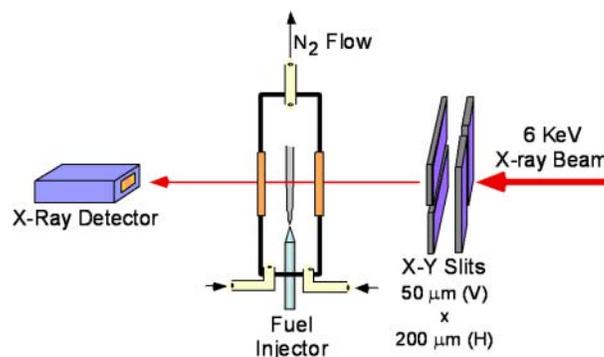
- Analysis of the measurement results is continuing. Initial results have shown significant differences in the fuel distribution of the sprays at different ambient pressures. Publication of this work is expected in early 2005 and will include the measurement results, comparisons with the conventional spray measurements performed at Sandia, and modeling results from Helsinki University.
- Measurements of the Detroit Diesel heavy-duty injector have been completed, and the funding has been shifted to the X-Ray FuelSpray project and the Caterpillar Cooperative Research and Development Agreement (CRADA). Further x-ray measurements of sprays from heavy-duty injectors will be part of the Caterpillar CRADA and will be performed on modern Caterpillar injection systems.

## 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 laser diagnostics over the last 20 years, scattering of light from the large number of droplets surrounding the spray prevents penetration of the 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 to date 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 Corp. with specially-fabricated single-hole nozzles. The injector and nozzles are similar to those which have been studied at Sandia National Laboratory 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 will allow 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



**Figure 1.** Schematic of the Experimental Setup

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 [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

$$\frac{I}{I_0} = \exp(-\mu_M M)$$

where  $I$  and  $I_0$  are the transmitted and incident intensities, respectively;  $\mu_M$  is the mass absorption constant; and  $M$  is the mass of fuel. The constant  $\mu_M$  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. Our work will be compared to the existing data that has been acquired by Sandia National Laboratory using a similar injection system. This will allow us to extend the Sandia database into the region very near the nozzle, and we will be able to determine whether

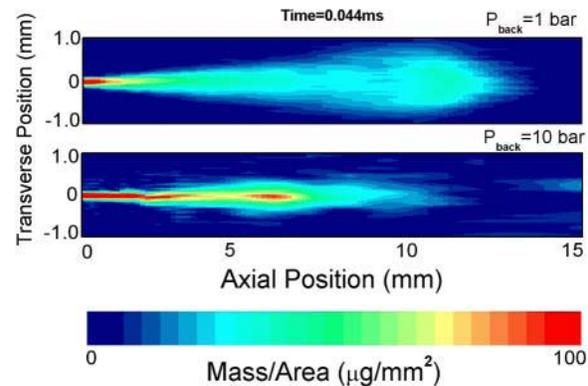
parameterizations that have been developed based on the Sandia data apply in this region. We will also collaborate with spray modelers to incorporate this previously unknown knowledge of the near-nozzle region of the spray into new models. This will lead to an increased understanding of the mechanisms 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 Corp. 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 allow comparison to similar measurements made in the past at Sandia. The nozzle diameter had a strong effect on the spray penetration and angle, as expected from the Sandia work. Additional optical imaging was performed using a microscopic lens, allowing a detailed measurement of the spray boundaries and shape. These images were compared to the images generated from the x-ray measurements; the two techniques showed good agreement in the near-nozzle region.

Another series of conventional spray measurements was made using the Bosch rate-of-injection (ROI) meter. 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 Sandia. Also, the mass flow measured in this way can be compared to the mass measurements made using the x-ray absorption method.

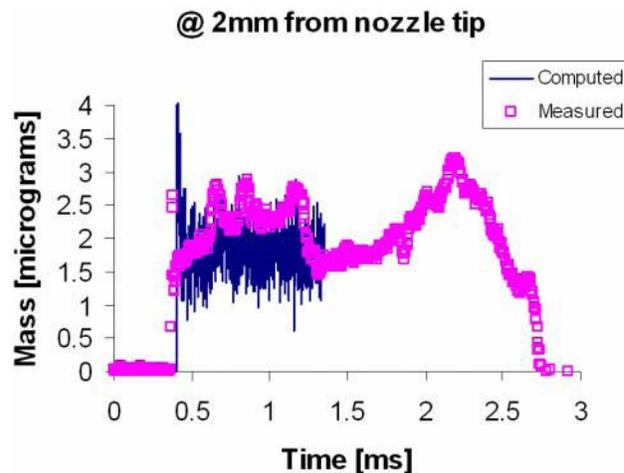


**Figure 2.** X-ray Image Reconstructions Showing the Effect of Ambient Pressure on the Spray

X-ray measurements were performed on three different nozzles under otherwise identical conditions. The first nozzle had an orifice diameter of 180  $\mu\text{m}$  and orifice length-to-diameter ratio ( $L/D$ ) equal to four, the second had a diameter of 250  $\mu\text{m}$  and  $L/D = 4$ , while the third had a diameter of 250  $\mu\text{m}$  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  $\text{N}_2$  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 diameter) 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. An interesting breakup process in the high mass density region was observed near the beginning of the injection event between  $\sim 22$ -26  $\mu\text{s}$  after the start of injection. It was also observed that increasing the ambient pressure from 1 to 10 bar resulted in a narrower and shorter spray than that observed with 1 bar backpressure before 50  $\mu\text{s}$  after start of injection (see Figure 2). Later in the spray event, the cone angle at 10 bar ambient pressure gets wider than the spray measured at 1 bar.

All of the measurements made using the x-ray technique are made as a function of time. This allows the dynamic features of the sprays to be



**Figure 3.** Preliminary Results Comparing the Mass Versus Time Measured Using X-rays and Calculated Using STAR-CD

studied and compared. Changes in the mass flux through the beam were observed as the probe was moved farther from the nozzle. The time-resolved mass 0.2 mm away from the nozzle was nearly flat, while fluctuations developed in the measured mass flux further downstream. This indicates that some physical effect is causing fluctuations to develop in the mass versus time as the spray moves away from the nozzle, and that this is taking place external to the nozzle. Several possible mechanisms could cause this behavior, including air entrainment, variations in speed along the spray axis, and transverse motion of the fuel. Careful theoretical modeling may be able to reproduce the features shown in these plots and would be an important development in the study of the mechanisms of spray atomization.

One very important accomplishment in FY 2004 was the establishment of a collaboration 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 is attempting to reproduce them with modeling using STAR-CD. Preliminary results of the measured and calculated mass flux through the x-ray beam are shown in Figure 3; a full publication of these results is expected in early 2005. 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 2004 Publications/Presentations

1. "Near-Nozzle Spray Characteristics of Heavy-Duty Diesel Engine", Essam M. EL-Hannouny, Sreenath Gupta, Christopher F. Powell, Seong-Kyun Cheong, Jinyuan Liu, Jin Wang and Raj R. Sekar, SAE, 2003-01-3150.
2. Presentation at DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation, Argonne National Laboratory, May, 2004.
3. "X-Ray Measurements on Near-Nozzle Spray for Heavy-Duty Diesel Injectors", poster at the DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation, Argonne National Laboratory, May, 2004.
4. "Lagrangian Diesel Spray Modeling and Near Nozzle X-Ray Measurements", Ari Saarinen, Essam EL-Hannouny, and Sreenath Gupta, SAE 2005, to be published.

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## II.A.3 Low-Temperature Automotive Diesel Combustion

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### Objectives

- Provide the physical understanding of the in-cylinder combustion processes needed to meet future diesel engine emissions standards while retaining the inherent efficiency and low CO<sub>2</sub> 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 effects 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.
- Measure engine performance, fuel economy, and emissions in a non-optical test engine with the identical geometry.
- Compare in-cylinder measurements and engine emissions and performance to model predictions.
- Refine and improve models and engine operating strategies.

### Accomplishments

- Experimentally evaluated a late-injection, low-temperature diesel combustion regime for a wide variety of system parameters, including injection pressure, swirl ratio, O<sub>2</sub> concentration (exhaust gas recirculation rate), start of injection (SOI), and intake temperature. Identified optimum swirl level and rate-limiting factors at various stages of the combustion process.
- Identified the formation of large-scale, mixing-enhancing flow structures as a dominant factor responsible for accelerated late-cycle heat release.
- Constructed a phenomenological picture of the progression of this low-temperature combustion regime in the equivalence ratio-temperature ( $\phi$ - $T$ ) plane.
- Analyzed an extensive set of in-cylinder velocity data obtained at various engine speeds, measurement locations, and swirl ratios to establish a data base for comparison with model predictions of the turbulent stresses. Performed a detailed comparison with predictions obtained using the industry standard  $k$ - $\epsilon$  model.

## Future Directions

- Evaluate alternative low-temperature combustion systems and identify the rate-limiting factors that prevent their application over a wider speed/load range.
- Investigate the mixture formation process in early-injection combustion systems, and evaluate the potential of in-cylinder fluid mechanical process to improve the mixture preparation process.
- Analyze the performance of more advanced turbulence models, including their influence on the prediction of large-scale flow structures, turbulence energy, and anisotropy. Emphasis will be placed on models which utilize minimal computing resources.

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## Introduction

Direct-injection diesel engines have the highest fuel efficiency and the lowest CO<sub>2</sub> emissions of any reciprocating internal combustion engine technology. This efficiency comes at the cost, however, of NO<sub>x</sub> and particulate matter (soot) emissions, which are high in relation to future emission standards. 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. Recently, the potential of low-temperature combustion (LTC) regimes to dramatically reduce NO<sub>x</sub> and soot emissions has been demonstrated. A key aspect of many LTC systems is reliance on high levels of exhaust gas recirculation (EGR). High EGR levels reduce in-cylinder O<sub>2</sub> concentrations to achieve low combustion temperatures, thereby requiring that a greater mass of ambient fluid be rapidly mixed with the fuel than is needed for conventional diesel combustion. Other LTC systems rely on extensive pre-mixing to overall fuel-lean conditions prior to ignition. In both cases, mixing processes are central to the success of the combustion strategy.

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 thus 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

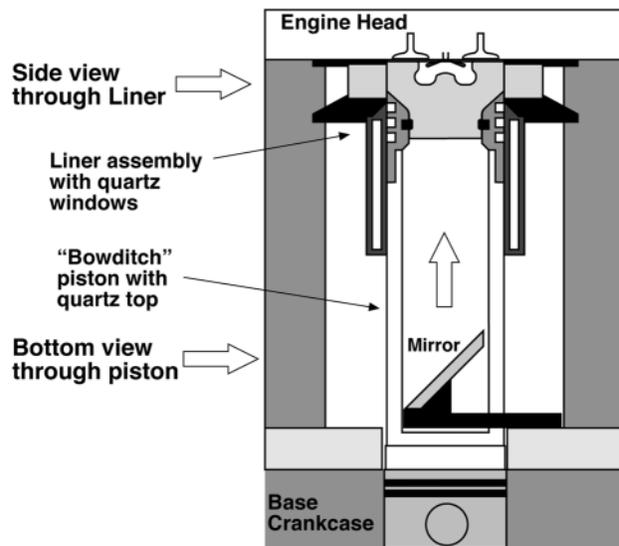
The research approach involves three parallel efforts in a closely coordinated project. Detailed

flow and thermochemical property measurements are made in an optically-accessible laboratory test engine; emissions, performance and fuel consumption measurements are made in a traditional single-cylinder test engine; and computer simulations are performed and compared to the data obtained in both the optical and traditional test engines. Natural synergies emerge among these three efforts. For example, detailed measurements of the 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. Similarly, traditional test engine measurements serve to identify interesting operating parameter trade-offs that bear further investigation either numerically or experimentally in the optical engine.

## 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 faithfully maintains the combustion chamber geometry, is a unique aspect of this facility. 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.

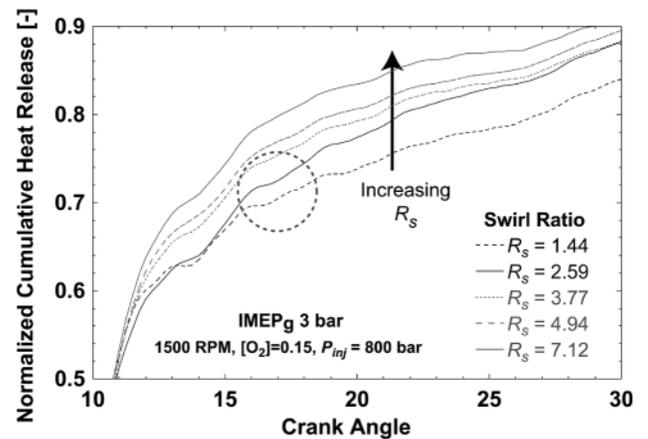
A major thrust of the research performed in FY 2004 was directed towards obtaining a better understanding of late-injection low-temperature



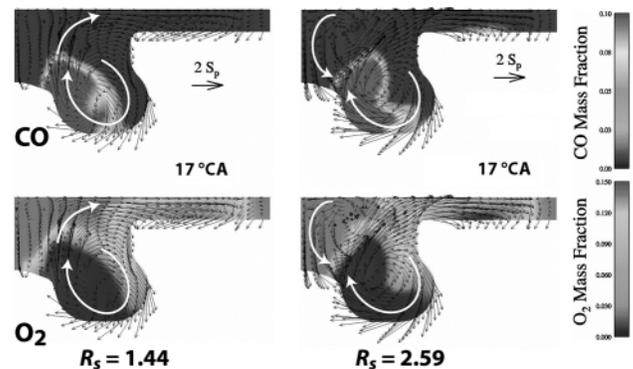
**Figure 1.** Schematic view of the optical engine, depicting the quartz piston top with a realistic combustion chamber geometry.

combustion systems, similar to the Nissan “MK”<sup>1</sup> or AVL “HPLI”<sup>2</sup> systems. In these systems, late-cycle mixing processes are key to obtaining acceptable emissions and retaining good fuel economy. Enhanced swirl is one method employed to increase the late-cycle mixing rates. Figure 2 shows the variation in the cumulative apparent heat release as swirl is increased for a typical LTC operating condition. From the divergence of the curves beyond approximately 11 °CA, it is clear that the apparent heat release rate increases with increased swirl. Numerical simulations indicate that this is not associated with increased heat transfer, but rather with increased chemical heat release associated with higher mixing rates. Through examination of the spatial distribution of the unburned fuel and air in the combustion chamber, the probable source of this increased mixing can be identified.

In-cylinder flow fields and distributions of CO and air are shown in Figure 3. The CO serves to mark the locations of the partially-oxidized products of rich combustion produced during the earlier part of the combustion event. The crank angle shown, 17 °CA, is typical of the period during which the cumulative heat release curves (see Figure 2) are diverging rapidly for the two swirl levels shown,  $R_s=1.44$  and 2.59. At the lower swirl ratio, the flow structure in the vertical plane is characterized by a

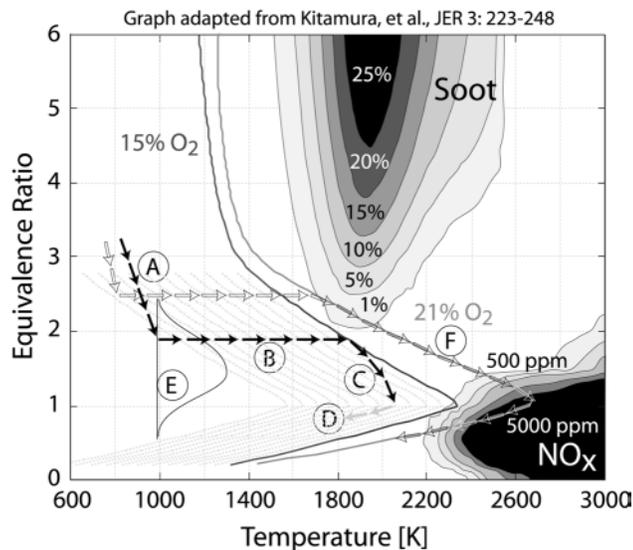


**Figure 2.** Variation in the cumulative apparent heat release with flow swirl. Accelerated heat release for  $R_s = 2.59$  as compared to  $R_s = 1.44$  (indicated by the dashed circle) corresponds to the formation of the flow structures seen in Figure 3.



**Figure 3.** Flow structures formed in the mixing-controlled portion of the combustion process. The double-vortex structure seen for  $R_s = 2.59$  is believed to be the dominant factor responsible for the increased heat release rate observed in Figure 2.

single dominant vortex. Fuel and air thus “follow” each other around the combustion chamber and are only mixed by the random turbulent motions superimposed on the mean flow structure shown. In contrast, at the higher swirl ratio, a double-vortex mean flow structure is formed which greatly enhances the mixing process. The lower vortex transports the partially-burned fuel to an interfacial region which is simultaneously being fed fresh air by the upper vortex. At the interface, high turbulence levels are also generated by sharp gradients in swirl



**Figure 4.** Equivalence ratio-temperature map illustrating the zones of formation of both soot and  $\text{NO}_x$ , as well as the approximate path taken by a “typical” fuel element during a late-injection low-temperature combustion event.

velocity and by vertical-plane flow deformation associated with the counter-rotating vortices.<sup>3</sup> The bulk transport of fuel and air to a common interface, coupled with high turbulence levels at the interface, results in significantly increased mixing rates. At the higher swirl levels (e.g.  $R_s=3.77$ ), this interface forms earlier.

A series of tests involving variable swirl ratio, engine speed, injection pressure, SOI, and intake temperature was conducted to better understand the rate-limiting processes that prevent the application of late-injection LTC systems to a wider speed and load range. To illustrate the progress of the combustion event, it is helpful to follow the path of a “typical” fuel element as combustion proceeds (Figure 4). Initially, the fuel and air are premixed near-adiabatically in mixing processes that are dominated by the injection event (path A), resulting in a range of mixture equivalence ratios just prior to ignition, as indicated by the distribution (E). Thermodynamic analysis and in-cylinder soot formation suggest that the mean equivalence ratio of the mixture at ignition is between 1 and 2, and that a significant fraction of the fuel can be found in mixtures with equivalence ratios greater than 2. Ignition and combustion of this mixture are indicated by the idealized path (B),

which represents chemical reaction occurring over a short period in which additional mixing is small. This path ends near the adiabatic flame temperature characteristic of the mixture composition prior to ignition, which is indicated by the dark line labeled “15%  $\text{O}_2$ .” The majority of the soot is likely formed near the end of path (B). From this point on, the combustion is limited by mixing (C), much like conventional diesel combustion (F). If the combustion proceeded at constant volume, path (C) would closely follow the adiabatic flame temperature curve. However, due to cylinder volume expansion, the gases are cooling and path C bends downward. Completing the mixing process before falling temperatures quench chemical reaction is critical to the successful application of this LTC system. Even after combustion is complete, additional mixing (D) can be beneficial as it represents a path away from the high temperatures characteristic of  $\text{NO}_x$  production.

### Conclusions

- Mixing rates in the late-cycle period can be significantly enhanced by bulk flow structures that transport fuel and air to a common interface.
- An analysis of the progression of low-temperature, late-injection combustion systems indicates that the late-cycle mixing process is critical to obtaining good fuel economy and low emissions of CO and unburned hydrocarbons.
- The flow development is a multifaceted process involving mutual interactions between intricate combustion chamber geometry, high-pressure sprays, and a complex flow structure. Development of an economical, accurate numerical simulation capability will be key to optimizing low-emission diesel engines of the future.

### Special Recognitions & Awards/Patents Issued

1. SAE Award for Excellence in Oral Presentation, for presentation of SAE Paper 2004-01-1678, March 2004.
2. Sandia National Laboratories Employee Recognition Award for Individual Technical Excellence, June 2004.

3. Paul Miles of Sandia National Laboratories was selected as Co-Vice-Chair of Combustion for SAE's Fuels and Lubricants Activity.

### **FY 2004 Additional Presentations**

1. Miles PC. "Low-Temperature Engine Combustion: New Challenges for In-Cylinder Mixing," Keynote address, CECOST and Energy Related Fluid Mechanics Annual Seminar, Gothenburg, Sweden, November 2003.
2. Miles, PC. "Turbulent Flow Structure Development in HSDI Diesel Engines," Invited Seminar, Volvo Car & Volvo Technology Corporation, Gothenburg, Sweden, November 2003.
3. Choi, D. "Heat Release Analysis and Imaging of Combustion Luminosity for MK-like Combustion," DOE OFCVT Advanced Engine Combustion Meeting, Livermore, CA, January 2004.
4. Miles PC. "Recent Progress in the HSDI Diesel Engine Laboratory," DOE OFCVT Advanced Engine Combustion Meeting, Livermore, CA, January 2004.
5. Miles PC. "Engine Turbulence Modeling Support at Sandia National Laboratories" & "Mixing Processes in Swirl-Supported Diesel Engines," Invited Seminars, General Motors Powertrain and R&D, February 2004.
6. Miles PC. "Automotive Low-Temperature Combustion Research," DOE OFCVT Advanced Engine Combustion Peer Review, Argonne, IL, May 2004.
7. Miles PC. "Identification of Dominant Turbulence Generation Mechanisms in Bowl-in-Piston Combustion Chambers," DOE OFCVT Advanced Engine Combustion Meeting, Southfield, MI, June 2004.
3. Choi D, Miles PC. "A Parametric Study of Low-Temperature, Late-Injection Combustion in an HSDI Diesel Engine," Paper presented at the 6<sup>th</sup> Intl. Symp. on Diagnostics and Modeling of Combustion in IC Engines: COMODIA 2004. August 2-5, Yokohama, 2004.
4. Miles PC, Choi D, Pickett LM, Singh IP, Henein N, RempelEwert BH, Yun H, Reitz RD. "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, 2004.
5. Miles PC. "Light-Duty (Automotive) Diesel Combustion," DOE OFCVT Annual Report, 2003.
6. Zhong L, Henein NA, Bryzyk W. "Effect of Smoothing the Pressure Trace on the Interpretation of Experimental Data for Combustion in Diesel Engines," SAE Paper No. 2004-01-0931, 2004. Also presented at the 2004 SAE World Congress, March 2004. (*Selected for inclusion in 2004 SAE Transactions*)
7. Liu Y, Amr AA, Reitz RD. "Simulation of the Effects of Valve Pockets and Internal Residual Gas Distribution on HSDI Diesel Combustion and Emissions," SAE Paper No. 2004-01-0105, 2004. Also presented at the 2004 SAE World Congress, March 2004. (*Selected for inclusion in 2004 SAE Transactions*)

### **FY 2004 Publications**

1. Miles PC. "In-Cylinder Turbulent Flow Structure in Direct-Injection, Swirl-Supported Diesel Engines," Ch. 1 in *Flow and Comb. in Automotive Engines*, C. Arcoumanis, ed. Springer-Verlag, 2004. (*Invited book chapter, final version submitted*)
2. Miles PC, Choi D, Megerle M, RempelEwert BH, Reitz RD, Lai MC, Sick V. "The Influence of Swirl Ratio on Turbulent Flow Structure in a Motored HSDI Diesel Engine –A Combined Experimental and Numerical Study," SAE Paper No. 2004-01-1678, 2004. Also presented at the 2004 SAE World Congress, March 2004. (*Selected for inclusion in 2004 SAE Transactions*)
1. Kimura S, Ogawa H, Matsui Y and Enomoto Y. "An experimental analysis of low-temperature and premixed combustion for simultaneous reduction of NO<sub>x</sub> and particulate emissions in direct injection diesel engines," *Int. J. Engine Res.*: vol 3: no 4: pp 249-259, 2002.
2. Weißbäck M, Csató J, Glensvig M, Sams T and Herzog P. "Alternative brennverfahren – ein ansatz für den zukünftigen pkw-dieselmotor," *MTZ*: vol 64: pp 718-727, 2003.
3. Miles PC, RempelEwert BH, Reitz RD. "Squish-Swirl and Injection-Swirl Interaction in Direct-Injection Diesel Engines," 6<sup>th</sup> Intl. Conf. on Engines for Automobiles: ICE 2003. Sept. 14-19, Capri, 2003.

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## II.A.4 The Role of Radiative Heat Transfer on NO<sub>x</sub> Formation in a Heavy-Duty Diesel Engine

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### Objectives

- The overall objective of this project is to advance the understanding of diesel engine spray, combustion, and emissions formation processes 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 diesel engines.
- Specific objectives for FY 2004 include:
  - Continue to modernize and upgrade laboratory hardware and capabilities, adding exhaust NO/NO<sub>x</sub> measurement capability and upgrading the common-rail fuel injection system to deliver fuel rail pressures up to 2000 bar (30,000 psi).
  - Explore the factors that affect in-cylinder NO<sub>x</sub> formation under conditions with large premixed burning. Measure soot temperature/radiation and NO<sub>x</sub> as injection timing is retarded and premixed burning becomes significant. Also, investigate the role of soot radiative cooling on NO<sub>x</sub> formation as injection pressure, intake temperature, and EGR rates are varied.

### Approach

- Optical detection of in-cylinder NO<sub>x</sub> is difficult, and quantitative in-cylinder measurements are even more challenging, if not impossible. By contrast, exhaust NO<sub>x</sub> measurements are relatively easy, well established, and highly quantitative. Therefore, to provide quantitative insight into in-cylinder NO formation processes, highly quantitative exhaust NO<sub>x</sub> measurements were married with in-cylinder optical diagnostics of other measurable phenomena.
  - An exhaust NO<sub>x</sub> chemiluminescence analysis capability was implemented in the laboratory to measure NO and NO<sub>x</sub> emissions from the optical engine.
  - A soot thermometry diagnostic was developed to measure soot temperature and radiation to measure in-cylinder temperatures for correlation with exhaust emissions.

### Accomplishments

- Implemented exhaust NO<sub>x</sub> analysis capability in optical engine.
  - Facilitates comparison of quantitative exhaust NO and NO<sub>x</sub> measurements with in-cylinder optical diagnostic data.
- Added new higher-pressure (2000 bar) common rail fuel injection pump to optical engine.
  - Part of ongoing hardware upgrade of optical engine facility to reflect new developments in production hardware.
- Developed new soot temperature/heat transfer diagnostic tool.
  - “3-color” soot thermometry using filtered photodiode detectors.

- Examined  $\text{NO}_x$  formation under large premixed burn conditions.
  - Radiative cooling from hot soot and compression heating of burned gases contribute to increased exhaust  $\text{NO}_x$  with premixed burning.

### Future Directions

- Examine radiation and  $\text{NO}_x$  emissions with multiple/early injections.
  - Early injections: large, slower premixed burn.
  - Pilot injections: can reduce premixed burning,  $\text{NO}_x$ .
  - Split injections: affect soot radiation and  $\text{NO}_x$ .
- Apply other optical diagnostics to low-temperature (exhaust gas recirculation) early injection.
  - Liquid fuel penetration (Mie scatter).
  - Soot formation (laser-induced incandescence and luminosity).
  - Flame development and ignition (planar laser-induced fluorescence of OH and chemiluminescence).

### Introduction

In the near future (2007-2010), air quality regulations for new on-road heavy-duty diesel engines in the United States will require a ten-fold reduction in exhaust emissions from current levels. Although aftertreatment technologies to reduce emissions of particulate matter (PM) and oxides of nitrogen ( $\text{NO}_x$ ) in the exhaust are being aggressively pursued, significant improvements must yet be realized before they may be practically utilized, especially for  $\text{NO}_x$  aftertreatment. Accordingly, reduction of engine-out emissions of  $\text{NO}_x$  (*i.e.*, prior to aftertreatment) remains an important strategy for regulatory compliance.

Several chemical pathways for NO (and hence,  $\text{NO}_x$ ) formation in combustion systems have been identified. In diesel engines, flame temperatures are high enough that oxygen and nitrogen molecules in the air react to form NO. This pathway, called the “thermal NO mechanism,” is expected to be the dominant NO formation pathway in diesel engines. Thermal NO formation increases exponentially with temperature. Hence, NO formation may be reduced significantly by reducing flame temperatures, which can be accomplished by charge dilution, for example, using exhaust gas recirculation (EGR). Indeed, engine-out  $\text{NO}_x$  has been shown to correlate exponentially with the calculated adiabatic flame temperature as EGR is varied [1]. This degree of success attests to the importance of flame temperature and thermal NO formation in diesel

engines. Although flame temperature reduction by EGR has a dominant effect on  $\text{NO}_x$ , other factors can also affect NO formation significantly.

It has long been recognized that diesel combustion occurs in both premixed modes (immediately following ignition) and non-premixed modes (latter part of combustion). A correlation between diesel premixed burning and engine-out  $\text{NO}_x$  emissions has been demonstrated in numerous investigations, especially when caused by fuel cetane number effects [2]. The increase in exhaust  $\text{NO}_x$  with increasing premixed burning often cannot be explained by changes in the calculated adiabatic flame temperature. In some instances, the differences in the energy contents of the fuels and the phasing of combustion may be responsible, but in many other studies, the increase in exhaust  $\text{NO}_x$  cannot be explained by these factors.

Hence, understanding of the factors that affect  $\text{NO}_x$  formation for conditions with increased premixed burning is currently incomplete. Many new diesel engine combustion strategies are currently being developed, and many of these strategies employ enhanced fuel premixing prior to combustion, and consequently, increased premixed burning. An improved understanding of the mechanisms responsible for increased  $\text{NO}_x$  emissions could provide new insight into strategies to mitigate  $\text{NO}_x$  emissions.

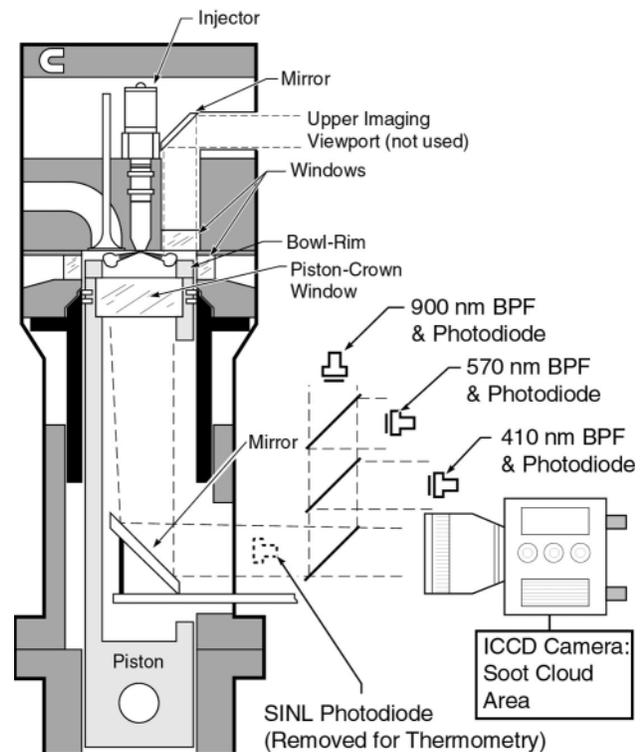
One potential explanation for the increase in  $\text{NO}_x$  formation with increased premixing is changes in the actual flame temperature caused by changes in radiative heat transfer from hot soot. Previous measurements of radiation for highly sooting diesel conditions show that radiative heat transfer can be significant [3]. As premixed burning is increased, the soot in the jet can decrease, so that radiative heat transfer should also decrease. This could yield higher flame temperatures. Prior to the current study, the magnitude of this effect, and thus its importance on NO formation, had not been quantified.

It is the objective of this study to examine the role of radiative heat transfer on in-cylinder flame temperatures and in-cylinder NO formation. 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. Additional access for imaging and/or laser diagnostics is provided by a window inserted in the cylinder head in place of one of the exhaust valves, and by five windows inserted in the cylinder wall. The engine is capable of operating under fired conditions over the full range of conditions typical of production diesel engines.

In the current study, a soot thermometry diagnostic was developed to measure soot temperature and radiative heat transfer. As shown in Figure 1, the diagnostic utilizes three photodiode detectors and an imaging camera. Narrow bandpass filters, centered at 410 nm, 570 nm, and 900 nm, were placed in front of the photodiodes so that they

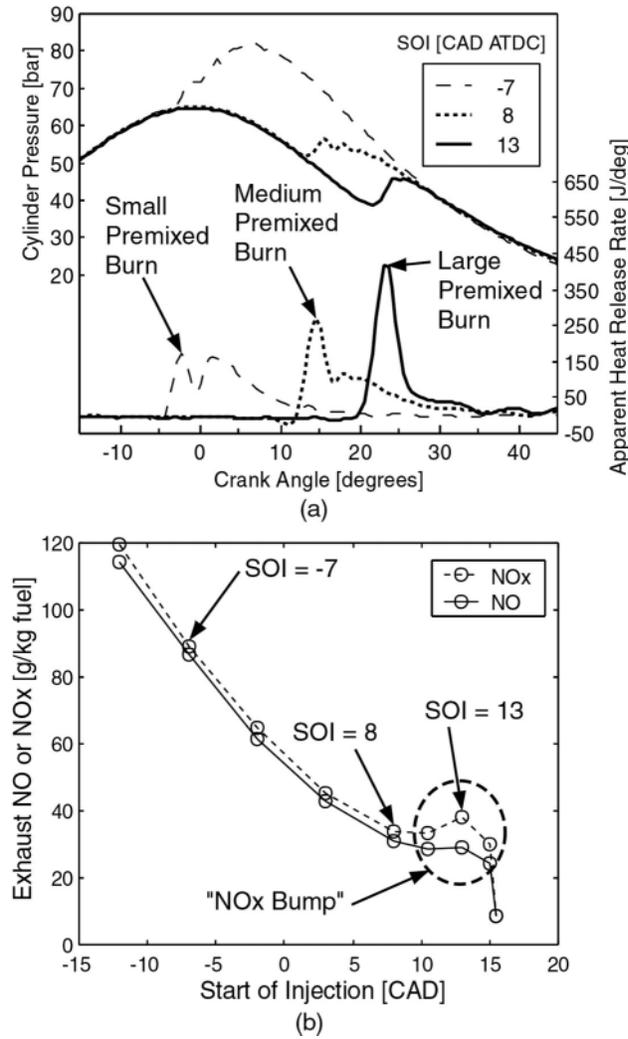


**Figure 1.** Schematic Diagram Showing Optical Engine and Soot Thermometry Diagnostic

measure the light emitted during combustion at three different colors. Soot particles, formed during combustion and heated to high temperatures, emit light in a broadband spectrum, and the intensities at various colors depend on the temperature and concentration of the soot. Hence, the intensity measurements from the photodiodes at three different colors can be used to determine the soot temperature and concentration. The area of the emitting soot cloud, which is provided by the imaging camera shown in Figure 1, is also necessary to determine the soot temperature and concentration. Other necessary improvements to the laboratory facility include the addition of an exhaust gas chemiluminescence  $\text{NO}_x$  analyzer and a new higher-pressure fuel delivery system for the common-rail fuel injector.

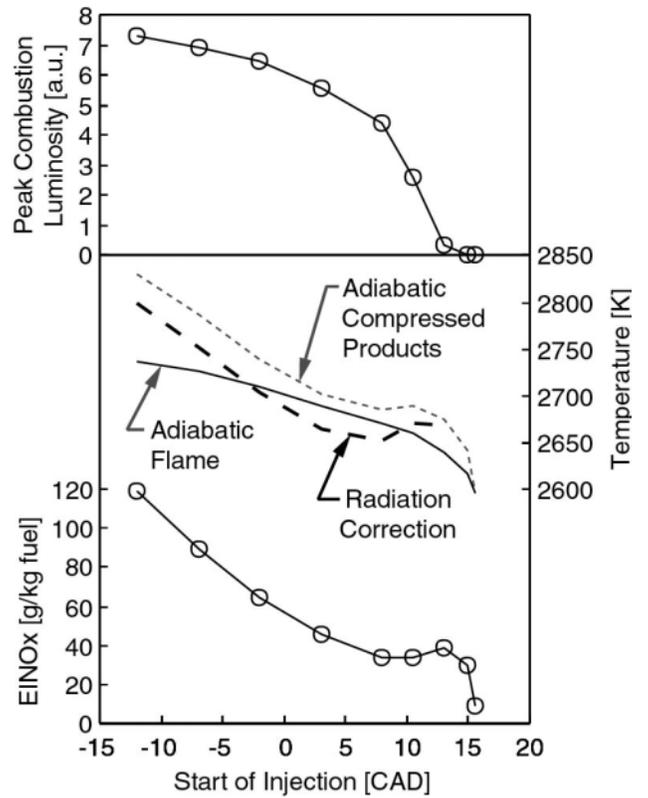
### Results

Shown at the bottom of Figure 2 are exhaust NO and  $\text{NO}_x$  measurements for a start of injection (SOI) timing sweep from -12 crank angle degrees (CAD) after top dead center (ATDC) to +15.5 CAD ATDC. The emissions index of the exhaust  $\text{NO}_x$  ( $\text{EINO}_x$ ) is



**Figure 2.** (a) Cylinder pressure and apparent heat release rate for three different SOI timing conditions. (b) Exhaust index of NO and NO<sub>x</sub> for a sweep of SOI timings. The circled region indicates the location of the “NO<sub>x</sub> bump.”

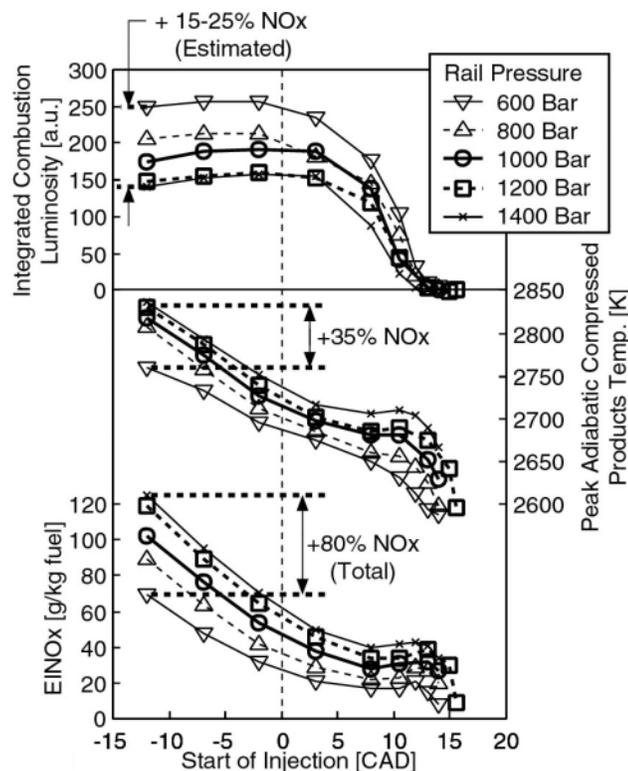
largest at early SOI and decreases as the SOI is retarded. Near SOI = +8, the EINO<sub>x</sub> trend changes, as it begins to increase with further retard of SOI, reaching a peak at SOI = +13. This peak in EINO<sub>x</sub> at late SOI is termed the “NO<sub>x</sub> bump,” as indicated in Figure 2. Shown at the top of Figure 2 are representative cylinder pressure and apparent heat release rates for SOI = -7, +8, and +13. For the early injection conditions, the heat release rate displays a small premixed burn, as typified by the SOI = -7 condition. At SOI = +8, the magnitude of the premixed burn becomes moderate, and at SOI = +13, where the EINO<sub>x</sub> increases, the premixed burn



**Figure 3.** Variation with SOI timing of (top) combustion luminosity, (middle) peak adiabatic flame, adiabatic and radiation-corrected compressed burned gas temperature, and (bottom) measured EINO<sub>x</sub>.

becomes large. This observation is an example of the correlation between diesel premixed burning and increased exhaust NO<sub>x</sub> emissions.

The peak adiabatic flame temperature for each SOI in Figure 2 is shown in the middle of Figure 3, and the EINO<sub>x</sub> data from Figure 2 is shown at the bottom of Figure 3 for reference. As the SOI is retarded, the peak adiabatic flame temperature monotonically decreases, even through the NO<sub>x</sub> bump. Hence, the increase in EINO<sub>x</sub> at the NO<sub>x</sub> bump cannot be explained by changes in the adiabatic flame temperature. A larger premixed burn, however, does increase the compression of burned gases after they pass through the flame. Compression of burned gases for conditions with early injection or large premixed burning can yield gas temperatures even higher than the flame temperature, yielding increased NO formation. Shown as a dotted line in the middle of Figure 3, the



**Figure 4.** Variation with SOI timing of (top) combustion luminosity, (middle) peak adiabatic compressed burned gas temperature, and (bottom) measured EINO<sub>x</sub> for a range of fuel rail pressures, as indicated in the legend.

calculated peak temperature of the compressed burned gases increases slightly near the NO<sub>x</sub> bump, but this increase is insufficient to cause the entire NO<sub>x</sub> bump.

Concurrent with the EINO<sub>x</sub> data, soot luminosity (*i.e.*, light emitted by hot in-cylinder soot) was measured with one of the photodiodes in Figure 1, and the peak soot luminosity at each SOI is shown at the top of Figure 3. From SOI = +8 to SOI = +13 where the NO<sub>x</sub> bump develops, the combustion luminosity decreases precipitously, suggesting that radiative heat transfer from the soot may also decrease as premixed burning becomes large. If the cooling effect of radiative heat transfer decreased, the gas temperature would increase. Using the soot thermometry diagnostic, the radiative heat transfer from the hot soot was measured, and this was used to correct the compressed burned gas temperature for the cooling effect of soot radiation, as shown in Figure 3 as a dashed line. The radiation correction

yields a larger increase in temperature near the NO<sub>x</sub> bump and is large enough to nearly account for the entire NO<sub>x</sub> bump. Hence, the combination of increasing burned-gas compression and decreasing soot radiative cooling can cause the peak gas temperature to increase as premixed burning becomes large. Based on the data acquired in the current study, these two effects are the primary factors responsible for the correlation between premixed burning and increased exhaust NO<sub>x</sub> emissions.

Another practical example of the role of radiation and burned-gas compression on in-cylinder temperatures and NO formation is the well-known increase in exhaust NO<sub>x</sub> that accompanies increased injection pressure. Shown in Figure 4 are the EINO<sub>x</sub>, compressed burned gas temperature, and combustion luminosity for a series of timing sweeps acquired with fuel rail pressures ranging from 600 bar to 1400 bar. As shown at the bottom of Figure 4, as the injection pressure is increased, the EINO<sub>x</sub> generally increases with fuel rail pressure. At SOI = -12, for example, the EINO<sub>x</sub> increases by 80% from the lowest to the highest fuel pressure. As shown in the middle of Figure 4, the compressed burned gas temperature increases by 75 K, which corresponds to an increase in EINO<sub>x</sub> of about 40%. The peak combustion luminosity, shown at the top of Figure 4, decreases by about half, which corresponds to an estimated increase in EINO<sub>x</sub> of 15-25%. (Complete soot thermometry data were not acquired for the fuel rail pressure sweep, but soot luminosity data is indicative of changes in radiative heat transfer.) The combination of these two effects predicts that EINO<sub>x</sub> should change by a factor of  $1.4 \times 1.2 = 1.7$ , *i.e.*, a 70% increase, compared to the 80% increase that was actually measured. This is good agreement, considering the simplifying assumptions employed in this analysis. With the improved understanding of the factors that affect NO formation provided by this study, other trends in NO emissions observed with advanced diesel operational strategies will be better understood, helping to improve the development process.

## Conclusions

Through comparison of exhaust NO<sub>x</sub> measurements with in-cylinder soot thermometry,

the influence of soot radiative cooling and burned-gas compression on  $\text{NO}_x$  formation was studied. Analysis of the data supports the following conclusions:

- For the injection timing sweeps examined in this study, changes in exhaust  $\text{NO}_x$  with increasing premixed burning cannot be explained by changes in the adiabatic flame temperature.
- As the premixed burn increases in magnitude, the cooling effect of in-cylinder soot radiation decreases, yielding a hotter flame, contributing to the increase in exhaust  $\text{NO}_x$ .
- Compression of burned gases also yields hotter estimated temperatures, further contributing to the increase in exhaust  $\text{NO}_x$ .
- Other practical examples of changes in exhaust  $\text{NO}_x$  that cannot be explained by changes in adiabatic flame temperature, such as the increase of exhaust  $\text{NO}_x$  with fuel injection pressure, may be explained by these two factors.

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2. Musculus, M. P. B. and Pickett, L. M. "Diagnostic Considerations for Soot Extinction Diagnostic in Transient High Pressure Combustion Environments," submitted to Combustion and Flame, June 2004.
3. Musculus, M. P. B., "On the Correlation between  $\text{NO}_x$  Emissions and the Diesel Premixed Burn," SAE Paper 2004-01-1401, SAE International Congress and Exposition, March 2004.
4. Musculus, M. P. B., and Dec., J. E., "Effects of the In-Cylinder Environment and Diffusion Flame Lift-Off in a Heavy-Duty Diesel Engine," Department of Energy Annual Project Report, November 2003.
5. Musculus, M. P. B., Dec, J. E. and Tree, D. R., "Effects of Fuel Parameters and Diffusion Flame Lift-Off on Soot Formation in a Heavy-Duty DI Diesel Engine," SAE Paper 2002-01-0889, SAE International Congress and Exposition, Published in SAE Transactions, September 2003.
6. "On the Correlation between  $\text{NO}_x$  Emissions and the Diesel Premixed Burn," SAE International Congress and Exposition, Detroit, MI, March 2004.
7. "The Influence of Soot Radiative Heat Transfer on In-Cylinder Temperatures and  $\text{NO}_x$  Formation," Advanced Engine Combustion Meeting, Sandia National Laboratories, January 2004.
8. "On  $\text{NO}_x$  Formation and the Diesel Premixed Burn," Advanced Engine Combustion Meeting, Sandia National Laboratories, June 2003.

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## II.A.5 Low Flame Temperature Diesel Combustion and Effects of Jet-Wall Interaction

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### Objectives

- Identify methods for producing low-flame-temperature, soot-free, mixing-controlled diesel combustion to minimize nitrogen oxide ( $\text{NO}_x$ ) and particulate matter (PM) emissions.
- Investigate the minimum flame temperature limits for mixing-controlled diesel combustion.
- Determine how jet-wall interaction affects soot formation. Make the distinction between jet-wall impingement effects and subsequent jet-jet interactions.

### Approach

- Utilize advanced optical diagnostics coupled with a unique optically-accessible diesel combustion simulation facility (DCSF) to conduct these investigations.
- Vary flame temperature by adjusting exhaust gas recirculation (EGR) level (ambient gas oxygen concentration).
- Perform quantitative soot and combustion measurements in a plane wall jet and “confined” jet configuration.

### Accomplishments

- Demonstrated that diesel combustion is soot-free for an ambient gas oxygen concentration of 8% and typical diesel ambient gas temperature (1000 K). Flame temperatures are also simultaneously low (less than 1800 K), implying that this combustion has minimal  $\text{NO}_x$  formation.
- Found that combustion efficiency remains high for mixing-controlled diesel combustion with flame temperatures as low as 1500-1600 K for conditions where the ambient gas temperature is greater than 1000 K. This low flame temperature limit is less than that of propagating flame processes in engines but close to that of homogeneous charge compression ignition (HCCI) combustion.
- Showed that the mass of soot downstream of the wall impingement location is approximately a factor of two less in a plane wall jet compared to a free jet. Possible mechanisms for the reduced soot formation include enhanced air entrainment and thermal interaction (cooling) of the jet.
- In a confined geometry that simulates adjacent jet interaction, we found the effect of wall interaction has an opposite effect: soot levels increase compared to a free jet or a plane wall jet. Soot increases when redirected combustion gases shorten the lift-off length, thereby making the fuel-air mixture at the lift-off length more fuel-rich.

## Future Directions

- Determine the low temperature limit for soot formation in a reacting diesel fuel jet.
- Investigate how very high EGR affects diesel soot formation by performing quantitative measurements for ambient oxygen concentrations ranging from 21% to 10%.
- Investigate injection rate modulation and orifice geometry effects on diesel combustion and emissions processes.

## Introduction

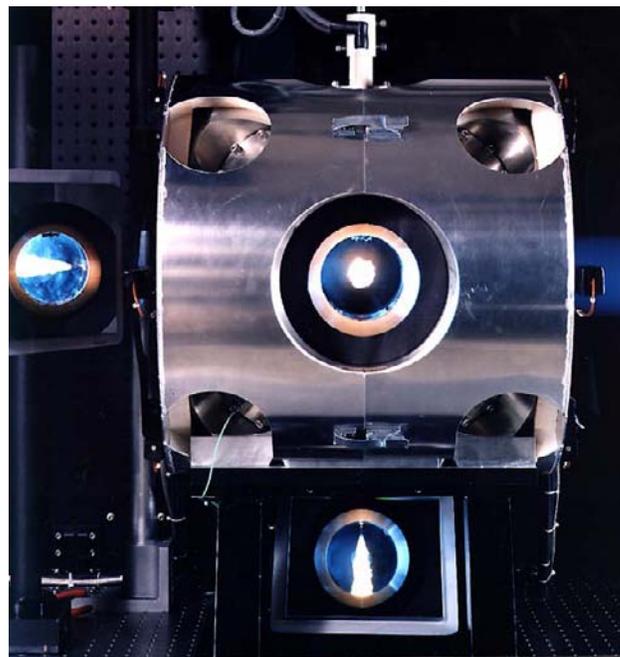
A major objective for experiments in the DCSF this year was to determine what factors affect soot formation during mixing-controlled diesel combustion with flame temperatures less than approximately 2000 K—too low for significant  $\text{NO}_x$  formation. A second objective was to determine if diesel combustion at temperatures far below 2000 K is possible. These low-temperature combustion regimes are of great interest for diesel combustion because of the potential for engine-out  $\text{NO}_x$  minimization without the use of aftertreatment. Interest in mixing-controlled diesel combustion is also motivated by the fact that mixing-controlled heat release remains closely coupled to injector controls, and many of the benefits of diesel combustion are inherently connected to this characteristic. The work is further motivated by results from the previous year, which showed that under some conditions it is possible to produce soot-free, low-temperature reacting diesel jets.

The third objective was to identify how realistic engine effects, such as jet-wall interaction, affect diesel combustion and soot formation. The wall has an effect on the mixing and combustion processes of the fuel jet through impingement and redirection of the fuel jet, and the wall also confines the fuel jet such that it turns back on itself and interacts with the adjacent fuel jets. At realistic diesel conditions (high temperature and pressure), a direct comparison of mixing and soot production between a free jet and a plane wall jet or spray has not been addressed experimentally. Moreover, the effect of jet-wall interaction has not been isolated from the ensuing jet-jet interaction. Wall jet experiments at diesel conditions would help the diesel engine community to better understand the basic processes governing soot production. This information, in turn, could help extend results to more complex and realistic engine conditions.

## 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.

Diesel flame temperatures were controlled by varying ambient gas oxygen concentration to simulate the effect of EGR in an engine. Combustion



**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  $45^\circ$  next to the bottom and left-side windows show side views of the burning spray.

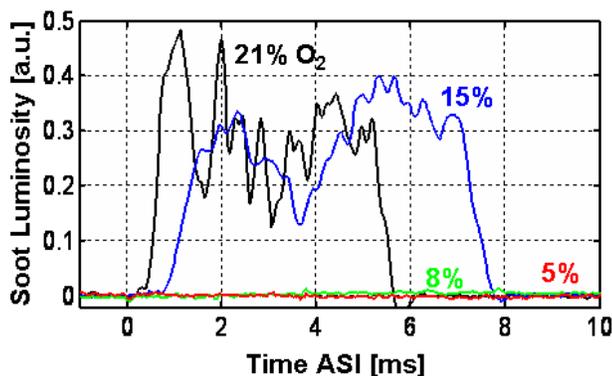
was studied after autoignition and premixed burn so that the diesel combustion would be dominated by mixing-controlled combustion [1].

The effects of jet wall interaction were investigated in the DCSF in two experimental configurations: a jet impinging on a plane wall without any additional geometrical constraints and a “confined” jet (a box-shaped geometry simulating secondary interaction with adjacent walls and jets in an engine). In this way, the effects of adjacent geometry and jet interaction were separated from the effects of plane wall interaction. Details of the experimental setup can be found in Reference [2].

**Results**

Figure 2 shows soot luminosity during the time of injection at various ambient oxygen levels. The figure demonstrates that there is no soot formation with 5% or 8% ambient oxygen, corresponding to very high EGR levels in an engine. The discovery that soot formation is impeded at low oxygen concentration is significant because flame temperatures are also very low. These results were achieved with a conventional injector nozzle (180 μm), as opposed to reports from previous years in which a small injector nozzle (50 μm) was needed to achieve non-sooting, low-temperature combustion.

Summarizing research from this year and last year, a schematic illustrating how the three different methods avoid soot formation and produce low flame

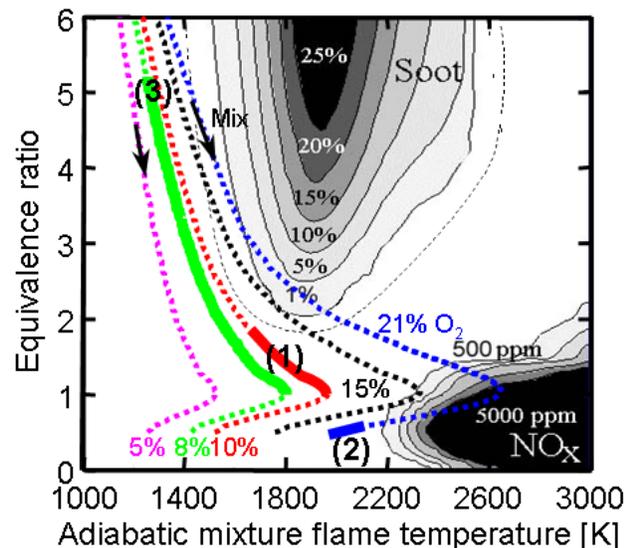


**Figure 2.** Spatially-integrated natural luminosity for four ambient gas oxygen concentrations. The ambient gas temperature and density were 1000 K and 30.0 kg/m<sup>3</sup>, respectively, and the orifice size was 180 μm.

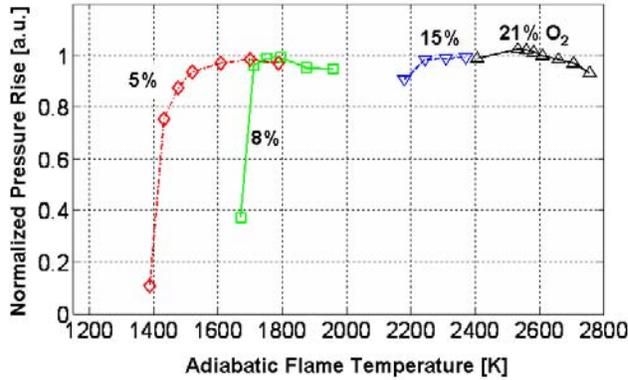
temperature is shown in Figure 3. Figure 3 is a plot of equivalence ratio versus temperature, with contours indicating the locations where soot and NO<sub>x</sub> formation occur for a diesel-like fuel. Overlaid on the plot are curves (dashed) showing the predicted adiabatic flame temperatures for fuel-air mixtures at the given equivalence ratios for five ambient oxygen concentrations.

The first two methods for low-temperature combustion were discussed last year and involve fast mixing coupled with EGR (1) or fuel-lean mixing-controlled combustion (2) by inducing very high fuel-air mixing prior to the lift-off length. The lean mixture avoids both soot formation and a high-temperature stoichiometric diffusion flame. The third method (3), discovered this year, relies on the use of very high EGR (8% ambient oxygen), resulting in mixtures in the fuel jet that are rich, but with peak adiabatic flame temperatures that are too cool for soot inception at diesel timescales.

Despite the low flame temperature at high-EGR conditions, pressure-rise measurements show that combustion efficiency remains high for flame temperatures as low as 1500-1600 K, as shown in Figure 4. This is true for conditions where the ambient gas temperature is greater than 1000 K. This



**Figure 3.** Three methods for soot-free, low-flame-temperature, mixing-controlled diesel combustion shown on a schematic of equivalence ratio versus adiabatic mixture flame temperature.

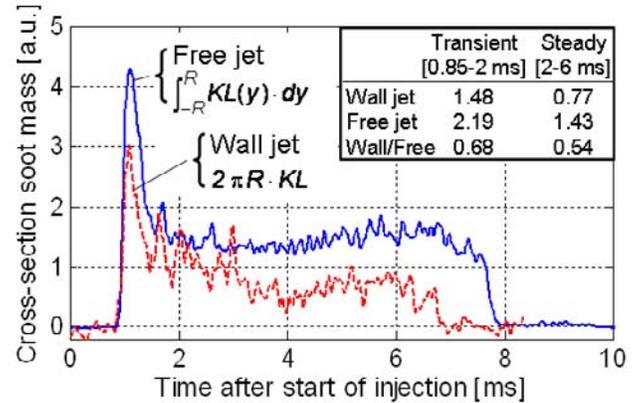


**Figure 4.** Normalized maximum pressure rise of diesel combustion *versus* flame temperature at four ambient oxygen concentrations.

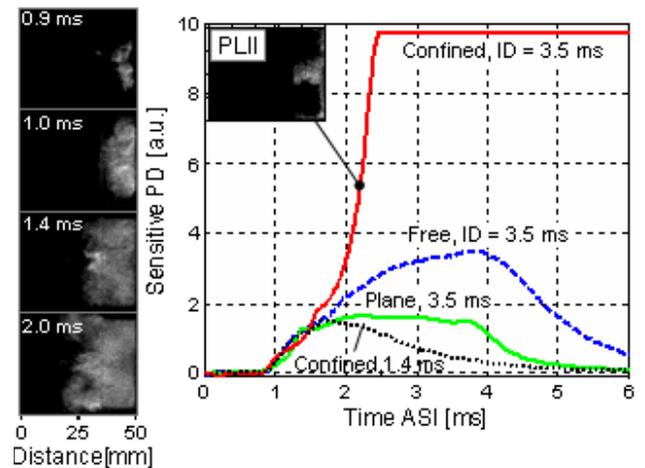
low flame temperature limit is less than that suggested for propagating flame processes in engines and is close to that observed for HCCI combustion.

The effects of plane wall interaction on soot formation processes of a diesel fuel jet are shown in Figure 5. The figure shows integrated soot mass measurements in a free jet or plane wall jet at a downstream cross-section of the jet at identical ambient and injector conditions. Soot levels are significantly lower in a plane wall jet compared to a free jet. At other operating conditions, sooting free jets become soot-free as plane wall jets. Possible mechanisms to explain the reduced or delayed soot formation upon wall interaction include an increased fuel-air mixing rate and a wall-jet cooling effect [2].

In a confined-jet configuration, however, there is an opposite trend in soot formation. Figure 6 shows that jet confinement causes combustion gases to be redirected towards the incoming jet, causing the lift-off length to shorten and soot to increase. The figure shows highly sensitive photodiode measurements of fuel jet luminosity at two different injection durations (ID) for various wall-jet configurations. The sensitivity of the photodiode is such that if soot formation occurs, the soot luminosity saturates the detector. Therefore, detectable levels of luminosity for the photodiode are due to chemiluminescence of non-sooting diesel combustion. Images of chemiluminescence are shown at the left for the “confined” jet configuration. The free jet and plane wall jet are non-sooting with an injection duration of 3.5 ms. However, the confined jet is non-sooting

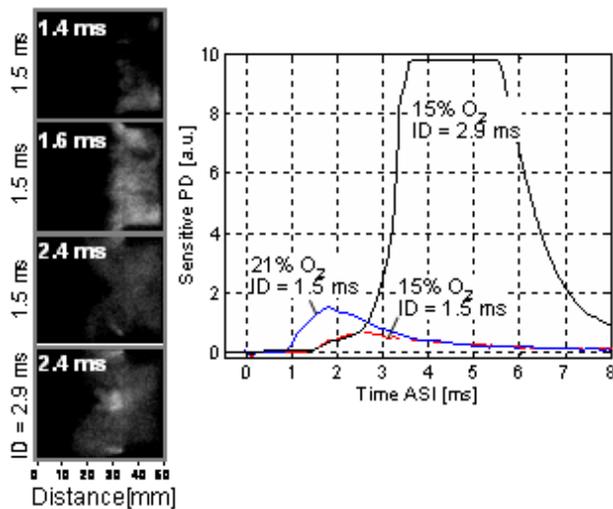


**Figure 5.**  $KL$  integral (soot mass) versus time for a free jet and a plane wall jet. Ambient gas temperature and density were 1000 K and 14.8 kg/m<sup>3</sup>, respectively. The  $KL$  measurement positions were  $x = 70$  mm for the free jet and  $R = 20$  mm for the plane wall jet with a wall position of  $x = 50$  mm. Time-integrals of the soot mass profile are indicated in the legend.



**Figure 6.** Time sequence of OH chemiluminescence images (left) and flame luminosity emission images (right) for various wall configurations. Ambient gas temperature was 900 K. Injection duration (ID) is indicated on the graph. ID was 3.5 ms ASI for the OH chemiluminescence image sequence. A PLII image showing that soot formation corresponds to a rapid rise in luminous emission is inset on the graph.

only with an injection duration of 1.4 ms. The time-sequence of chemiluminescence for the confined jet shows that combustion gases are redirected back towards the injector for extended injection durations.



**Figure 7.** Time sequence of OH chemiluminescence images (left) and flame luminosity emission (right) for a confined jet with an ambient gas oxygen concentration of 15%.

The redirected combustion gases cause the lift-off length to shorten, thereby making the fuel-air mixture at the lift-off length more fuel-rich. The time after the start of injection of soot formation corresponds to the time shortly after this time of jet interaction with redirected combustion gases. The figure also shows that if the injection event is concluded prior to this jet interaction event, soot formation is avoided.

Jet interaction with redirected combustion products may also be avoided using reduced ambient oxygen concentration, as shown in Figure 7. One might suspect that EGR would increase the likelihood of combustion gas interactions at the lift-off length. This is because the lift-off length increases with the use of EGR and also there is less available oxygen in the confined region of the jet. However, Figure 7 shows that the use of EGR did not increase the sooting tendency of a confined jet for similar injection durations. Soot luminosity levels do not saturate the detector for an ignition delay of 1.5 ms, indicating that combustion is non-sooting.

The surprising result that there was no soot formation at 15% ambient oxygen appears to be caused by an increase in the ignition delay. Figure 7 shows that autoignition for the 15% oxygen condition is nearly coincident with the end of

injection at 1.5 ms after start of injection (ASI), compared to 0.9 ms ASI for 21% oxygen. The time sequence of OH chemiluminescence for the 15% oxygen condition is consistent with the rise in spatially integrated flame luminosity. At 1.4 ms ASI, ignition kernels are shown within the confines of the box-shape. The OH chemiluminescence quickly fills the box-shape by 1.6 ms ASI. However, because injection has ended, the opportunity for combustion product interaction and its effect on lift-off length is avoided. At 2.4 ms ASI, for example, there is only weak chemiluminescence within the box region. If injection is continued (ID = 2.9 ms), reaction races back towards the injector as shown in the lower left image at 2.4 ms ASI. Soot formation follows shortly thereafter.

## Conclusions

A new method for soot-free, low-flame-temperature, mixing-controlled diesel combustion was demonstrated using conventional injector technology. Also, combustion efficiency remains high for flame temperatures as low as 1500-1600 K. The lack of soot formation and low flame temperatures realized suggest that there is a potential for a simultaneous soot and  $\text{NO}_x$  reduction in an engine, while maintaining a mixing-controlled heat release rate. Jet-wall interaction studies on soot formation show decreased soot formation for plane wall interaction only and increased soot formation when the jet is confined. The identification of important mechanisms affecting combustion and soot formation is expected to be useful for understanding these processes in more complex and realistic diesel engine geometries and also provides guidance to engine designers on directions to proceed to lower soot and  $\text{NO}_x$  emissions.

## Presentations

1. Pickett, L.M., López, J.J., "Jet-Wall Interaction Effects on Soot Formation in a Diesel Fuel Jet," COMODIA 2004, Yokohama, Japan, August 2004.
2. Pickett, L.M., Siebers, D.L., "Low Flame Temperature Limits for Mixing-Controlled Diesel Combustion," 30th International Symposium on Combustion, Chicago, IL, July 2004.
3. Pickett, L.M., "Low Temperature Limits for Soot Formation in Diesel Fuel Jets," AEC meeting, Detroit, MI, June 2004.

4. Pickett, L.M., "Low Flame Temperature Diesel Combustion with Jet-Wall Interaction," DOE Advanced Combustion Engine Annual Review, Chicago, IL, May 2004.
5. Pickett, L.M., Siebers, D.L., "Non-Sooting, Low Flame Temperature Mixing-Controlled DI Diesel Combustion," SAE World Congress, Detroit, MI, March 2004.
6. Pickett, L.M., López, J.J., "Jet-Wall Interaction Effects on Soot Formation in Diesel Fuel Jets," SAE World Congress, AEC meeting, Livermore, CA, January 2004.
7. Pickett, L.M., Siebers, D.L., "Fuel Effects on Soot Processes of Fuel Jets at DI Diesel Conditions," SAE Powertrain and Fluid Systems Conference, Pittsburgh, PA, October 2003.
8. Pickett, L.M., and Siebers, D.L., "Non-Sooting, Low-Flame Temperature, and Mixing-Controlled DI Diesel Combustion," 9<sup>th</sup> Diesel Engine Emissions Reduction Conference, Newport, RI, August 24-28, 2003.
5. 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.
6. López, J.J., and Pickett, L.M., "Jet/Wall Interaction Effects on Soot Formation in a Diesel Fuel Jet," accepted to COMODIA 2004, Yokohama, Japan, August 2-5, 2004.
7. Pickett, L.M., and Siebers, D.L., "Non-Sooting, Low Flame Temperature Mixing-Controlled DI Diesel Combustion," SAE World Congress, 2004-01-1399 (accepted for Transaction of the SAE 2004).
8. Pickett, L.M., and Siebers, D.L., "Soot in Diesel Fuel Jets: Effects of Ambient Gas Temperature, Ambient Density and Injection Pressure," Combustion and Flame, 138:114-135, 2004.
9. Pickett, L.M., and Siebers, D.L., "Fuel Effects on Soot Processes of Fuel Jets at DI Diesel Conditions," SAE Powertrain and Fluid Systems Conference, 2003-01-3080 (accepted for Transaction of the SAE 2003).
10. Pickett, L.M., and Siebers, D.L., "Non-Sooting, Low-Flame Temperature, and Mixing-Controlled DI Diesel Combustion," 9<sup>th</sup> Diesel Engine Emissions Reduction Conference, Newport, RI, August 24-28, 2003.

### **Publications**

1. Pickett, L.M., and López, J.J., "Jet-Wall Interaction Effects on Diesel Combustion and Soot Formation," submitted to SAE World Congress, 2005.
2. Pickett, L.M., "Low Flame Temperature Limits for Mixing-Controlled Diesel Combustion," 30th International Symposium on Combustion, Chicago, IL, July 25-30, 2004.
3. Musculus, M.P.B., and Pickett, L.M., "Diagnostic Considerations for Optical Laser-Extinction Measurements of Soot in High-Pressure Transient Combustion Environments," submitted to Combustion and Flame, 2004.
4. 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.

### **References**

1. Pickett, L.M., and Siebers, D.L., "Non-Sooting, Low Flame Temperature Mixing-Controlled DI Diesel Combustion," SAE World Congress, 2004-01-1399.
2. Pickett, L.M., and López, J.J., "Jet-Wall Interaction Effects on Diesel Combustion and Soot Formation," submitted to SAE World Congress, 2005.

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

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### Objectives

- Explore potential of expanding the HECC speed/load operation range in a light-duty diesel engine while relying on production-like controls.
- Demonstrate HECC operation under road-load type conditions.
- Characterize effect of transition pathway from original equipment manufacturer (OEM) to HECC operation on emissions and performance.

### Approach

- Explore potential strategies for achieving HECC operation on a Mercedes 1.7-L diesel engine with reliance only on production-like controls.
- Explore effect of transition pathway from OEM to HECC operation on emissions and performance.
- Perform detailed emissions and combustion characterization to improve understanding of efficient advanced combustion modes.

### Accomplishments

- Explored potential of achieving HECC over a range of speeds and loads. Based on these experiments, modifications will be made to the experimental setup in FY 2005 in an attempt to increase the HECC operation window for this engine.
- Demonstrated efficient operation with a 90% reduction in oxides of nitrogen (NO<sub>x</sub>) and a 50% reduction in particulate matter (PM) emissions under road-load type conditions (20% load, 1500 rpm) without excessive hydrocarbon (HC) emissions.
- Investigated transition from OEM to HECC operation. Experimental results indicate that the transition pathway has strong impact on achieving efficient operation.

### Future Directions

- Upgrade engine control system for greater flexibility in injection timing and frequency as well as improved transient capability.
- Modify experimental setup to include a low-pressure exhaust gas recirculation (EGR) system and a diesel atomizer for partially premixed strategies to explore expanding the effective HECC speed/load range.
- Investigate techniques for entering and exiting HECC modes and consider potential diagnostic tools for feedback control when transitioning between these modes. Methods for transitioning between conventional diesel and HECC operation may have an important role in minimizing harmful emissions and maintaining efficiency.

## **Introduction**

Researchers at Oak Ridge National Laboratory (ORNL) have been exploring the potential of new combustion regimes that exhibit simultaneous low  $\text{NO}_x$  and PM emissions. An improved understanding of these combustion modes is critical for lowering the performance requirements for post-combustion emissions control devices and meeting future U.S. emissions and efficiency goals. Through proper combustion management, ORNL has achieved significant reductions in  $\text{NO}_x$  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 acceptance of significant fuel penalties.

Another important aspect of operating diesel engines in advanced combustion modes is the ability to transition in and out of these modes with minimal adverse effects on emissions or performance. ORNL researchers were able to demonstrate seamless transitions with no significant emissions excursions or effects on performance.

## **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 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 specific injection parameters. EGR was used to achieve a low- $\text{NO}_x$ , 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 OEM condition to HECC operation using this approach was also investigated using the advanced controller.

## **Results**

Extensive experiments have been performed to develop approaches for achieving HECC operation in a light-duty diesel engine. The results of an example road-load condition are summarized in Table 1. The OEM condition is 1500 rpm at 2.6 bar brake mean effective pressure (BMEP). Results are shown for the OEM condition, the low- $\text{NO}_x$  low-PM condition (LTC), and the HECC condition, which may also be referred to as an "efficient LTC" condition. Note that the phrase LTC as used in the literature typically refers to a low- $\text{NO}_x$  low-PM condition only and provides no information concerning efficiency. In this document, the LTC condition should be thought of as an intermediate condition which was explored during the search for HECC operation. Comparing the OEM and HECC conditions in Table 1, a 90% reduction in  $\text{NO}_x$  and a 30% reduction in PM is shown between the two cases with no degradation to engine efficiency or increase in HC emissions. Also note that this was achieved with conventional rail pressures and a single fuel injection event.

The average heat release profiles for the conditions in Table 1 are shown in Figure 1. A significant shift in the heat release profile was observed with increasing EGR, as seen in comparing Figures 1(a) and 1(b). The heat release profile is recovered (or improved) by re-phasing the combustion process with injection timing to achieve HECC operation, as illustrated in Figure 1(c). Recall from Table 1 that the pilot injection was disabled during HECC operation. The 10-50% heat release interval was shorter for HECC operation as

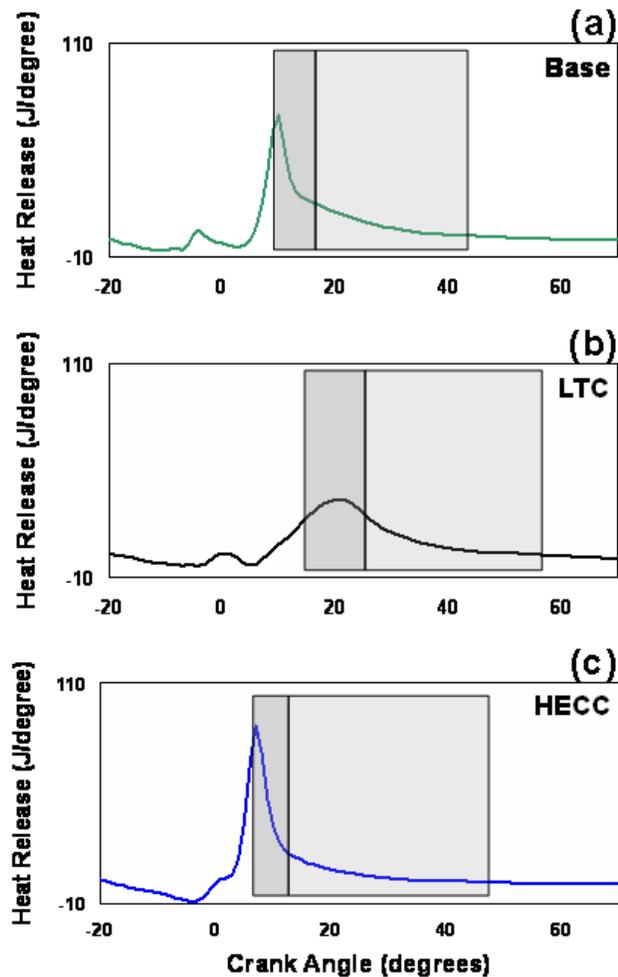
**Table 1.** Example of HECC Operation at Road-Load Conditions (1500 rpm, 2.6 bar BMEP)

	OEM	LTC	HECC
EGR (%)	21	49	48
BSFC (g/hp-hr)	211	240	209
NO <sub>x</sub> (g/hp-hr)	1.2	0.1	0.1
PM (g/hp-hr)	0.38	0.51	0.29
THC (g/hp-hr)	2.68	4.54	2.46
Intake Temp (°C)	43	129	94
Exhaust Temp (°C)	205	244	199
Main Timing (BTDC)	2	2	12
Pilot Timing (BTDC)	18	18	Off
Rail Pressure (bar)	320	320	328

compared to OEM operation, indicating a higher fraction of premixed (or kinetically controlled) combustion. Conversely, the 50-90% heat release interval was longer for HECC operation, indicating a slower mixing-controlled combustion phase, potentially due to the increased EGR level under the HECC condition.

HECC operation using high levels of EGR results in a reduction in volumetric efficiency due to the increase in the temperature of the inducted intake charge. For the case summarized in Table 1, the temperature of the intake charge increased from 43°C for the OEM condition to 94°C for the HECC condition, but the thermal efficiency remained unchanged at approximately 30% for the two conditions. Therefore, some form of a reduction in losses occurred during the engine cycle. Further analysis is necessary to determine whether the reduction in losses is due to heat transfer effects or the combustion process. A more detailed first- and second-law thermodynamic analysis will be applied to this and other HECC data during the next phase of this activity. Not shown in the average heat release profiles is the effect of these different operating modes on engine stability. The coefficient of variation (COV) in indicated mean effective pressure (IMEP) increased with EGR level but returned to a comparable OEM level during HECC operation.

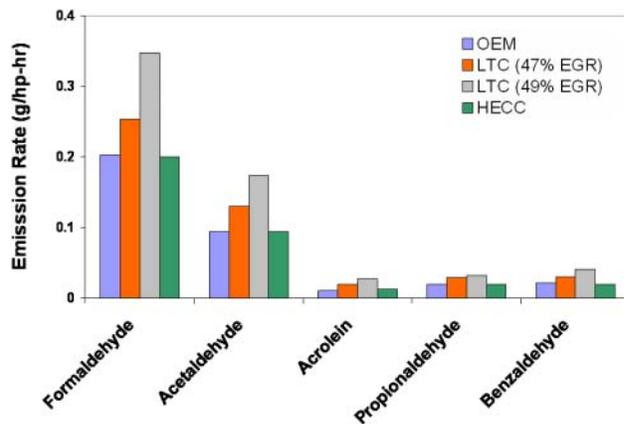
Exhaust constituents were analyzed in detail to characterize the production of aldehyde emissions for



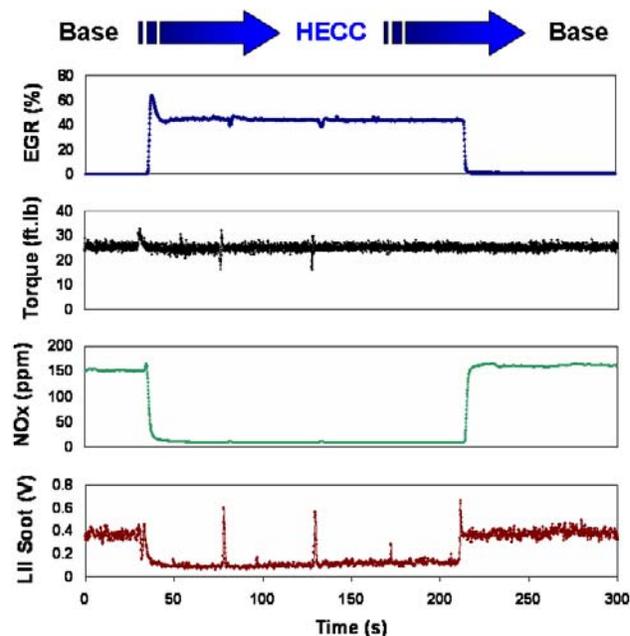
**Figure 1.** Heat release profiles for OEM (a), LTC (b), and HECC (c) engine operation under road-load conditions. The darker shaded region corresponds to the 10-50% heat release interval and the lighter shaded region corresponds to the 50-90% heat release interval.

Table 1. The results of this analysis are shown in Figure 2 and indicate a sharp increase in aldehyde emissions as EGR is increased to achieve LTC operation. The increase in aldehyde emissions is believed to be the result of slower or delayed combustion and is not necessarily due to increased locally rich combustion. Re-phasing of the combustion process and removal of the pilot injection to achieve HECC operation resulted in a reduction in aldehyde emissions to levels similar to those observed for the OEM condition.

Controlled transition experiments were performed to investigate potential emissions and performance problems which may be associated with



**Figure 2.** Aldehyde Emissions for OEM, LTC, and HECC Engine Operation under Road-Load Conditions



**Figure 3.** Controlled Transition between OEM and HECC Operation under Road-Load Conditions

transitioning in and out of HECC operation. The results shown in Figure 3 are for conditions similar to those summarized in Table 1. The most significant differences are that the base condition for the transition experiments is 0% EGR and a different engine (though the same model, Mercedes Benz 1.7-L) was used for these experiments. No significant PM or NO<sub>x</sub> spikes were observed during

transitions in and out of HECC operation. In addition, brake-specific fuel consumption (BSFC) was the same for both modes with no significant excursions in performance.

### Summary and Conclusions

- HECC operation under road-load conditions is possible in light-duty diesel engine applications and was achieved with a reduction of engine-out NO<sub>x</sub> (90%) and PM (30-50%) without excessive HC emissions and with no efficiency penalty.
- HECC operation is characterized by an increased fraction of premixed combustion.
- Engine-out aldehyde emissions do not increase with HECC operation but are of levels similar to those observed for the OEM condition.
- Transitioning between OEM and HECC conditions does not result in significant PM or performance excursions under road-load conditions.

### FY 2004 Publications/Presentations

1. C. S. Sluder, R. M. Wagner, S. A. Lewis, and J. M. Storey, "A Thermal Conductivity Approach for Measuring Hydrogen in Diesel Exhaust," SAE Paper No. 2004-01-2908 and SAE Transactions (Tampa, FL, USA; October 2004).
2. 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).
3. R. M. Wagner, C. S. Sluder, S. A. Lewis, and J. M. Storey, "Achieving High Efficiency Clean Combustion in Diesel Engines," 10th Diesel Engine Emissions Reduction Conference (San Diego, CA, USA; August 2004).
4. R. M. Wagner, C. S. Sluder, S. A. Lewis, and J. M. Storey, "Chemical Composition of the Exhaust from Low-NO<sub>x</sub> Low-PM Diesel Combustion," 2004 Internal Combustion Division of ASME and the CIMAC World Congress (Kyoto, Japan; June 2004).
5. C. S. Sluder, R. M. Wagner, S. A. Lewis, and J. M. Storey, "Exhaust Chemistry of Low NO<sub>x</sub> Low PM Diesel Combustion," SAE Paper No. 2004-01-0114 and SAE Transactions (Detroit, MI, USA; March 2004).

## **II.A.7 Large Eddy Simulation (LES) Modeling Applied to LT/Diesel/H<sub>2</sub> Combustion Research**

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*DOE Technology Development Managers: Kevin Stork*

### **Objectives**

- New project (as of January 2004) aimed at combining state-of-the-art LES and high-performance computational capabilities with the Advanced Combustion Engine R&D activities and expertise in optical engine experiments at the Sandia Combustion Research Facility (CRF).
- Establish one-to-one coupling of LES with experimental hydrogen-fueled internal combustion engine research:
- Generate baseline time-varying 3D multiblock grid of optical research engine, which is being designed and built simultaneously.
- Begin detailed unsteady analysis of gas injector processes and provide support for pattern optimization.
- Perform progressive verification and validation of fully-coupled model framework for treatment of in-cylinder hydrogen-air combustion processes.

### **Approach**

- Application of unique state-of-the-art software and computational resources.
- Implementation of a sophisticated set of subgrid-scale models that are consistent with the Direct Numerical Simulation (DNS) technique in the limit as the LES grid cut-off is refined toward smaller scales.
- Rigorous validation of models using data acquired from the carefully selected target experiments.
- Detailed characterization of complex turbulent combustion processes through joint-analysis of respective data.

### **Accomplishments**

- Preliminary time-varying 3D multiblock grid that matches the geometry of the Sandia National Laboratories optically assessable hydrogen-fueled research engine has been completed.
- Progressive interdisciplinary verification and validation of model base and boundary conditions are in progress.
- Hydrogen fuel injector analysis and optimization are in progress.

### **Future Directions**

- High-fidelity LES calculations will be synchronized with the development of the hydrogen-fueled internal combustion engine (IC-engine) and homogeneous charge compression ignition engine experiments being developed concurrently at Sandia National Laboratories.
- Detailed analysis of local in-cylinder engine processes will be conducted:
  - Hydrogen fuel injector pattern optimization and analysis.
  - Progressive refinement of grid geometry (valve-port) configuration.

- Joint experimental-numerical characterization of unsteady mixing and low-temperature combustion process over full engine cycles.
  - Work toward critical needs and challenges:
    - Power density limitations and maximum fuel efficiency.
    - NO<sub>x</sub> emissions (kinetics-dominated, exhaust gas recirculation alone not sufficient).
    - Flame structure, stability, effects of stratification.
- 

## **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 (SNL). The objective is to use high-fidelity science-based simulations in a manner that directly complements select optical engine experiments. The simulations will be carried out using a highly specialized state-of-the-art massively-parallel flow solver designed for LES of turbulent reacting multiphase flows that was brought to SNL by J. C. Oefelein. Respective case studies will make use of unique high-performance computational resources available internally and at various DOE facilities such as the National Energy Research Scientific Computing Center. After systematic validation of key processes, quantitative data can be extracted from the simulations that are not otherwise available.

The investment in time and resources will provide two significant benefits. Results from this work will provide both a detailed description of intricately coupled processes not measurable by experimental diagnostics and the 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 enhance the accuracy and confidence in these models. The combination of experiments and high-fidelity LES will provide a unique and unparalleled capability to study in-cylinder combustion and transport processes and will facilitate analysis of dynamically coupled processes over the full range of physically relevant time and length scales (i.e., from the largest geometrically dominated turbulence scales to the smallest reactive-diffusive scales). No single approach is capable of achieving this goal.

## **Approach**

The approach involves five key steps: 1) application of unique software capabilities and computational resources that are not typically available in industry and academia, 2) development of fundamental subgrid-scale models that treat turbulence-chemistry interactions and complex thermo-physics in a direct manner consistent with the application of a Direct Numerical Simulation (DNS), 3) adherence to the strict algorithmic requirements that enable LES to effectively eliminate the effects of numerical errors on respective subgrid-scale models, 4) rigorous validation of respective models using data acquired from carefully selected target experiments, and 5) detailed characterization and analysis of key processes by performing tightly coupled joint-analysis of the characteristic unsteady and transient in-cylinder combustion processes associated with a given experiment. Each of the proposed tasks requires considerable high-level expertise, labor, and computational resources. They significantly exceed the time and resources available in industry and academia and are consistent with a National Laboratory's role of using high-performance computing to enable fundamental exploration of complex combustion phenomena.

## **Results**

Given that this project commenced in January of 2004, efforts to date have been focused primarily on establishing a fully synchronized project that is tightly coupled with key target experiments. Figure 1 illustrates the key components. Tasks are being carried out using a unique and unified theoretical-numerical framework developed by Oefelein [1-2]. This framework is currently one-of-a-kind and has been designed for application of both LES and DNS. It solves the fully coupled conservation equations of mass, momentum, total energy and species for complex chemically reacting flows (gas or liquid), in



**Figure 1.** Sequence of Accomplishments Planned for FY 2004

full geometries. The numerical formulation treats the fully coupled compressible form of the conservation equations but can be evaluated in the incompressible limit. Thus, incompressibility is treated as a limiting extreme. The code is fully modular, self-contained, and written in standard American National Standards Institute (ANSI) Fortran 90.

The theoretical framework handles both multicomponent and mixture-averaged systems, with a generalized treatment of the equation of state, thermodynamics, and transport processes. It can accommodate high-pressure, real-gas phenomena, along with the full range of simplified extremes (such as ideal calorically perfect gas mixtures). This framework has been designed to handle turbulent multiple-scalar mixing processes, finite-rate chemical kinetics and multiphase phenomena (or respective simplifications and modeled approximations) in a fully coupled manner. The overall formulation provides full thermophysical coupling (compressible and incompressible) over a wide range of conditions, and in a fundamental manner.

For LES applications, the instantaneous conservation equations are filtered and models are applied to account for the subgrid-scale (SGS) mass, momentum and energy transport processes. The baseline SGS closure is obtained using the mixed dynamic Smagorinsky model by combining the models of Erlebacher, Hussaini, Speziale and Zang [3] and Speziale [4] with the dynamic modeling procedure [5-9] and the Smagorinsky eddy viscosity model [10]. There are no tuned constants employed anywhere in the closure. The property evaluation scheme is based on the extended corresponding states

model [11-12] and is designed to handle full multicomponent systems. This scheme has been optimized to account for thermodynamic nonidealities and transport anomalies over a wide range of pressures and temperatures, and is based on research conducted over many decades [13-21].

Unlike all approaches to date, the filtered energy and chemical source terms are closed directly using an appropriately specified chemical kinetics mechanism and a moment-based reconstruction methodology similar to that of Sarkar et al. [22-23]. The local instantaneous scalar field ( $p$ ,  $T$ ,  $Y_1, \dots, Y_N$ ) is estimated using an approximate deconvolution operation that requires the statistical filtered moments of respective scalars to match to a specified order. The estimated scalar field is then used as a surrogate for the exact scalar field to calculate the SGS contribution to the filtered chemical source terms. This approach is completely consistent with the dynamic modeling procedure and facilitates simultaneous treatment of multiple-scalar mixing processes and key rate of progress variables associated with the chemical kinetics.

The baseline numerical scheme provides a fully implicit all-Mach-number time advancement using a fully explicit multistage scheme in pseudo-time. A unique dual-time multistage scheme is employed with a generalized (pseudo-time) preconditioning methodology that treats convective, diffusive, geometric, and source term anomalies in an optimal and unified manner. The implicit formulation allows one to set the physical time step based solely on accuracy considerations. This attribute alone typically provides a 2 to 3 order of magnitude increase in the allowable integration time step compared to other contemporary methods, especially in the limit of zero-Mach-number flow.

The spatial scheme is designed using a staggered methodology in generalized curvilinear coordinates that provides non-dissipative spectrally clean damping characteristics and discrete conservation of mass, momentum and total energy. The scheme can handle arbitrary geometric features, which typically dominate the evolution of turbulence in a flow. The differencing methodology includes appropriate switches to handle shocks, detonations, flame-fronts, and contact discontinuities. A Lagrangian-Eulerian formulation is employed to accommodate

particulates, sprays, or Lagrangian-based combustion models, with full coupling applied between the two systems. The numerical algorithm has been designed using a fully consistent and generalized treatment for boundary conditions based on the method of characteristics.

The algorithm is massively-parallel and has been optimized to provide excellent parallel scalability attributes using a distributed multiblock domain decomposition with a generalized connectivity scheme. Distributed-memory message-passing is performed using Message Passing Interface and the Single-Program—Multiple-Data model. It accommodates complex geometric features and time-varying meshes with generalized hexahedral cells while maintaining the high accuracy attributes of structured spatial stencils. The numerical framework has been ported to all major platforms and provides highly efficient fine-grain scalability attributes. Sustained parallel efficiencies above 90 percent have been achieved with jobs as large as 1600 processors.

### **Conclusions**

- Combination of detailed experiments and high-fidelity LES provides unique ability to study key in-cylinder processes.
  - Use of advanced predictive capability to perform both fundamental and applied analysis at relevant conditions.
  - Systematic improvements to KIVA-like engineering models through unique multilayered coupling with key target experiments.
- Tasks specifically address need to resolve intricately-coupled turbulent combustion processes in IC engines.
  - Time-accurate simulations over full range of relevant dynamic scales.
  - Dynamic modeling to evaluate model coefficients, no tuned constants.
  - More universal applicability over broader range of flow regimes.

### **FY 2004 Publications/Presentations**

1. J. C. Oefelein. Large eddy simulation for turbulent combustion and propulsion (invited). *Progress in Aerospace Sciences*, submitted.
2. H. H. Chiu and J. C. Oefelein. Modeling liquid-propellant spray combustion processes (invited). Chapter 6, *Liquid Rocket Thrust Chambers, Aspects of Modeling, Analysis and Design*, in print. *Progress in Astronautics and Aeronautics*. American Institute of Aeronautics and Astronautics, 2004.
3. J. C. Oefelein. Thermophysical characteristics of shear-coaxial LOX-H<sub>2</sub> flames at supercritical pressure. *Proceedings of the 30th International Symposium on Combustion*, 30: in print, 2004.
4. J. C. Oefelein. Hydrogen fuel and lean combustion (invited). *Proceedings of the workshop on Lean Combustion Technology II: Promise and Practice*, Tomar, Portugal, April 25-29, 2004.
5. J. O. Keller, G. A. Richards, J. C. Oefelein and R. W. Schefer. Hydrogen combustion research for gas turbine engines (invited). *Proceedings of the Spring Technical Meeting on Combustion Fundamentals and Applications*, Central States Section of the Combustion Institute, Austin, Texas, March 21-23 2004.
6. J. C. Segura, J. C. Oefelein and J. K. Eaton. Large eddy simulation of turbulence modification by particles. *Proceedings of the Thermal and Fluid Sciences Affiliates Program*, Department of Mechanical Engineering, Stanford University, February 4-6, 2004.
7. J. C. Oefelein. Simulation of combustion and thermophysics in practical propulsion systems (invited). *42nd AIAA Aerospace Sciences Meeting and Exhibit, Paper 2004-0159*, January 5-8 2004. Reno, Nevada.
8. J. C. Oefelein, R. W. Schefer and R. S. Barlow. High-fidelity LES and target flame validation experiments in the Turbulent Combustion Laboratory (invited). *42nd AIAA Aerospace Sciences Meeting and Exhibit, Invited Topical Workshop of the Technical Committees*, January 5-8 2004. Reno, Nevada.
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11. J. O. Keller, J. C. Oefelein, R. W. Schefer, and G. A. Richards. Joint program for advanced simulation of fuel flexible gas turbines (invited). *Proceedings of the 1st International Conference on Industrial Gas Turbine Technologies*, Brussels, Belgium, July 10-11 2003.
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## **II.A.8 Nitrogen-Enriched Air for the Reduction of NO<sub>x</sub> Emissions in Heavy-Duty Diesel Engines**

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### **Objectives**

- Evaluate the performance of nitrogen-enriched intake air (NEA) as an alternative to exhaust gas recirculation (EGR) for NO<sub>x</sub> reduction in heavy-duty diesel engines.
- Optimise NEA generation system using gas separation membranes.
- Test the NEA generation system installed on a heavy-duty diesel engine using an engine dynamometer.
- Demonstrate the NEA system's durability and effectiveness on a heavy-duty vehicle.

### **Approach**

- Evaluate EGR data for baseline tests and relate target engine requirements to NEA performance.
- Develop parametric membrane model that accounts for bundle volume and fiber size.
- Characterize available gas separation membranes.
- Match membrane to target engine requirements.
- Test prototype on engine test stand (13-mode test).
- Test prototype performance in a vehicle (transient and durability testing).

### **Accomplishments**

- The EGR engine tests (baseline tests) were performed and the data was evaluated. The target engine's requirements were related to engine performance.
- A parametric membrane model that accounts for bundle volume and fiber size was developed and modified to enable comparison of system power requirements.
- A gas separation membrane characterization bench was designed and built to provide data at higher flows and pressures required for heavy-duty diesel engines.
- Six gas separation membrane prototypes have been tested using the new membrane characterization bench.
- Five reports were delivered to Mack Trucks Inc., detailing the characterization results of four gas separation membranes and system power requirements.

### Future Directions

- Re-evaluate the membrane characterization test data and optimize the gas separation membranes form factor (fiber dimensions), using the membrane model to more closely determine system power requirements per Mack Truck needs.
- Complete the enhanced, power-enabled model results and build an NEA system for use with heavy-duty diesel engines.
- Conduct a test of the NEA system on a heavy-duty diesel engine using the Environmental Protection Agency’s 13-mode test.
- Conduct transient and durability testing on a heavy-duty vehicle.

### Introduction

EGR has been used to reduce NO<sub>x</sub> emissions for decades in spark-ignited engines. Recently, due to increasingly stringent emissions regulations, diesel engines are beginning to use this technology. EGR reduces NO<sub>x</sub> emissions by adding CO<sub>2</sub> as a diluent to lower in-cylinder combustion temperatures. When used in a diesel engine, large quantities of exhaust gas are needed at low loads since the engine operates extremely lean at these points and the exhaust gas has a low percentage of CO<sub>2</sub> (see Figures 1 and 2). Large quantities of EGR must be cooled to keep the volumetric efficiency of the engine at normal levels. This increases the heat load of the radiator. A larger radiator is a problem for heavy-duty diesel vehicles since manufacturers have been trying to reduce the radiator size to lower aerodynamic drag. EGR in diesel engines also introduces particulate matter (PM) and acids into the cylinder which are corrosive and abrasive, increasing engine wear.

A solution to the problems inherent in EGR is to use nitrogen as a diluent. Nitrogen can be used to replace CO<sub>2</sub> to lower in-cylinder combustion temperatures and control NO<sub>x</sub> emissions. Gas separation membranes can be used to remove oxygen from the intake air, making it nitrogen-rich. A gas separation membrane works by dividing the air into two streams: one is nitrogen-rich, and the other is oxygen-rich. The higher the driving pressure through the membrane, the higher the purity. Relatively low pressures are needed since the oxygen level only needs to be reduced from 21% to 17% (typical intake oxygen concentrations with EGR). Since exhaust gas is not used, PM is not introduced into the cylinder, decreasing engine wear. Also, since nitrogen is taken directly from the intake air and does not require extra cooling, there is no increased heat load to the engine.

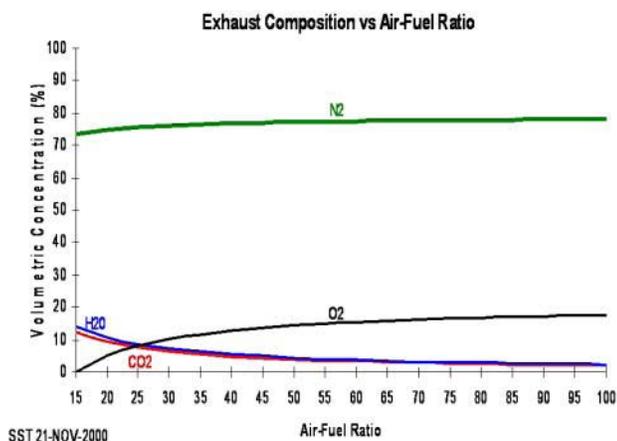


Figure 1. Exhaust Gas Composition at Different Air-Fuel Ratios

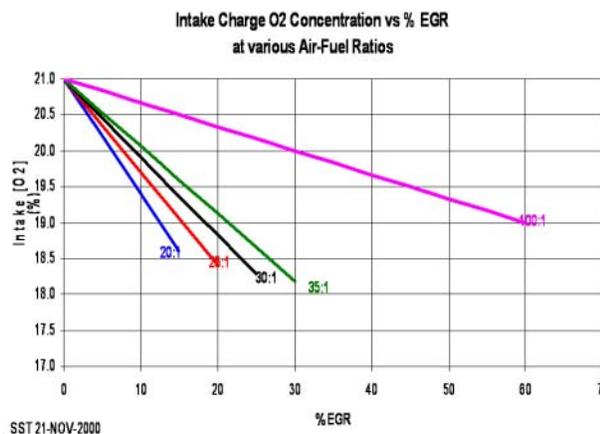


Figure 2. Amount of EGR Required to Lower Intake Air Oxygen Concentration at Different Air-Fuel Ratios

## **Approach**

Typically, the first step in a research project is to develop baseline data to use in evaluating the changes that occur during testing. For a baseline data set, a heavy-duty diesel engine was operated at four different EGR levels and 3 different beginning of injection (BOI) timings over a 13-mode test. The EGR data for baseline tests was evaluated, and target engine requirements were related to NEA performance. This data was used to develop a parametric membrane model that accounts for bundle volume and fiber size.

Previous studies have indicated that the best way to generate nitrogen onboard a vehicle would be to use a gas separation membrane. Several gas separation membrane manufacturers were contacted, and prototype membrane bundles were requested. A new membrane characterization bench was developed since the heavy-duty diesel engine required higher boost pressures that the previous bench could not supply. Four of the six gas separation membranes have been characterized, and the remaining gas separation membranes will be characterized in the near future.

Once the membranes are characterized, the membrane data is evaluated using the model to match the gas separation membrane to target engine requirements. It is perceived that some form factor changes such as membrane thickness or fiber size may have to change to meet the engine requirements. After a suitable membrane is identified, a full-scale NEA unit will be built and evaluated using the 13-mode test on an engine test stand. At the conclusion of the engine tests, the NEA unit will be installed in a heavy-duty vehicle. Transient response and durability will then be evaluated in prototype performance testing.

## **Results**

Originally, four membrane manufacturers were willing to supply prototype membranes for this project. Because some suppliers requested anonymity, the modules will be designated as A, B, C, D, E and F. Analysis done by the membrane manufacturer of A concentrated on three different membrane variants: a high-selectivity membrane, a

high-permeability membrane, and a membrane of intermediate performance. The manufacturer's initial conclusion was that their existing membrane technology required more energy than allowed and required more storage volume than available. They reviewed our feedback and concluded that they could develop an alternative module. However, it would have a higher-permeability material with improved separation factor, and it would cost a significant amount of money to produce. They were not willing to spend the money required to produce this module variant due to other product priorities.

Membrane manufacturer B submitted a prototype for evaluation. The prototype was polymeric, consisting of bundled fibers, three elements (bundles) in a single chamber 7 inches in diameter x 40 inches long. These modules had been previously run in a high-contaminant environment. The modules were tested under the following conditions: feed pressures to 40 psig; feed to retentate pressures differential of less than 5 psi; permeate pressure and temperature at ambient conditions; and retentate flows up to 15 SCF/min. During testing, membrane module B achieved target nitrogen enrichment while remaining stable at elevated pressures and after repeated cycles of testing. However, the module required excess power and exceeded the module size limits.

Membrane manufacturer C supplied a low-selectivity, high-permeability, single-element polymeric fiber, bundled in a container 5 inches in diameter x 20 inches long. Test conditions for membrane C were as follows: feed pressures to 50 psig; feed to retentate pressures less than 6 psi; permeate set at ambient pressure and temperatures; and retentate flows up to 25 SCF/min. Membrane C achieved the target nitrogen enrichment while slightly exceeding the power and size limits (see Figures 3 and 4). The membrane was chosen to be resized. Model results showed that if the low-selectivity, high-permeability membrane modules are sized at 18 inches in diameter and the maximum flow is corrected to 70 lb/min, two membrane bundles are needed if the fiber bore diameter is opened to twice its original size. With advanced coatings and optimization, this could be reduced to one bundle. A new bundle has been requested with a larger bore diameter.

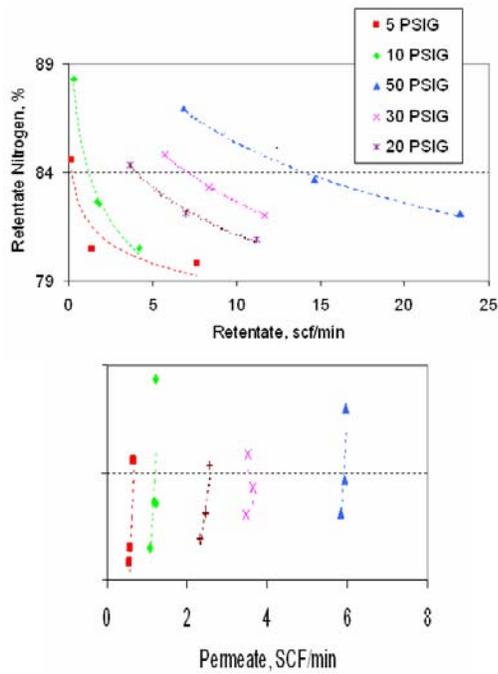


Figure 3. Retentate and Permeate Flows for Membrane C

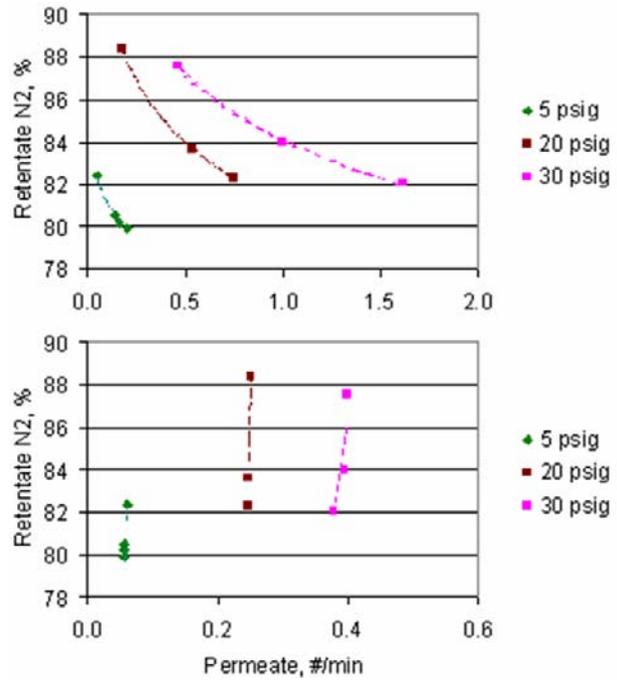


Figure 5. Retentate and Permeate Flows for Membrane D

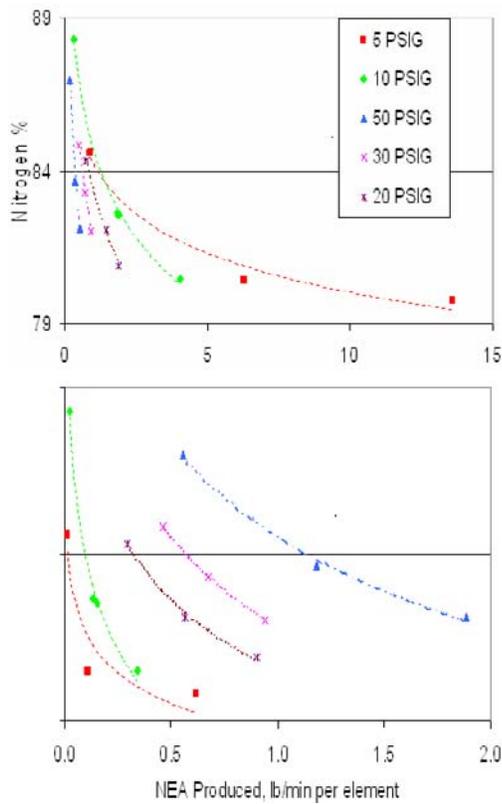


Figure 4. Power and Size Requirements for Membrane C

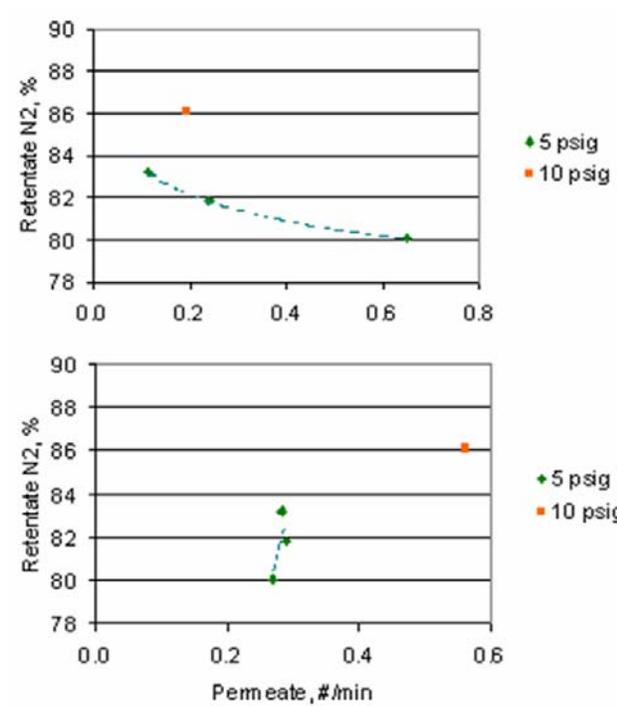


Figure 6. Retentate and Permeate Flows for Membrane E

promising and full analysis is being completed (see Figures 5, 6 and 7).

Modules D, E, and F have been tested. Preliminary results of analysis at low pressures look

System power requirements are now more stringent according Mack Truck's needs than originally envisioned. Further analysis of power

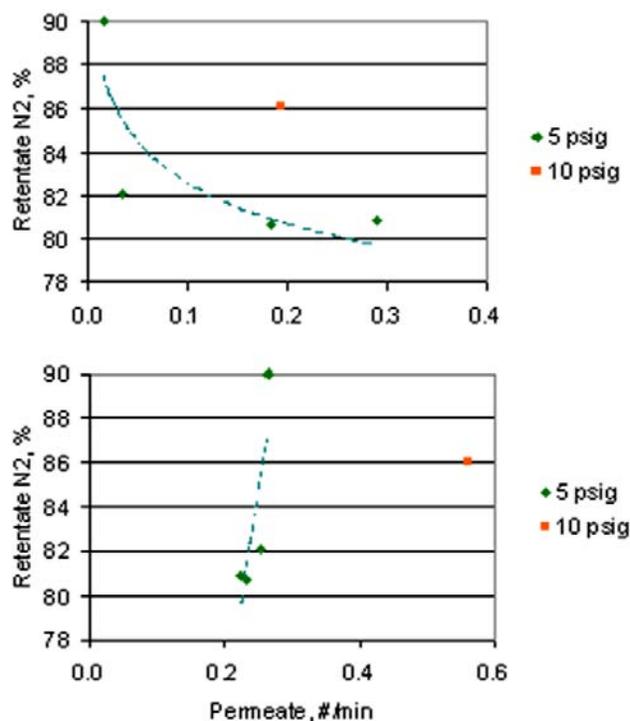


Figure 7. Retentate and Permeate Flows for Membrane F

requirements is in progress as inputs are gathered from Mack Truck (Table 1).

It is projected that an NEA system will be ready for engine testing when it can be placed in Mack Truck's test cell schedule.

### Conclusions

- A membrane model was developed and enhanced to incorporate Mack Truck's system power considerations.
- Membrane B achieved the required nitrogen enrichment but exceeded the power and size limits.
- Membrane C achieved the required nitrogen enrichment while slightly exceeding the power and size limits. Using the membrane model, membrane C was chosen to be resized and tested.
- Modules D, E and F have been tested. Preliminary results at low pressures look promising and analysis is in progress.

Table 1. Process Parameters for System Power Analysis

"13-Mode" Test Point	Compressor Flow #/min	Permeate Flow #/min	Retentate Flow #/min	Theoretical Intake N <sub>2</sub> , %	Module Feed Pressure, psig	Parasitic Power Loss as % of power
c-100	84	12	72	81	52	5
c-75	68	13	55	82	41	5
c-50	49	14	35	82	25	7
c-25	45	24	21	83	10	9
b-100	72	13	59	82	52	5
b-75	56	12	44	82	36	5
b-50	41	9	32	81	21	4
b-25	28	12	16	84	21	10
a-100	53	7	46	81	40	4
a-75	44	7	37	81	30	4
a-50	29	6	23	81	14	6
a-25	20	7	13	83	15	9

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

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### *Subcontractors:*

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University of Wisconsin-Madison, Madison, WI*

### **Objectives**

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

### **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**

#### Part 1. Analysis

- We have developed the most advanced and accurate analysis tools for HCCI combustion. During this year, we have applied this capability to perform a detailed analysis of experiments conducted at Lund Institute of Technology where two different cylinder geometries were considered: a high-turbulence cylinder with a square bowl in piston and a low-turbulence cylinder with a flat top piston. The purpose of the analysis is to determine the role of turbulence during HCCI combustion.
- We have extended our multi-zone analysis methodology to make it applicable to analysis of PCCI combustion. PCCI is a generalization of HCCI combustion where the fuel and air mixture may be partially stratified at the moment of ignition. Examples of PCCI engines include direct injected engines with early injection and controlled autoignition (CAI) engines that use variable valve timing and high residual fraction to control combustion.

#### Part 2. Experimental

- Experimental and computational work has shown the possibility to use an ion sensor to determine combustion timing in an HCCI engine. This is an important breakthrough, as there is a pressing need for reliable, inexpensive combustion sensors for HCCI combustion control.

## Future Directions

- The three fundamental problems of HCCI engines are the difficulty in controlling the engine, the low power achievable, and obtaining consistent timing in the different cylinders of a multi-cylinder engine. In this project, the analytical and experimental work is dedicated to solving these three problems.
- A possible solution to increase the engine power output and balance combustion is to partially stratify the charge (PCCI). We are developing analysis tools to accurately predict combustion and emissions under PCCI combustion.
- Our Volkswagen TDI engine is the ideal test bed for studying combustion balancing between the cylinders of a multi-cylinder engine. We will develop computer controls and inexpensive combustion sensors that will allow us to achieve efficient, controlled HCCI combustion.

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## Introduction

Homogeneous charge compression ignition (HCCI) engines can have efficiencies as high as diesel engines, while producing ultra-low emissions of oxides of nitrogen ( $\text{NO}_x$ ) and particulate matter (PM). HCCI engines can operate on gasoline, diesel fuel, and most alternative fuels. While HCCI has been demonstrated and known for quite some time, some issues have kept it from widespread commercialization. The main issue is combustion control. Other significant hurdles include low power output, high hydrocarbon and carbon monoxide emissions, and difficulty in starting the engine. In this project we use analytical and experimental approaches to address these issues and assist engine and vehicle manufacturers in producing efficient and clean HCCI engines.

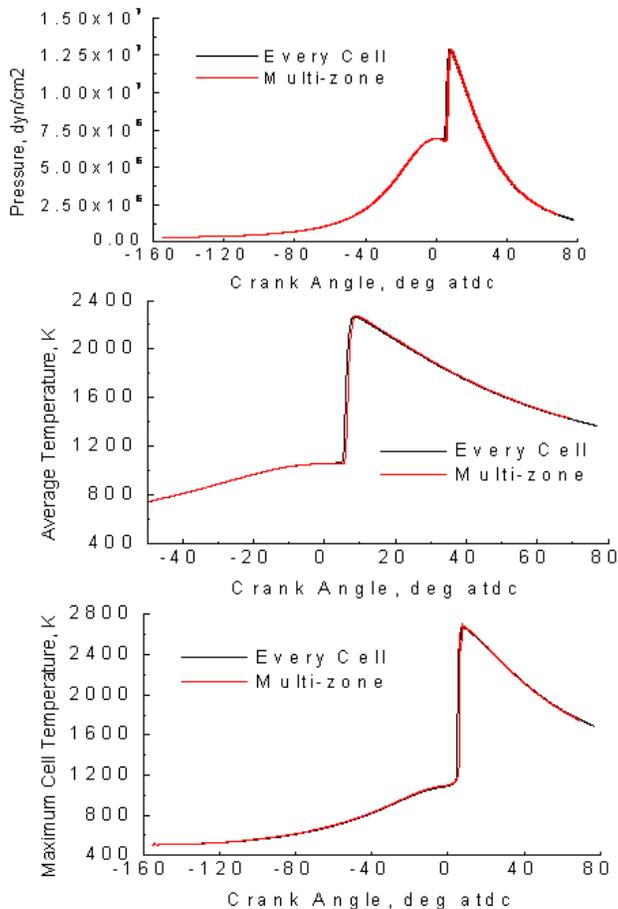
## Approach

Our work is a synergistic combination of analysis and experimental work. We have developed advanced analysis methodologies that combine chemical kinetics with fluid mechanics to analyze HCCI and PCCI engines with accuracy never before achievable for other types of engines. We have also developed systems analysis models for HCCI engines that have allowed us to optimize operating conditions to obtain maximum efficiency with minimum emissions. These analysis tools have also been used to guide the experimental effort. In the laboratory, we have tested new control methodologies and developed new combustion sensors for HCCI combustion.

## Results

We have applied a sequential fluid mechanics-chemical kinetics model for analyzing HCCI experimental data generated at Lund for two combustion chamber geometries: a flat top piston and a piston with a square bowl [1]. Our model uses a fluid mechanics code to determine temperature histories in the engine as a function of crank angle. These temperature histories are then fed into a chemical kinetics solver, which determines combustion characteristics for a relatively small number of zones (40). The results show that the methodology yields good results for both the flat top piston and the square bowl piston. The model makes good predictions of pressure traces and heat release rates. It is observed that the engine with the highest turbulence level (the square bowl) has longer burn duration than the engine with low turbulence (the flat top). This difference can be explained by our model, which indicates that the cylinder with the square bowl has a thicker boundary layer that results in a broader temperature distribution. This broader temperature distribution tends to lengthen the combustion, as cold mass within the cylinder takes longer to reach ignition temperature when compressed by the first burned gases.

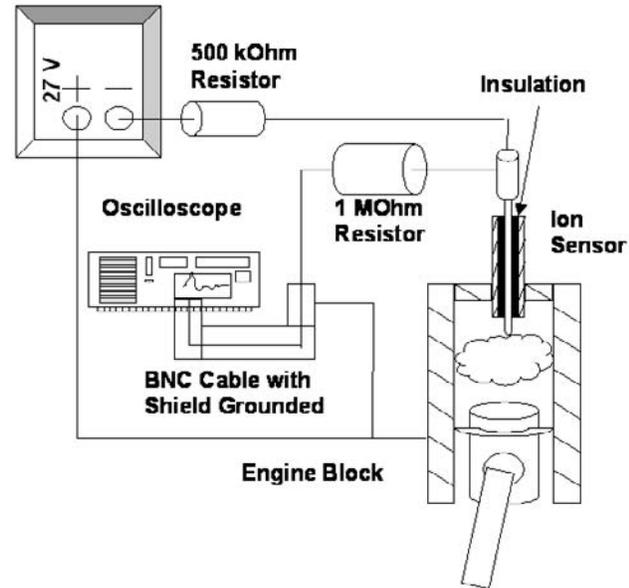
Our multi-zone method has been extended to analysis of PCCI engines when there is some stratification in the air-fuel distribution inside the cylinder at the time of combustion. Our analysis methodology has two stages. First, a fluid mechanics code is used to determine temperature and equivalence ratio distributions as a function of crank angle, assuming motored conditions. The



**Figure 1.** Comparison between results of the multi-zone model and results from an “exact” calculation where the chemical kinetics code is executed at every cell of a fluid mechanics grid. This “exact” solution is labeled “every cell” in the figure.

distribution information is then used for grouping the mass in the cylinder into a two-dimensional (temperature-equivalence ratio) array of zones. The zone information is then handed on to a detailed chemical kinetics model that calculates combustion, emissions and engine efficiency information [2]. We have tested the results for two fuels (methane and n-butane). The results show that the model can accurately predict pressure traces for the fuels being considered.

A second methodology that can be applied to PCCI combustion consists of running the fluid mechanics code for a time step and grouping the many fluid mechanics cells (of the order of



**Figure 2.** Circuit Used for Detecting Ion Signals in the Volkswagen TDI Engine

~100,000) into a few zones (100 or less). The chemical kinetics code is then run for the 100 zones, and the composition and heat release information obtained from the chemical kinetics code is sent back to the fluid mechanics code to conduct the calculations for the next time step. This method yields accurate results at a much reduced computational cost, since chemical kinetics is the most computationally intensive part of the problem. Our methodology yields accurate results for tested operating conditions (see Figure 1) [3].

We have also studied the ion current signal in HCCI to develop inexpensive combustion sensors [4]. Combustion timing is the key measured quantity used in combustion control systems for HCCI engines. In-cylinder pressure transducers are widely used in the laboratory setting for combustion timing measurement, but these sensors are very expensive and have short life (typically less than 100 hours). A promising alternative means of combustion sensing is to measure electrical current from chemi-ionization that occurs during the combustion event. Ion sensing has great potential as a low-cost and long-life alternative to in-cylinder pressure transducers. An experiment was conducted in the Volkswagen TDI engine, and the circuit used for ion sensing is shown in Figure 2. The results of the

experiments show that a measurable ion current exists even in the very lean combustion (equivalence ratio = 0.35) in an HCCI engine. Numerical models using detailed chemical kinetics for propane combustion, including kinetics for ion formation, support the experimental findings. The effects of the equivalence ratio, the intake mixture temperature, and the applied bias voltage on the ion signal have been studied through a series of experiments. The research shows that an inexpensive ion sensor may replace the expensive pressure transducers currently used in HCCI engines.

### **Conclusions**

Our analytical efforts this year focused on developing numerical techniques for analysis of PCCI combustion. We developed and tested two new methodologies that can be applied for cases where there is some air and fuel stratification at the time of ignition. The two methods yield accurate results. Further development and testing is required to be able to analyze direct injected engines.

Our experimental work has demonstrated the use of inexpensive ion sensors to determine combustion timing in HCCI engines. Determining combustion timing with an accurate and inexpensive sensor is crucial for implementing a successful HCCI engine controller. The experiments show that the ion signal can be successfully applied for determining combustion timing. The experimental results have been evaluated with a chemical kinetics code, and an ion chemical kinetics mechanism has been used to explain the results.

### **Special Recognitions & Awards/Patents Issued**

1. Lawrence Livermore National Laboratory (LLNL) HCCI program was featured in the April 2004 issue of LLNL's "Science and Technology Review."
2. Daniel Flowers was quoted in a recent issue of the Wall Street Journal (September 28, 2004), discussing the potential benefits of HCCI engines.
3. Daniel Flowers delivered an invited lecture at the SAE HCCI TopTech seminar, conducted in Berkeley, California, August 2004.

### **FY 2004 Publications/Presentations**

1. 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.
2. 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.
3. Combustion Timing in HCCI Engines Determined by Ion-Sensor: Experimental and Kinetic Modeling, Parag Mehresh, Jason Souder, Daniel Flowers, Uwe Riedel, Robert W. Dibble, Proceedings of the Combustion Institute, Vol. 30, 2004.
4. 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, Proceedings of the ASME Internal Combustion Engine Division, 2004.
5. 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.

### **References**

1. Magnus Christensen and Bengt Johansson, 2002, "The Effect of Combustion Chamber Geometry on HCCI Operation," SAE Paper 2002-01-0425.
2. Salvador M. Aceves, Daniel L. Flowers, Francisco Espinosa-Loza, Aristotelis Babajimopoulos, Dennis Assanis, 2005, "Analysis of Premixed Charge Compression Ignition Combustion with a Sequential Fluid Mechanics-Multizone Chemical Kinetics Model," Submitted to the SAE Congress, 2005.
3. Randy P. Hessel, Daniel L. Flowers, Salvador M. Aceves, 2005, "Estimating Combustion with CFD and Detailed Chemistry using an Equivalence Ratio-Temperature Multi-Zone Methodology," Submitted to the SAE Congress, 2005.
4. Parag Mehresh, Jason Souder, Daniel Flowers, Uwe Riedel, Robert W. Dibble, 2004, "Combustion Timing in HCCI Engines Determined by Ion-Sensor: Experimental and Kinetic Modeling," Proceedings of the Combustion Institute, Vol. 30.

## **II.A.10 HCCI and Stratified-Charge Compression-Ignition Engine Combustion Research**

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### **Objectives**

#### Project Objective

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

#### FY 2004 Objectives

- Investigate the factors affecting combustion phasing with changes in fueling rate.
- Investigate the relationship between intake temperature and in-cylinder bottom dead center (BDC) temperature, and the factors causing heating/cooling during intake.
- Conduct an initial investigation of the effect of intake pressure boost (for increased power) on HCCI combustion and emissions.
- Acquire chemiluminescence images to investigate the nature of HCCI combustion under various operating conditions.

### **Approach**

- Develop experimental techniques to isolate and evaluate the relative magnitude of each factor that affects HCCI combustion phasing with changes in fueling rate.
- Combine detailed analysis of experimental data with guidance from cycle-simulation modeling to determine the BDC temperature at various operating conditions.
- Design an experimental matrix to evaluate the effects of intake boost and fueling rate on HCCI combustion for various fuel types.
- Bring the optically accessible HCCI engine to full operational status, and establish a capability for low-light-level imaging.
- Work cooperatively with Lawrence Livermore National Laboratory (LLNL) and the University of Michigan on computational fluid dynamics (CFD) and multi-zone modeling of our experiments.

### **Accomplishments**

- Determined the relative magnitude of the factors affecting changes in combustion phasing with changes in fueling rate. Showed how the effect of fuel chemistry on changes in combustion phasing with changes in fueling rate depends on fuel type.
- Established a methodology for computing the in-cylinder BDC temperature from easily obtained parameters.
- Investigated the effect of intake pressure boost on HCCI combustion for gasoline and other representative fuel constituents.

- Conducted an investigation of the lowest temperature for complete combustion of hydrocarbon fuels over a wide range of conditions. Showed that the peak temperature must exceed 1500 K at 1200 rpm, regardless of fuel type or combustion timing.
- Completed installation and shakedown testing of the optically accessible HCCI engine.
- Applied chemiluminescence imaging to investigate the characteristics of well-mixed and mixture-stratified HCCI.

### **Future Directions**

- Evaluate the potential for increasing the naturally occurring thermal stratification by increasing wall heat-transfer rates to extend HCCI operation to higher loads.
- Investigate combustion timing retard as a means to extend the high-load limit of HCCI.
- Combine multi-zone Senkin modeling with experimental data to investigate how thermal stratification affects HCCI heat release rates with normal and retarded timing, and to determine the potential for extending the high-load limit with thermal stratification.
- Conduct detailed exhaust speciation study of HCCI at various operating conditions.
- Set up a high-pressure common-rail diesel fuel injection system for investigations of diesel-fueled HCCI.
- Apply laser-based and other optical imaging diagnostics to investigate the effects of thermal and mixture stratification on HCCI combustion.

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### **Introduction**

HCCI engines have significant efficiency and emissions advantages over conventional spark-ignition and diesel engines, respectively. However, several technical barriers must be addressed before HCCI can be implemented in practical engines. Among these, controlling combustion phasing as the fueling rate is varied and extending both the high- and low-load operating limits are some of the most important. As outlined under the accomplishment bullets above, the work conducted for this project during FY 2004 involved several investigations that provide new understanding related to overcoming these technical barriers.

### **Approach**

To obtain the necessary fundamental understanding of HCCI, an HCCI engine laboratory has been established that has been equipped with both all-metal and optically accessible HCCI engines of the same basic design. The majority of the investigations in FY 2004 involved the all-metal engine, which has been fully operational since 2001. These investigations provide substantial information, but it is also advantageous to obtain a detailed understanding of in-cylinder processes through the application of advanced optical imaging diagnostics.

Accordingly, installation and shakedown testing of the optically accessible engine was completed, and a low-light-level imaging capability was established.

This HCCI engine research facility is designed to allow operation over a wide range of operating conditions using various fueling techniques. It also has several features to provide precise control of parameters such as combustion phasing and mass flow rates of fuel and air, so that data are repeatable even for relatively small changes in operating conditions. For some investigations, computational modeling was applied to complement the experiments. In most cases this involved single-zone chemical kinetic modeling using the Senkin application of CHEMKIN. In addition, we have worked with LLNL to apply Kiva and multi-zone modeling to our experiment, and a collaborative modeling effort has also been established with the University of Michigan.

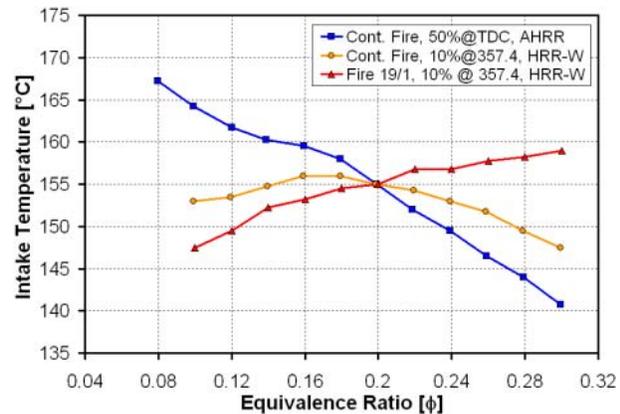
### **Results**

Combustion phasing in HCCI engines can be affected by many operating parameters, and two investigations were conducted to provide an understanding of the factors that affect combustion phasing with changes in operating conditions.

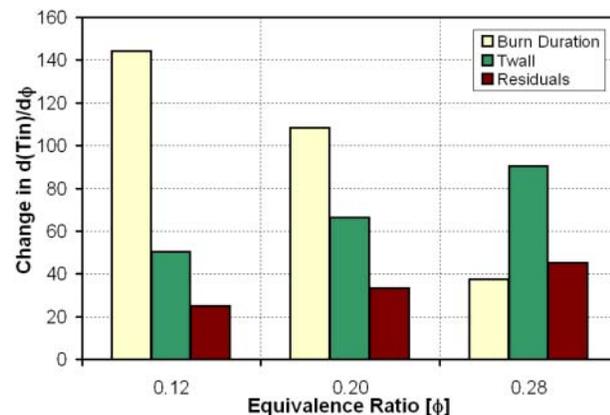
For the first investigation, the factors that affect combustion phasing with changes in fueling rate were analyzed. As the fueling rate is increased in an HCCI engine, the combustion phasing, as measured by the 50% burn point (CA50, the engine crankshaft angle at 50% burned), will become more advanced unless the intake temperature is reduced. This occurs for all fuels tested (gasoline, toluene, iso-octane, PRF80 [primary reference fuel, 80 octane], and PRF60), suggesting that fuel autoignition chemistry is faster for all fuels as the mixture becomes richer. However, more careful examination shows that four other factors besides fuel chemistry change as the fueling rate is varied, and each of these can affect the combustion phasing. These factors include changes in the burn duration, wall temperature, residuals, and heating/cooling during induction. To determine the relative importance of these factors, the experiment was altered in a series of steps to sequentially remove each factor, isolating the effects of fuel chemistry.

A sample of the results is shown in Figure 1 (with iso-octane as the fuel). The three curves in this figure show the changes in required intake temperature with changes in fueling for the following scenarios: 1) the base condition with CA50 at top dead center (TDC), 2) with the effect of changes in burn duration with  $\phi$  removed by maintaining constant “ignition” phasing as measured by the 10% burn point, and 3) with the changes in wall temperature and residuals removed by using a novel alternate firing technique, fire 19/1 [1]. For the base condition, the intake temperature must be decreased with increased fueling (equivalence ratio,  $\phi$ ), as discussed above, but with the removal of changes in burn duration, wall temperature, and residuals, the curve shows the opposite trend. Analysis of these temperature curves and other data provides the relative magnitude of these factors, as shown in Figure 2. At low loads ( $\phi < 0.2$ ), the change in burn duration is the main reason that the intake temperature must be adjusted to maintain CA50 at TDC, while at higher loads ( $\phi > 0.25$ ), the effect of wall heating is the dominant effect.

With the effects of fuel chemistry isolated, three fuels were examined to determine how the role of fuel chemistry on combustion phasing varied with fuel type. The results showed that for single-stage ignition fuels such as iso-octane and gasoline, the autoignition chemistry is only slightly enhanced by



**Figure 1.** Comparison of the change in required intake temperatures with changes in fueling ( $\phi$ ) for three conditions: 1) the base condition with CA50 at TDC, 2) with constant 10% burn point, and 3) with constant wall temperature and residuals.



**Figure 2.** Relative magnitude of the effects of burn duration, wall temperature, and residuals on changes in required intake temperature with changes in fueling rate, at three equivalence ratios.

increased equivalence ratio. Thus, the changes in required intake temperature are dominated by the sum of the other effects. However, for fuels exhibiting two-stage ignition (*i.e.*, cool-flame chemistry), such as PRF80 (or by inference, diesel fuel), the autoignition kinetics are greatly enhanced with increased  $\phi$ , and kinetics are dominant over the other effects [1].

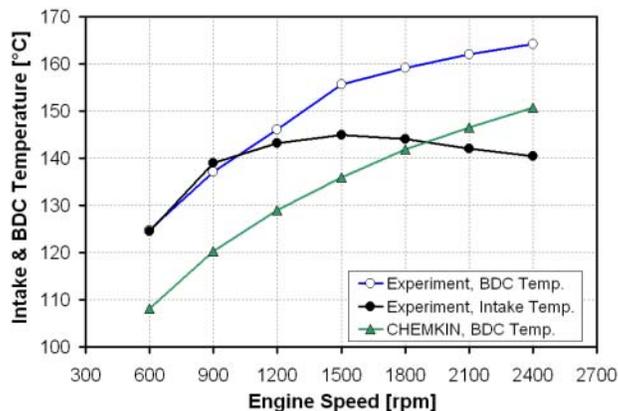
For the second investigation related to factors that affect combustion phasing, the effect of heating and cooling during induction was examined in detail.

In addition, a straightforward algorithm was developed to compute the in-cylinder temperature at the end of induction ( $T_{BDC}$ ). This investigation showed that there are four main effects that cause the  $T_{BDC}$  to differ from the measured intake temperature: 1) heat transfer during induction, 2) heating of the charge due to flow dynamics, “dynamic heating”, 3) cooling due to fuel vaporization, and 4) mixing with residuals. The technique for estimating  $T_{BDC}$  is based on a detailed analysis of experimental data with the dynamic heating being computed for one base condition per engine speed using a cycle-simulation model, as described in detail in Ref. [2].

An example of the application of this technique is shown in Figure 3. As can be seen, the kinetics model (CHEMKIN) predicts that  $T_{BDC}$  must be increased with engine speed to maintain the same combustion timing since there is less real time for the autoignition/combustion reactions to occur. In contrast, the required intake temperature for the experiment shows little change above 900 rpm, which seems unrealistic. However, when the experimental  $T_{BDC}$  is computed as outlined above, it shows a monotonic increase similar to CHEMKIN. Similar validity of the technique for computing  $T_{BDC}$  has been demonstrated for fuel vaporization and wall heat-transfer effects [2].

Boosting the intake pressure can increase the power output of HCCI engines, but it can also affect the autoignition timing and the propensity for knock. To better understand the effects and tradeoffs of intake boosting, tests were conducted over a range of intake pressures for gasoline and several representative commercial-fuel constituents, including: iso-octane, methyl-cyclohexane, toluene, and a mixture of toluene and n-heptane. These studies showed that due to the ignition enhancement with increased intake pressure, the amount of boost is typically limited by the lowest intake temperature that can be achieved or by engine knock. The onset of these limits is strongly related to fuel-type, and for some fuels, boost causes the shift from single-stage to dual-stage ignition, which further reduces the allowable boost before the limits are reached.

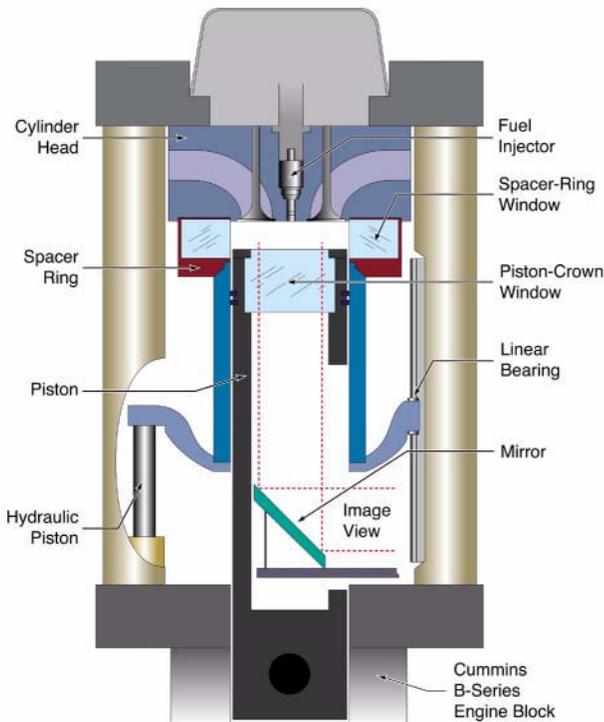
In another study, the effect of fuel type was found to be directly related to the minimum fueling



**Figure 3.** Changes in intake or BDC temperature required to maintain CA50 at TDC as engine speed is varied. The CHEMKIN  $T_{BDC}$  is lower than the experimental  $T_{BDC}$  because the model is adiabatic.

rate for complete bulk-gas combustion, *i.e.* the low-load limit [3]. This investigation showed that for complete combustion, the peak combustion temperature must exceed 1500 K at 1200 rpm, independent of combustion phasing or hydrocarbon fuel-type. (This required temperature varies from 1460 to 1550 K for engine speeds from 600 to 2400 rpm, respectively.) Thus, for fuels with low ignition temperatures (*e.g.*, PRF80 or diesel fuel), a higher equivalence ratio must be used to reach these required peak temperatures, or some other technique such as charge-mixture stratification must be applied. In addition, a combined computational and experimental study was conducted in cooperation with LLNL [4] that showed how the thermal boundary layer affects the minimum fueling rate for complete combustion.

In order to better understand the nature of HCCI combustion, chemiluminescence images were acquired at various operating conditions using the optically accessible HCCI engine (Figure 4). Figure 5 shows an example of an image sequence with fully premixed intake conditions. Despite the well-mixed intake, the images show significant turbulent structure, and the change in the appearance of the images through the sequence indicates significant thermal stratification. The first image shows ignition/combustion over broad areas, but dark regions suggest colder regions that have not yet ignited. By 363° CA, the first-ignited regions appear

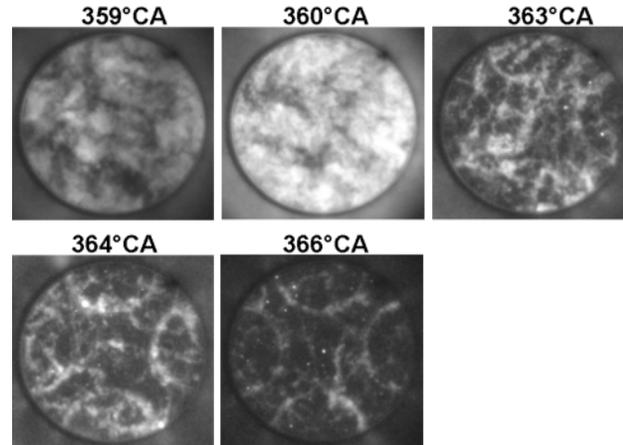


**Figure 4.** Schematic of the optically accessible HCCI engine.

to have burned out as indicated by the large dark regions. Combustion is now confined to more narrow “string-like” regions, that are thought to correspond to the colder regions that had not yet ignited in the earlier images. Near the end of the heat release (364 - 366° CA), combustion occurs in the valve-pocket crevices where the mixture is even colder. Understanding the nature of thermal stratification in HCCI engines and how it can be affected by operating parameters is a key element for slowing the heat release rate to extend HCCI operation to higher loads.

## **Conclusions**

- In addition to fuel chemistry, several factors affect combustion phasing as the fueling rate is varied. The most important factors are changes in burn duration at low loads ( $\phi < 0.2$ ), and wall heating at higher loads ( $\phi > 0.25$ ).
- The autoignition chemistry is only slightly enhanced by increased fueling for single-stage ignition fuels such as iso-octane and gasoline, but for fuels with two-stage ignition (significant cool-flame chemistry), the enhancement in the



**Figure 5.** Chemiluminescence images of HCCI combustion for well-mixed intake charge. Fuel is iso-octane,  $\phi = 0.24$ . Images were acquired through the piston-crown window as shown in Figure 4.

autoignition chemistry is substantial and can be dominant over the other factors.

- The in-cylinder temperature at the end of induction ( $T_{BDC}$ ) is a valuable parameter for analyzing HCCI, and a technique has been developed to estimate  $T_{BDC}$  with good accuracy.
- Boosting the intake pressure can significantly increase the power output, but operating range becomes limited by knock and/or the minimum available intake temperature.
- For complete combustion, peak temperatures must exceed 1500 K at 1200 rpm, regardless of combustion phasing or hydrocarbon fuel-type.
- Chemiluminescence imaging was found to provide significant insight into the nature of HCCI combustion and how it is affected by thermal and mixture stratification.

## **Special Recognitions & Awards/Patents Issued**

1. Invited speaker and panelist for SAE panel discussion on HCCI at the 2003 SAE Fall Powertrain and Fluid Systems Conference, Pittsburgh, PA, October, 2003.
2. Invited speaker at the SAE Homogeneous Charge Compression Ignition Symposium, Berkeley, CA, August, 2004.

**FY 2004 Publications/Presentations**

1. Dec, J. E. and Sjöberg, M., "Isolating the Effects of Fuel Chemistry on Combustion Phasing in an HCCI Engine and the Potential of Fuel Stratification for Ignition Control," SAE Paper 2004-01-0557, 2004.
2. Sjöberg, M. and Dec, J. E., "An Investigation of the Relationship between Measured Intake Temperature, BDC Temperature, and Combustion Phasing for Premixed and DI HCCI Engines," SAE paper 2004-02-1900, 2004.
3. Sjöberg, M. and Dec, J. E., "An Investigation into Lowest Acceptable Combustion Temperatures for Hydrocarbon Fuels in HCCI Engines," presented at and to be published in the proceedings of the 2004 International Combustion Symposium, 2004.
4. Aceves, S. M., Flowers, D. L., Espinosa-Loza, F., Martinez-Frias, J., Dec, J. E., Sjöberg, M. and Dibble, R. W., Hessel, R. P., "Spatial Analysis of Emissions Sources for HCCI Combustion at Low Loads Using a Multi-Zone Model," SAE paper 2004-01-1910, 2004.
5. Sjöberg, M. and Dec, J. E., "Combined Effects of Fuel-Type and Engine Speed on Intake Temperature Requirements and Completeness of Bulk-Gas Reactions for HCCI Combustion," SAE paper 2003-01-3173, 2003, presented at the 2003 SAE Fall Powertrain Conference, October 2003.
6. Dec, J. E. and Sjöberg, M., "The Role of Optical Diagnostics in the Development of HCCI Engines," presented at the SAE 2003 Fall Powertrain and Fluid Systems Conference, October 2003.
7. Sjöberg, M. and Dec, J. E., "An Investigation of the Relationship between Measured Intake Temperature, BDC Temperature, and Combustion Phasing for Premixed and DI HCCI Engines," Advanced Engine Combustion Working Group Meeting, January 2004.
8. Dec, J. E. and Sjöberg, M., "Update on Recent Progress in the HCCI Dual-Engine Laboratory," Advanced Engine Combustion Working Group Meeting, January 2004.
9. Dec, J. E. and Sjöberg, M., "HCCI and Stratified-Charge CI Engine Combustion Research," Advanced Combustion R&D Peer Review, May 2004.
10. Sjöberg, M. and Dec, J. E., "Enhanced Natural Thermal Stratification and Combustion Timing Retard for Smoothing of HCCI Heat-Release Rates," Advanced Engine Combustion Working Group Meeting, June 2004.
11. Dec, J. E. and Sjöberg, M., "Insights into HCCI Combustion Using Chemiluminescence Imaging," Advanced Engine Combustion Working Group Meeting, June 2004.
12. Dec, J. E. and Sjöberg, M., "HCCI Combustion Inefficiency and Potential Solutions," SAE Homogeneous Charge Compression Ignition Symposium, August 2004.
13. Dec, J. E. and Sjöberg, M., "Factors Affecting HCCI Combustion Phasing for Fuels with Single- and Dual-Stage Chemistry," International Energy Agency (IEA) Task Leaders Meeting, August 2004.
14. Dec, J. E. and Sjöberg, M., "Factors Affecting HCCI Combustion Phasing for Fuels with Single- and Dual-Stage Chemistry," presented at and to be published in the proceedings of the 10<sup>th</sup> Diesel Engine Emissions Reduction Workshop (DEER 2004), San Diego, CA, Aug.-Sept. 2004.

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1. Dec, J. E. and Sjöberg, M., "Isolating the Effects of Fuel Chemistry on Combustion Phasing in an HCCI Engine and the Potential of Fuel Stratification for Ignition Control," SAE Paper 2004-01-0557, 2004.
2. Sjöberg, M. and Dec, J. E., "An Investigation of the Relationship between Measured Intake Temperature, BDC Temperature, and Combustion Phasing for Premixed and DI HCCI Engines," SAE paper no. 2004-02-1900, 2004.
3. Sjöberg, M. and Dec, J. E., "An Investigation into Lowest Acceptable Combustion Temperatures for Hydrocarbon Fuels in HCCI Engines," to be published in the proceedings of the 2004 International Combustion Symposium, 2004.
4. Aceves, S. M., Flowers, D. L., Espinosa-Loza, F., Martinez-Frias, J., Dec, J. E., Sjöberg, M. and Dibble, R. W., Hessel, R. P., "Spatial Analysis of Emissions Sources for HCCI Combustion at Low Loads Using a Multi-Zone Model," SAE paper no. 2004-01-1910, 2004.