II.A.11 Automotive HCCI Combustion Research

Richard Steeper
Sandia National Laboratories, MS 9053
P.O. Box 969
Livermore, CA 94551-0969

DOE Technology Development Managers: Kevin Stork and Gurpreet Singh

Objectives

The focus of the Automotive HCCI Combustion project is on applying advanced optical diagnostics to characterize homogeneous charge compression ignition (HCCI) fuel injection and fuel-air mixing processes, and to understand how mixture preparation strategies affect the combustion and emission performance of automotive HCCI engines. Objectives for FY 2004 are as follows:

- Benchmark fired operation of the recently completed Automotive HCCI Optical Engine Facility.
- Identify a laser-induced fluorescence (LIF) diagnostic suitable for quantitative equivalence ratio measurements in the HCCI engine.
- Apply selected LIF diagnostics to begin characterizing the fuel-mixture preparation process in the fired HCCI engine.

Approach

- Perform fired tests of the automotive HCCI engine to identify its viable operating range, and benchmark the engine's combustion performance across the range of operating conditions.
- Perform bench-top experiments to match the volatility of LIF tracers to the primary reference fuels (PRF) that they are meant to track in the engine.
- Perform engine experiments to assess the quality of LIF measurements of in-cylinder fuel distribution.
- Apply LIF imaging to characterize the effects of fuel-injection timing on charge preparation.

Accomplishments

- Benchmark tests of the optical HCCI engine were completed using PRF fuels with inlet temperatures up to 220°C, inlet pressures up to 1.75 bar absolute, and loads up to 4 bar indicated mean effective pressure (IMEP). Skip-fired operating conditions viable for optical experiments were identified for PRFs with octane numbers less than 80.
- Bench-top evaporation tests identified several LIF tracers that improve fuel tracking by better matching the volatility of PRF fuels. LIF tracers formulated to co-evaporate well with iso-octane, as shown in prior gasoline direct injection (GDI) work, were shown here to properly co-evaporate with the full range of PRF mixtures.
- The same group of LIF tracers was tested in the fired engine to assess the ability to quantify in-cylinder equivalence ratios. Two co-evaporative tracers with sufficient signal strength at appropriate concentrations were identified. A technical paper describing the results of the bench-top and engine tests of the LIF tracers was submitted to SAE.
- In-cylinder equivalence ratio distributions were measured and converted to probability density function (PDF) statistics to quantify the effects of injection timing on charge preparation.

Future Directions

- Characterize the charge-preparation process for alternative injectors and injection strategies, including liquid injection, wall wetting, and fuel-air mixing.
- Correlate the characterization measurements with combustion and emissions performance as measured using pressure records, combustion-luminosity images, and emissions measurements.

Introduction

Major challenges to the implementation of HCCI combustion—including phasing control, operating-range extension, and emissions control—may well require advanced, non-homogeneous, fuel-air mixing strategies. Alternative injection strategies such as retarded or multiple injections can be used to modify the local equivalence ratios at which combustion takes place, thereby affecting rate of heat release, combustion efficiency, and engine-out emissions. The focus of the current project is the application of in-cylinder optical diagnostics to characterize the fuel-air mixing process and to correlate mixing with the subsequent HCCI combustion.

Approach

Four activities were undertaken in FY 2004. The first activity comprised engine experiments to benchmark the performance of the automotive HCCI engine. Modifications to convert the facility to HCCI operation were completed at the end of the last reporting period. Second, bench-top evaporation experiments tested several LIF tracer/PRF fuel mixtures to determine whether they properly co-evaporate—a necessary condition for quantitative LIF diagnostics. Third, the LIF tracers were tested in the fired engine to assess their signal-to-noise ratios. Finally, measurements of in-cylinder fuel-air mixing were commenced, producing PDF statistics of mixing as a function of injection timing.

Results

Benchmark tests of the optical HCCI engine were performed under the following conditions: compression ratio = 11.8; low residual cams; premixed and direct injection (DI) fueling; fuels = PRF 50, 80, and 100; speed = 1200 rpm; intake temperatures 220°C and intake pressure = 1.75 bar IMEP. A wide range of loads were obtainable using the PRF-50 fuel. For the PRF-80 fuel, the operating range was reduced, with appropriate combustion phasing only possible at elevated intake temperatures and pressures. During tests with PRF 100 (iso-octane) at loads near the limit of the optical engine, phasing near top center was not achievable, even at the limit of our intake temperature and pressure range. Operation with PRF 100 in the future may be possible with residual-enhanced intake temperatures or fuel additives.

The second activity comprised bench-top evaporation experiments to test four selected LIF tracers: 10% 3-pentanone, 9% 3-hexanone + 1% 3-pentanone, 3% toluene, and 1.2% 3-hexanone. Some of these tracers have been previously tested for use with the common GDI surrogate fuel iso-octane, and the current experiments extended the tests to cover the full range of PRF mixtures commonly used as HCCI fuels. Results of the tests for the four tracers are shown in Figure 1. Each graph summarizes data for one of the tracers mixed in four different PRF mixtures: PRF 0, 50, 80, and 100.

The x-axes of the graphs represent the progress variable (remaining liquid mass fraction) during the evaporation of tracer/PRF mixtures, measured using a mass scale. On this axis, time progresses from right (100% mass remaining) to left (zero mass remaining). The open symbols indicate the rate of evaporation of the total mixture, with values read on the left y-axis. The closed symbols, read on the right axis, are derived from LIF measurements of the vapor leaving the evaporation chamber. These data are proportional to the evaporation rate of the tracer alone. By comparing the open and closed symbol data, we can determine if the tracer co-evaporates with the fuel—a necessary condition for the tracer to properly track the fuel during in-cylinder mixing.

The fact that in each graph the open and closed symbols (taken separately) fall on a single curve indicates that the evaporation behavior of all these tracers is the same regardless of the PRF selected as

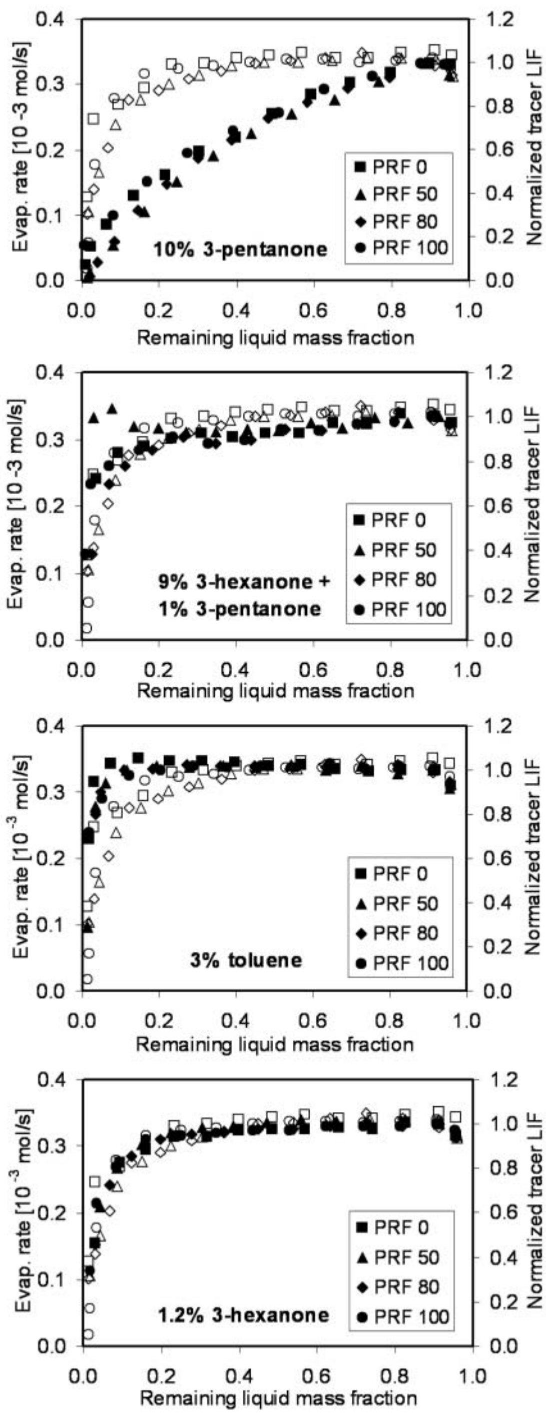


Figure 1. Evaporation histories of mixtures of LIF tracers and PRFs. X-axis: evaporation progress variable = remaining liquid mass fraction, read from left to right; Left axis: total mixture evaporation rate (open symbols); Right axis: normalized vapor-phase tracer LIF signal, proportional to tracer evaporation rate (closed symbols).

fuel. This is due to the close match of the physical properties of the iso-octane and n-heptane components of PRFs. In the top graph, however, it is clear that tracer evaporation (closed-symbol data) does not match the total mixture evaporation rate (open-symbol data). This indicates that 3-pentanone does not properly match the evaporation of the PRFs. In contrast, the other three graphs indicate excellent co-evaporation of tracer and fuel, implying that these tracers will more faithfully track the fuel during in-cylinder evaporation.

Tests of the tracers during LIF imaging in the engine (Activity 3) showed that while signal levels are not as good as 3-pentanone, the 9% 3-hexanone + 1% pentanone signal is satisfactory. The 3% toluene tracer has about the same signal level as the 9% 3-hexanone + 1% pentanone, but the current configuration of our diagnostic is not optimal for this tracer—further gains in signal-to-noise ratio are possible. The fourth tracer, 1.2% 3-hexanone, shows the perfect co-evaporation of an azeotrope mixture, but its signal in the engine tests was too low to be useful for equivalence ratio measurements. The LIF tracer test results will be published in a paper submitted to the 2005 SAE Congress.

The final activity this year comprised engine measurements initiating the characterization of fuel-air mixing in the fired HCCI engine. Using a current-design, 8-holed injector and varying start of injection (SOI) from 300 to 60 crank angle degrees (CAD) before top center of compression, we recorded sets of LIF images to reveal the effect of injection timing on fuel distribution. Data for each SOI timing were reduced to equivalence ratio PDF plots representing the state of mixing in the cylinder just prior to cool-flame ignition. Figure 2 combines PDF plots for the injection timing sweep into a 3-D PDF graph. The rear plane represents early injection, and the narrow PDF peak is characteristic of the resulting homogeneous mixture. As injection is retarded (moving forward in the 3-D graph), the mixture becomes progressively stratified, and the PDF broadens. The goal is to compare these fuel distribution measurements with combustion and emission data to guide the development of mixing strategies that enhance HCCI combustion by, for instance, reducing CO, HC, and NO_x emissions or by moderating heat release rates.

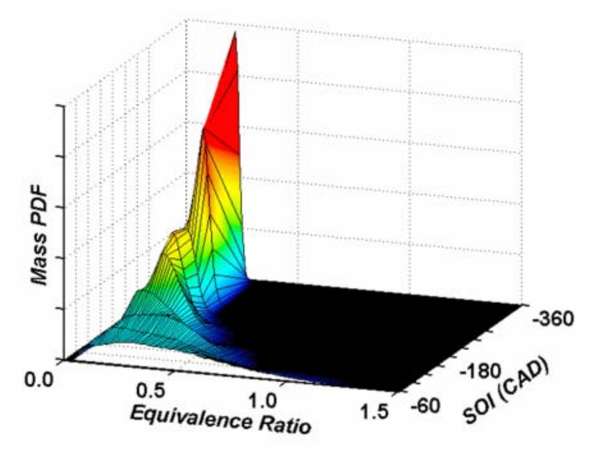


Figure 2. 3-D graph of equivalence ratio PDF curves for a range of SOI timings. Operating conditions: 1200 rpm, 120°C and 1.2 bar intake temperature and pressure, 8-hole injector, PRF-50 fuel, 0.24 equivalence ratio

Conclusions

Following completion of HCCI-enabling modifications to the light-duty optical engine, benchmark tests were performed to map the viable operating range of the automotive HCCI engine. Bench-top comparison of several candidate LIF tracers highlighted three tracers whose evaporation rates match the primary reference fuels far better than 3-pentanone. Tests in the HCCI engine revealed that the signal strength of one of them was too low to be useful. Finally, measurements of fuel-air mixing were commenced in the fired HCCI engine, producing PDF statistics of the effect of injection timing on fuel distribution prior to ignition.

Special Recognitions & Awards/Patents Issued

1. Richard Steeper of Sandia National Laboratories was selected as Co-Vice-Chair of Combustion for SAE's Fuels and Lubricants Activity.

FY 2004 Presentations

1. R. R. Steeper, "HCCI Fuel-Air Mixing Experiments," DOE AEC Working Group Meeting, Sandia National Laboratories, Livermore, January, 2004.
2. R. R. Steeper, "Progress Report: Automotive HCCI Engine Research," Invited seminar, General Motors Research, Detroit, March, 2004.
3. R. R. Steeper, "Automotive HCCI Combustion Research," DOE Advanced Combustion Engine Peer Review, Argonne National Laboratory, Chicago, May, 2004.
4. R. R. Steeper, "Automotive HCCI Engine Progress Report," DOE AEC Working Group Meeting, USCAR, Detroit, June, 2004.

FY 2004 Publications

1. D. Han and R. R. Steeper, "Examination of Iso-octane/Ketone Mixtures for Quantitative LIF Measurements in a DISI Engine," SAE Transactions 111-4: 313-324, 2002.
2. R. R. Steeper, "Automotive HCCI Combustion Research," DOE Advanced Combustion Engine Annual Report, 2003.
3. M. Davy, P. Williams, D. Han, and R. R. Steeper, "Evaporation Characteristics of the 3-Pentanone/Isooctane Binary System," Experiments in Fluids 35: 92-99, 2003.
4. R. R. Steeper, S. De Zilwa, and A. Fayoux, "Co-Evaporative Tracer-PRF Mixtures for LIF Measurements in Optical HCCI Engines," submitted to 2005 SAE Congress, 2004.

II.A.12 HCCI Engine Optimization and Control Using Diesel Fuel

Profs. Rolf D. Reitz (Primary Contact), Dave Foster, Jaal Ghandhi, Kevin Hoag and Chris Rutland
Engine Research Center
University of Wisconsin-Madison
1500 Engineering Drive
Madison, WI 53706

DOE Technology Development Manager: Kevin Stork

Subcontractor:
Prof. D. Haworth, Penn State University

Objectives

- Develop methods to optimize and control homogeneous charge compression ignition (HCCI) engines, with emphasis on diesel-fueled engines.
- Use engine experiments and detailed modeling to study factors that influence combustion phasing, unburned hydrocarbon (UHC) and carbon monoxide (CO) emissions.
- Provide criteria for transition to other engine operation regimes (e.g., standard diesel and low-temperature combustion).

Approach

- Use two fully-instrumented engines with prototype fuel injection systems and combustion sensors to map and define HCCI combustion regimes, and apply optimization techniques.
- Develop and apply engine performance models, including multi-, zero- and 1- dimensional global models for control system development.
- Use homogeneous and stratified charge Coordinating Fuel Research (CFR) engine and low and high injection pressure heavy-duty engine experiments to document fuel effects on HCCI ignition.
- Develop and apply modeling tools, including multi-dimensional codes (e.g., KIVA with state-of-the-art turbulent combustion and detailed and reduced chemistry models), to reveal combustion mechanisms.

Accomplishments

- Diesel HCCI combustion regimes have been identified on a Caterpillar 3401 engine using both low-pressure and high-pressure multiple injection strategies.
- Evaluated and selected combustion sensors and methodologies for engine control.
- Low-pressure diesel fuel injection has been shown to lead to significant fuel film formation on the cylinder wall that deteriorates engine performance.
- Models have been used successfully to propose methods to minimize wall film fuel and to provide start-of-combustion control via variable valve timing and variable geometry sprays.
- HCCI engine operating limits have been shown to be extended by operation with stratified combustion.
- Detailed combustion computations have been used to identify methodologies to increase mixing prior to ignition for emissions reduction.

Future Directions

- Use of multiple injections for diesel HCCI combustion control will be assessed.
- Guidelines for diesel HCCI will be obtained by experiments and modeling using variable intake valve actuation for combustion phasing control.

- Diesel HCCI will be investigated for fumigated/direct injection configurations including port fuel injection and high-pressure diesel in-cylinder injection systems.
- Efficient methods for including detailed kinetics will be implemented and applied in multidimensional models for more accurate combustion predictions.

Introduction

Advantages of HCCI operation include significantly reduced NO_x and particulate emissions. However, there are significant challenges associated with the successful operation of HCCI engines. One of the major difficulties is controlling the combustion phasing—mainly the assurance of auto-ignition at appropriate timings over a wide range of operating conditions. Another obstacle specific to diesel HCCI engine operation is the fact that the early injection required to provide time for fuel-air mixing can lead to wall impingement and, consequently, poor combustion efficiency. In addition, the formation of relatively high emissions of unburned hydrocarbons (HC) and carbon monoxide (CO) can occur due to incomplete combustion with low-temperature lean burn. The power output of the HCCI engine is also limited since the combustion can become unstable. The present research investigates methods to quantify and overcome these obstacles using a combined experimental and modeling approach.

Approach

In order to control the engine, it is necessary to know what variables to control. The six (6) technical tasks of the present work provide information about HCCI combustion mechanisms for use in knowledge-based engine control schemes. The experiments of Task 1 use a fully instrumented Caterpillar 3401 heavy-duty diesel engine that features electronically controlled fuel injection systems to map combustion regimes. Combustion sensors have been investigated for engine control, including acceleration (knock), ionization and cylinder-pressure detectors. Combustion diagnostics include engine-out particulate, NO_x, HC and other gaseous emissions measurements. Computer modeling, coupled with the engine experiments, is also being used to devise strategies for optimizing and controlling HCCI engine performance and reducing emissions over the speed-load range of interest in applications. The engine performance models include zero- and one-dimensional global models for control system development (Task 2). Task 3, In-cylinder Measurements (removed from the original proposal due to funding limitations, but now included with matching funding from industry), provides detailed validation data for chemical kinetics models. Additional model validation data is obtained using a CFR engine operated with various fuels (Task 4). The influence of turbulence, temperature and mixture inhomogeneity is revealed with highly resolved computational fluid dynamics (CFD) predictions (Tasks 5 and 6).

Results

Task 1: HCCI engine combustion optimization and regime mapping.

The Caterpillar 3401 heavy-duty diesel engine has been tested over a wide range of speeds and loads using low- and high-pressure injection systems and various injection strategies [1]. It was found that to achieve highly premixed combustion (HCCI-like) conditions, optimal dwell between the end of injection and the start of combustion is required to allow sufficient time for fuel-air mixing. The local mixture must be lean for soot/NO_x control [2]. With early injections (e.g., 50 degrees btdc), wall wetting is a significant problem. With high-pressure injection, an injection time earlier than 30 degrees before top dead center (btdc) can cause unacceptably high rates of pressure rise or lead to significant lost fuel due to wall impingement. On the other hand, combustion stability becomes a problem if the fuel is injected late in the cycle (e.g., more than 20 degrees after top dead center [atdc]). With low-pressure injection, the combustion process is complicated by a compromise between vaporization, mixing and ignition that is especially severe with the use of diesel fuel [3, 4]. A real-time control methodology based on a response surface method (RSM) technique has been established that uses a cylinder pressure sensor for feedback control. The methodology has been applied to optimize high

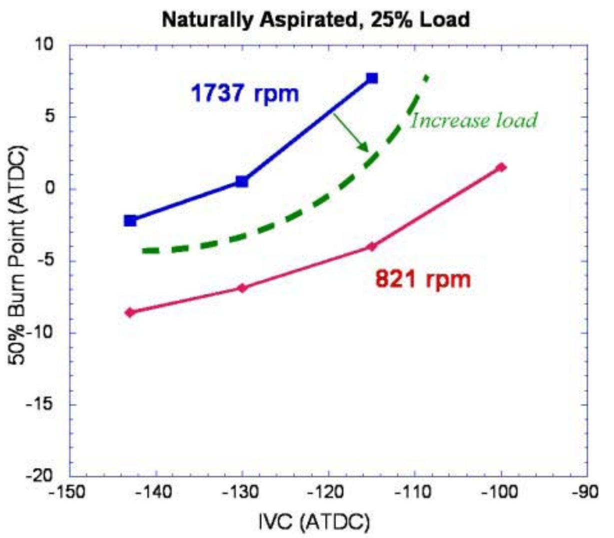


Figure 1. Combustion phasing control with variable valve timing. 50% burn point versus IVC for different engine speeds and loads.

injection pressure engine operation using a multiple injection strategy [5]. Detailed chemistry models have been developed using an efficient skeletal reaction mechanism to describe diesel fuel oxidation chemistry [6, 7, 8]. NO_x and soot emission models have been integrated into the mechanism such that the model successfully predicts the combustion process, as well as emissions trends. Acetylene is used as the soot formation species in the model formulation. Application of the model has shown that low soot emissions at early start-of-injection (SOI) timings (e.g., 20 btdc) is due to enhanced oxidation, while low soot emissions at late SOI (e.g., 5 atdc) is a result of less soot formation. The model is being further used to study combustion phasing control using variable intake valve camshaft (IVC) timing that has the same effects as varying the compression ratio [9]. Effects of load, boost and engine speed have been investigated, and the results have shown that the 50% burn point is retarded at high engine speed due to the shorter times available for chemical reactions. Combustion phasing can be optimized by increasing the engine load such that the IVC is within a controllable range, as shown in Figure 1. In addition, it is found that the 50% burn point is largely unaffected by boost, which can be used at higher loads to improve indicated mean effective pressure (IMEP). The present CFD models

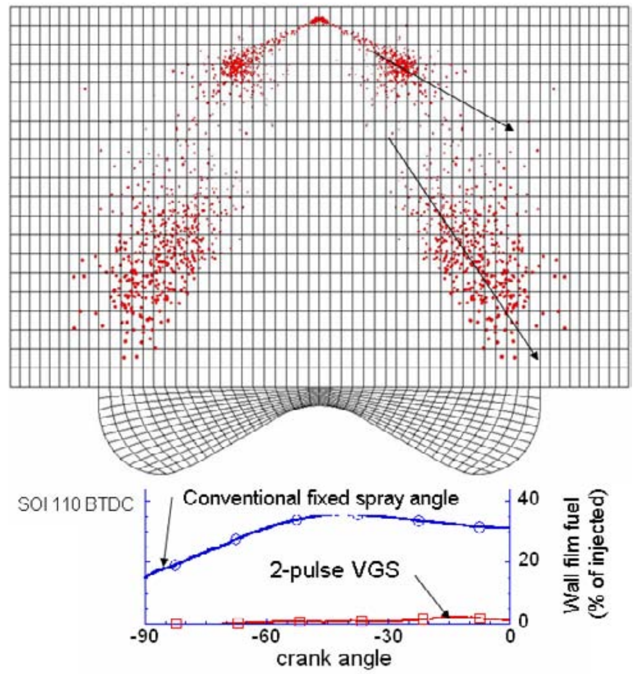


Figure 2. Optimized spray angle in each injection pulse gives improved fuel-air mixing and significantly reduced impinged fuel during the compression and combustion processes.

have also been used to explore the benefits of using variable geometry sprays (VGS) on mixture preparation for low-pressure direct in-cylinder injection HCCI operation. The results show that the amount of wall film fuel can be drastically reduced if the included spray angle is allowed to vary from a smaller angle at the beginning to a wider angle at the end of injection, as shown in Figure 2 [10]. Future modeling studies will include the optimization of intake valve timing with the VGS multiple injection strategy and exhaust gas recirculation (EGR). Models will also be used to help set up experimental port fuel injection/direct in-cylinder injection (PFI-DI) conditions to explore diesel HCCI low-emission operation.

Task 2: Combustion modeling and control.

Cycle simulation models are an important tool in understanding and developing viable combustion systems for HCCI operation. However, currently available cycle simulation codes lack advanced models for HCCI combustion. Under this project, advanced system-level modeling tools are being developed that can accurately predict direct injection diesel-fueled HCCI combustion. These are incorporated into control systems to study the basic time scales and feasibility of various control strategies during transient operations.

Commercially available full-cycle simulation codes are a convenient starting point as they readily model gas exchange processes. Three different approaches were used to couple advanced models with a cycle simulation program to capture the physics of HCCI combustion. The coupled simulations are used to study basic combustion controllers and to analyze fundamental aspects of speed/load transients in direct injection (DI) diesel HCCI operation. In the first approach, the GT-Power engine simulation code was integrated with Chemkin as a single-zone external combustion model to facilitate detailed chemistry calculations. In the second approach, an external cylinder model was developed and implemented into GT-Power. This model incorporates sub-models for fuel injection, vaporization, detailed chemistry calculations (Chemkin), heat transfer, and energy and species conservation. To improve the modeling accuracy, a multi-zone approach was used to account for temperature and fuel stratifications in the cylinder charge [11]. In the third approach, the multi-dimensional ERC-KIVA CFD code was coupled with GT-Power. The primary motivation for this coupling was to more accurately model the fuel injection process since it is critical in DI HCCI operation. To reduce run times, a validated coarse grid version of ERC-KIVA is being used.

The simulation results have been validated with experimental data from the Caterpillar 3401 engine modified for DI diesel HCCI operation. Parametric studies were conducted to identify the variables affecting ignition timing, and the coupled simulation was used to demonstrate transient operations in speed and load to develop closed loop control strategies, as shown in Figure 3. This example shows that a fuel savings of up to 3% is predicted with optimal control of fuel injection and intake valve closure timings. Future work aims at continued model development to make the system-level tools faster and more accurate, better understanding of the physics and relevant time scales for combustion control, and evaluation of relative advantages and disadvantages of various control concepts.

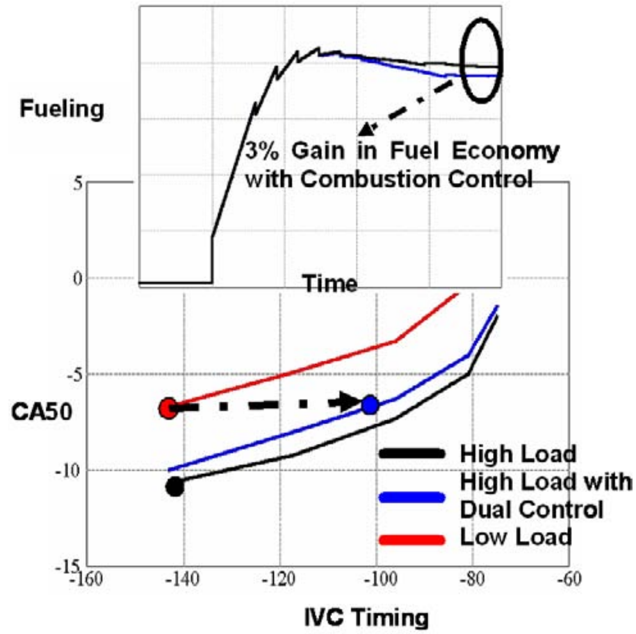


Figure 3. Simulation of load transient using simultaneous closed-loop control of fuel mass injected and variable intake valve closure. The use of variable valve closure demonstrates a 3% improvement in fuel economy.

Task 3: In-cylinder Measurements.

Near-wall planar measurements are being pursued in order to investigate the role of thermal stratification due to the cold cylinder walls. The experiment, however, cannot be performed in the manner of most planar laser-based measurements due to vignetting. [Vignetting is an optical effect that arises when an extended obstruction (e.g., the combustion chamber surface) is between the camera and the image plane, resulting in a reduction of the signal intensity near the obstruction, which is where one desires quantitative intensity information.] To overcome this problem, a through-the-wall illumination technique is being developed. Line-of-sight absorption measurements are being pursued to quantitatively measure the OH concentration as a function of temperature near the lean combustion limit. Presently, the design of the optical system is being undertaken. Finally, a modeless, wavelength-agile laser source has been developed to measure H_2O concentration and temperature. Measurements over a wide range of operating conditions will be pursued next. Wavelength-agile sources that will allow the measurement of other species are also being pursued.

Task 4: Ignition chemistry.

A focus of the research has been experimental engine tests on charge stratification as a means of extending the light-load operating range. The results show that there are operating windows at light-load conditions in which HCCI operation is improved via charge stratification [12]. Under these conditions, if the charge is premixed, the combustion quality is poor and the CO and HC emissions are very high. As the degree of stratification is increased, the CO and HC can be reduced. However, as the stratification is increased further, NO_x starts to increase.

A companion CFD modeling effort has attempted to quantify the threshold stratification for which combustion is improved, yet NO_x stays low. These simulations were conducted as full 3-D calculations that included the intake process, and sample results are shown in Figure 4. Five operating conditions have been simulated at 600 rev/min, compression ratio 16.6, equivalence ratio 0.15, with iso-octane as the fuel used in the simulation (the data are for PRF 91.8, the fuel that enabled us to explore the stratified operating conditions). Except for the premixed homogeneous case, all the fuel was directly injected into the cylinder. The injection profile for each case was created based on a validated spray model.

The trend of NO_x versus time of start of injection (SOI) is shown across the bottom of Figure 4. It is observed that the NO_x stays low when start of injection occurs earlier than 90^o btdc. Also, it was noted that there is significant stratification in both equivalence ratio and temperature right up to start of combustion for all cases investigated, even those in which the NO_x emission from the cylinder is low (see Figure 4). However, when NO_x increases as injection timing is retarded, it increases very rapidly.

Tasks 5 and 6: Multidimensional Modeling.

The impacts of mixing and fuel preparation on HCCI combustion phasing, specifically the study of ignition 'dwell' between end of fuel injection and start of combustion, are being studied using CFD. Temperature is known to have a large and direct impact on the timing and duration of ignition dwell. However, initial fuel-air distribution and mixing can also affect combustion phasing, with the advantage

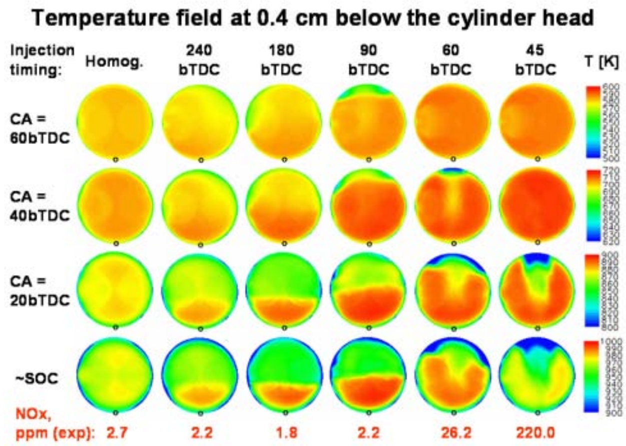


Figure 4. Predicted temperature distributions at different crank angles in a cut plane at the injector location for different SOI. The engine-out NO_x for each operating condition is given at the bottom of each column of images.

of a much faster response time than changes in temperature. To investigate the impact of mixing, variations in EGR percent, fuel injection timing, engine valve actuation and swirl ratio magnitude were simulated. To determine the extent of fuel-air mixing generated by these techniques, the equivalence ratio and temperature distribution, intermediate radical formation, mixing timescales and fuel vaporization were analyzed. The results showed that the initial fuel-air distribution did affect the ignition dwell, although to a smaller extent than changes in temperature [12].

Currently, work is in progress to incorporate several large eddy simulation (LES) models into the study. LES models are more accurate in depicting the large-scale fluid flow structures and will help understand details of mixing in the engine. Figure 5 shows a sample result using the standard Smagorinsky LES model. This image was used to study the details of the flow structure and temperature profiles during the intake stroke. These profiles were compared with earlier profiles from Reynolds Averaged Navier Stokes (RANS) models. It was observed that the LES profiles were able to capture important details of the flow structure. For example, in the top image, eddies are observed downstream of the valve stems in the intake manifold. These are caused by reverse flow at the beginning of the intake stroke and they result in the

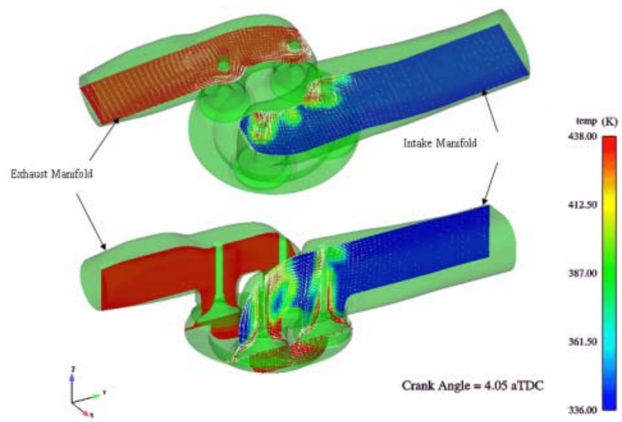


Figure 5. Cut-plane sections showing temperature contours through cylinder, intake and exhaust manifolds close to start of the intake stroke using LES turbulence models.

induction of cooler air into the cylinder later during the intake stroke. This affects the in-cylinder temperature and charge mass so that the LES predictions show a better match with experimental results.

Consistent hybrid particle/finite-volume probability density function (PDF) methods [13], detailed chemical kinetics [14, 15], and chemistry acceleration strategies [8, 16] have been developed for three-dimensional time-dependent simulations of autoignition and emissions in HCCI engines. The resulting model has been compared with experimental measurements in the CFR engine [17, 18], as shown in Figure 6. With no explicit tuning to match these experiments, the model captures the trends with variations in equivalence ratio and other operating conditions.

The influence of turbulence/chemistry interactions (TCI) on autoignition and emissions (CO and unburned hydrocarbons) has been examined by considering the joint PDF of up to 40 chemical species and mixture enthalpy. Variations in global equivalence ratio, wall temperature, swirl level, degree of mixture inhomogeneity (including direct in-cylinder fuel injection), and a top-ring-land crevice (TRLC) have been investigated, and sensitivities to model parameters and engine operating conditions have been established [19, 20]. Key findings are that, for nearly homogeneous reactants with low to moderate swirl and no TRLC,

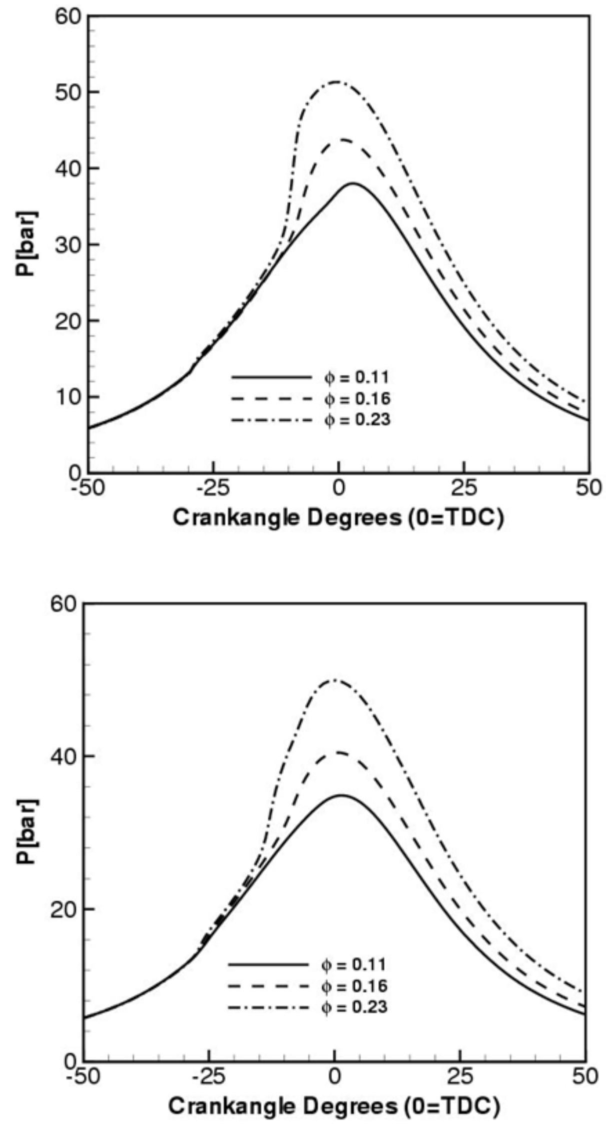


Figure 6. Computed (top) and measured (bottom) in-cylinder pressure with variations in equivalence ratio (Φ) for premixed n-heptane/air in the CFR engine. (From Ref. [18].)

TCI has little effect on ignition timing. However, even in that case, the influence of TCI on emissions is not negligible. In addition, with increasing levels of swirl, higher degrees of mixture inhomogeneity, and for cases that include a TRLC, TCI effects become increasingly important and result in significant changes in ignition timing, global in-cylinder temperature and pressure, and emissions. Finally, unburned fuel is a non-negligible contribution to UHC only in cases with high swirl or where a TRLC has been considered.

Conclusions

The engine tests have shown that operation at both very early and very late start-of-injection timings is effective for low emissions using high-pressure diesel fuel injection. A combustion control criterion based on the ignition/injection time delay has been formulated and has been implemented in a control algorithm for low-emissions operation. With low-pressure fuel injection and early injection for mixing, significant fuel wall impingement occurs and performance deteriorates. Multidimensional modeling has been applied successfully to provide guidelines to minimize wall fuel using variable geometry sprays. In addition, variable intake valve closure timing has been shown to be useful for combustion phasing control in diesel HCCI. Detailed turbulence and chemistry models have been developed and are being applied to study mixing and combustion in diesel HCCI engines. It is concluded that PDF methods are a practical and valuable approach for three-dimensional time-dependent modeling of HCCI autoignition and emissions.

Special Recognitions & Awards/Patents Issued

1. Reitz, R.D., Rutland, C.J., Jhavar, R., "Engine Valve Actuation for Combustion Enhancement", Awarded U.S. Patent 6,736,106, May 2004.

FY 2004 Publications/Presentations

1. UW DOE HCCI Working Group Presentation Meetings: January 29, 2004 (Sandia) and June 24, 2004 (USCAR).
2. Kong, S.-C., and Reitz, R.D., "3-D CFD Tools for PCCI Engine Simulations," SAE Homogeneous Charge Compression Ignition Symposium, Berkeley, CA, August 10-11, 2004.
3. Foster, D.E., "The Impact of Stratification on HCCI Operational Ranges," SAE Homogeneous Charge Compression Ignition Symposium, Berkeley, CA, August 10-11, 2004.
4. Kong, S.-C., Patel, A., and Reitz, R.D., "Development and Application of Detailed Chemistry-Based CFD Models for Diesel HCCI Engine Combustion Simulations," Proceedings of THIESEL 2004 Conference, Valencia, Spain, September 9-12, 2004.
5. Jhavar, R., Rutland C.J., "A Computational Study of the Impact of Mixing on HCCI," Proceedings of THIESEL 2004, Universidad Politecnica De Valencia, Spain, September 2004.
6. Tao, F., Reitz, R.D., Srinivas, S., and Foster, D.F., "Current Status of Soot Modeling Applied to Diesel Combustion Simulations," COMODIA 2004, The Sixth International Symposium on Diagnostics and Modeling of Combustion in Internal Combustion Engines, Yokohama, Japan, August 2-5, 2004.
7. Ra, Y., and Reitz, R.D., "The Role of Vaporization and Mixture Preparation on HCCI Engine Combustion," ILASS-04 Conference, Washington, DC, May 16-19, 2004.
8. Hruby, E.J., Ra, Y., and Reitz, R.D., "Parametric Study of Combustion Characteristics in a Diesel HCCI Engine with a Low Pressure Fuel Injector," ILASS-04 Conference, Washington, DC, May 16-19, 2004.
9. Canakci, M., and Reitz, R.D., "Experimental Optimization of a DI-HCCI-Gasoline Engine's Performance and Emissions Using Split Injections with Fully-Automated Micro-Genetic Algorithms," ASME Journal of Gas Turbines and Power, Vol. 126, No. 1, pp. 167-177, 2004.
10. Juneja, H., Ra, Y., and Reitz, R.D., "Optimization of Injection Rate Shape Using Active Control of Fuel Injection," SAE Paper 2004-01-0530, Presented at SAE Congress, Detroit, MI, 2004.
11. Patel, A., Kong, S.-C., and Reitz, R.D., "Development and Validation of a Reduced Reaction Mechanism for HCCI Engine Simulations," SAE Paper 2004-01-0558, Presented at SAE Congress, Detroit, MI, 2004.
12. 2010 ERC Diesel Emissions Reduction Consortium, Madison, WI, September 21, 2004.
13. Lee, K., and Reitz, R.D., "Investigation of Spray Characteristics from a Low-Pressure Common Rail Injection System for Use in a HCCI Engine," Measurement Science and Technology, Vol. 15, No. 3, pp. 509-519, 2004.
14. Volker, S., Kong, S.C., Foster, D.E., Morikawa, T., Iida, M., "A Computational Investigation into the Cool Flame Region in HCCI Combustion," SAE 2004-01-0552, Transactions, Presented at SAE Congress, Detroit, MI, 2004.
15. Aroonsrisopon, T., Werner, P., Sohm, V., Waldman, J., Foster, D.E., Morikawa, T., and Iida, M., "Expanding the HCCI Operation with Charge Stratification," SAE 2004-01-1756, Transactions, Presented at SAE Congress, Detroit, MI, 2004.
16. Zhang, Y.Z., "Hybrid Particle/Mesh PDF Methods for 3D Time-Dependent Flows in Complex Geometries," Ph.D. Thesis, Department of Mechanical & Nuclear Engineering, The Pennsylvania State University (2004).

17. Zhang, Y.Z., Kung, E.H. and Haworth, D.C., "A PDF Method for Multidimensional Modeling of HCCI Engine Combustion: Effects of Turbulence/Chemistry Interactions on Ignition Timing and Emissions," *Proc. Combust. Institute* **30** (2004), to appear.
18. Veljkovic, Plassmann, P.E. and Haworth, D.C., "Parallel Implementation of Scientific On-line Database for Efficient Function Approximation," *2004 Intern'l. Conference on Parallel and Distributed Processing Techniques and Applications*, Las Vegas, NV (21-24 June 2004).
19. Zhang, Y.Z., Kung, E.H. and Haworth, D.C., "A PDF Method for Three-Dimensional Time-Dependent Computations of HCCI Engine Autoignition and Emissions," *SIAM 10th International Conference on Numerical Combustion*, Sedona, AZ (9-12 May 2004).
20. Haworth, D.C., "A PDF Method for Multidimensional Modeling of HCCI Engine Combustion," *CD-adapco 5th ICE Work-Group Meeting*, London, England (17 March 2004).
21. Haworth, D.C., "Combustion in Internal Combustion Engines," *STAR-CD 12th European User Conference*, London, England (15-16 March 2004).
22. Zhang, Y.Z., Kung, E.H., and Haworth, D.C., "A PDF Method for Multidimensional Modeling of HCCI Engine Combustion: Effects of Turbulence/Chemistry Interactions on Ignition Timing and Emissions," *14th International Multidimensional Engine Modeling Users' Group Meeting*, Detroit, MI (7 March 2004).
23. Veljkovic, I., Haworth, D.C. and Plassmann, P.E., "Parallel Implementation of Scientific On-line Database," *SIAM Conference on Parallel Processing for Scientific Computing*, San Francisco, CA (25-27 February 2004).

References

1. Klingbeil, A., "Particulate and NO_x Reduction in a Heavy-Duty Diesel Engine Using High Levels of Exhaust Gas Recirculation and Very Early or Very Late Start of Injection," MS Thesis, University of Wisconsin-Madison, 2002.
2. Klingbeil, A.E., Juneja, H., Ra, Y. and Reitz, R.D., "Premixed Diesel Combustion Analysis in a Heavy-Duty Diesel Engine," SAE paper 2003-01-0341, 2003.
3. Canakci, M., and Reitz, R.D., "Experimental Optimization of a DI-HCCI-Gasoline Engine Using Split Injections with Fully-Automated Micro-Genetic Algorithms," International Journal of Engine Research, Vol. 4, No. 1, pp. 47-60, 2003.
4. Canakci, M., and Reitz, R.D., "Experimental Optimization of a DI-HCCI-Gasoline Engine's Performance and Emissions Using Split Injections with Fully-Automated Micro-Genetic Algorithms," ASME Journal of Gas Turbines and Power, Vol. 126, No. 1, pp. 167-177, 2004.
5. Von Der Ehe, J., "Closed-Loop Feedback Control of a Heavy-Duty Diesel Engine for Emissions Reduction," MS Thesis, University of Wisconsin-Madison, 2004.
6. Kong, S.-C., and Reitz, R.D., "Use of Detailed Chemical Kinetics to Study HCCI Engine Combustion with Consideration of Turbulent Mixing Effects," ASME Journal of Gas Turbines and Power, Vol. 124 (3), pp. 702-707, 2002.
7. Kong, S.-C., Patel, A., Yin, Q., Klingbeil, A., and Reitz, R.D., "Numerical Modeling of Diesel Engine Combustion and Emissions Under HCCI-Like Conditions with High EGR Levels," SAE paper 2003-01-1087, 2003.
8. Patel, A., Kong, S.-C., and Reitz, R.D., "Development and Validation of a Reduced Reaction Mechanism for HCCI Engine Simulations," SAE Paper 2004-01-0558, 2004.
9. Munnannur, A., Kong, S.-C., and Reitz, R.D., "Performance Optimization of Diesel Engines with Variable Intake Valve Timing via Genetic Algorithms," Submitted to 2005 SAE Congress, September, 2004.
10. Ra, Y., and Reitz, R.D., "The Use of Variable Geometry Sprays with Low Pressure Injection for Optimization of Diesel HCCI Engine Combustion," Submitted to 2005 SAE Congress, October, 2004.
11. Narayanaswamy, K., and Rutland, C.J., "Cycle Simulation Diesel HCCI Modeling Studies and Control," SAE Paper No. 2004-01-2997 (To appear SAE Powertrain Conference, Tampa, FL, October 25-28, 2004).
12. Aroonsrisopon, T., Sohm, V., Werner, P., Foster, D.E., Morikawa, T., and Iida, M., "An Investigation into the Effect of Fuel Composition on HCCI Combustion Characteristics," SAE Paper 2002-01-2830, 2002.
13. Jhavar R., Rutland C.J., "A Computational Study of the Impact of Mixing on HCCI," Proceedings of THIESEL 2004, Universidad Politecnica De Valencia, Spain, September, 2004.
14. Zhang, Y.Z., and Haworth, D.C., "A General Mass Consistency Algorithm for Hybrid Particle/Finite-Volume PDF Method," J. Comput. Phys. 194: 156-193 (2004).

15. Nordin, N., “Numerical Simulation of Non-Steady Spray Combustion Using a Detailed Chemistry Approach,” Thesis for the degree of Licenciate of Engineering, Department of Thermo and Fluid Dynamics, Chalmers University of Technology, Goteborg, Sweden, 1998.
16. Pope, S.B., “Computationally Efficient Implementation of Combustion Chemistry Using in Situ Adaptive Tabulation,” Combust. Theory & Modelling 1:41-63 (1997).
17. Veljkovic, I., Plassmann, P., and Haworth, D., “A Scientific On-line Database for Efficient Function Approximation,” in Computational Science and Its Applications – ICCSA 2003, Lecture Notes in Computer Science (LNCS 2667), Part I, pp. 643-653, Springer Verlag (2003).
18. Aroonsrisopon, T., Werner, P., Waldman, J.O., Sohm, V., Foster, D.E., Morikawa, T., and Iida, M., “Expanding the HCCI Operation Using the Charge Stratification,” SAE paper 2004-01-1756, 2004.
19. Zhang, Y.Z., “Hybrid Particle/Mesh PDF Methods for 3D Time-Dependent Flows in Complex Geometries,” Ph.D. Thesis, Department of Mechanical & Nuclear Engineering, The Pennsylvania State University, 2004.
20. Zhang, Y.Z., Kung, E.H. and Haworth, D.C., “A PDF Method for Multidimensional Modeling of HCCI Engine Combustion: Effects of Turbulence/Chemistry Interactions on Ignition Timing and Emissions,” Proc. Combust. Institute 30 (2004), to appear.

II.A.13 HCCI Engine Optimization and Control Using Gasoline

Dennis Assanis
University of Michigan (UM)
Mechanical Engineering
2045 W.E.Lay Auto. Lab.
1231 Beal Avenue
Ann Arbor, MI 48109-2133

DOE Technology Development Manager: Kevin Stork

Subcontractors:
Massachusetts Institute of Technology (MIT)
Stanford University (SU)
University of California, Berkeley (UCB)

Objectives

- Develop a homogeneous charge compression ignition (HCCI) engine control system.
- Develop full-cycle modeling tools.
- Investigate chemical kinetics for modeling gasoline HCCI combustion.
- Carry out detailed modeling studies of mixing and sprays using computational fluid dynamics (CFD) codes and validate with optical diagnostics.

Approach

- Carry out experimental tests of available HCCI control methods.
- Develop a range of models of HCCI engines, from simple single-zone to complex CFD codes, in order to incorporate and share the knowledge base on HCCI as it develops.
- Investigate critical chemical kinetic rates and mechanisms for gasoline, and develop and validate reduced kinetic mechanisms for computationally efficient use in these engine models.
- Validate models with engine experiments and combine models and experiments to develop a workable engine control system.

Accomplishments

- Experimentally demonstrated potential control methods using breathing and thermal effects on HCCI and identified characteristic times of in-cylinder effects (10 cycles) and thermal effects (100's of cycles).
- Developed controller algorithms and demonstrated them in engine tests.
- Developed a new heat transfer correlation specific to HCCI based on direct heat transfer measurements.
- Constructed a system model based on GT-Power software that integrates experimental data from experiments on heat transfer and kinetics. Validated the model with experimental data including spark ignition (SI)-HCCI transitions. Successfully represented gasoline with the combustion model for isooctane by use of a simple calibration factor.
- Developed an integrated CFD-kinetic model which shows the effect of mixing through the combustion event. Results show significant broadening of the temperature profile throughout the cycle, leading to decreasing burn rate for later combustion events.
- Carried out measurements of ignition delay in isooctane-air mixtures in shocktubes and the UM rapid compression facility. Benchmarked available detailed kinetic models against this data set and identified best performance models.

- Correlated ignition delay data with a simple autoignition integral and successfully integrated the correlation into the engine-vehicle system model.
- Obtained instantaneous and average images of fuel inhomogeneities in an optical engine, and identified effects of swirl and residual levels.
- Performed 0-D and 1-D counterflow reaction simulations to identify fundamental criteria of mixedness (mixture fraction) and rate of mixing (scalar dissipation rate) for different ignition regimes.
- Integrated KIVA-3V with a representative interactive flamelet (RIF) model as an advanced full-cycle simulation strategy.

Future Directions

- Engine control experiments will expand and refine current studies of mode transitions, thermal transients necessary for successful HCCI implementation. Control algorithms will be developed and validated in engine experiments.
- Chemical kinetic and computational studies along with shock tube and Rapid Compression Facility (RCF) experiments will feed improved models of gasoline into the engine simulation tools.
- Detailed kinetics, CFD and mixing models that have been developed will be applied to generate fast semi-empirical models of ignition and HCCI combustion for ongoing incorporation into the engine system model.
- The engine system model will be used to develop and evaluate workable HCCI control strategies, first for an engine alone and then in the full vehicle environment.

Introduction

Homogeneous charge compression ignition (HCCI) has the potential to dramatically reduce NO_x emissions from gasoline internal combustion engines while achieving high thermal efficiencies characteristic of diesels, with lower particulate emissions. Because the ignition is not controlled by a spark plug as in conventional gasoline engines but occurs indirectly as a result of the compression heating of the charge, HCCI has been difficult to implement in practical engines. Therefore, the primary objective of this research project is to develop, through experiments and modeling, the understanding of physical and chemical HCCI processes necessary to develop and apply practical control strategies. To meet the project objectives, we have formed a multi-university research consortium of experts in the areas of engine, optical diagnostics, numerical modeling, gas dynamics, chemical kinetics and combustion research from UM, MIT, SU, UCB.

Approach

Our research project, now in its third year, combines experiments and modeling at various levels of complexity in order to acquire and utilize the knowledge and technology to develop a robust control system for HCCI engines. Both single-cylinder and multi-cylinder engine experiments are addressing issues such as injection strategy, mixture homogeneity, valve timing, exhaust gas recirculation (EGR), intake temperature, fuel properties, cooling strategy, transients and engine mode transitions (e.g. SI-to-HCCI). A range of models of HCCI engines and combustion, from simple single-zone to complex CFD codes, is being used in close coordination with the engine experiments to incorporate the experience gained as it develops. At the same time, extensive studies are underway to develop accurate and reliable chemical kinetic models for practical engine fuels. Together, the kinetics, engine models, and experiments will be used to identify HCCI operating ranges and limits and to develop viable control strategies.

Results

Development of an HCCI engine control system

Potential control methods to handle load changes and mode transitions have been demonstrated at MIT, Berkeley (UCB), and Stanford, on single-cylinder engines employing backpressure valves,

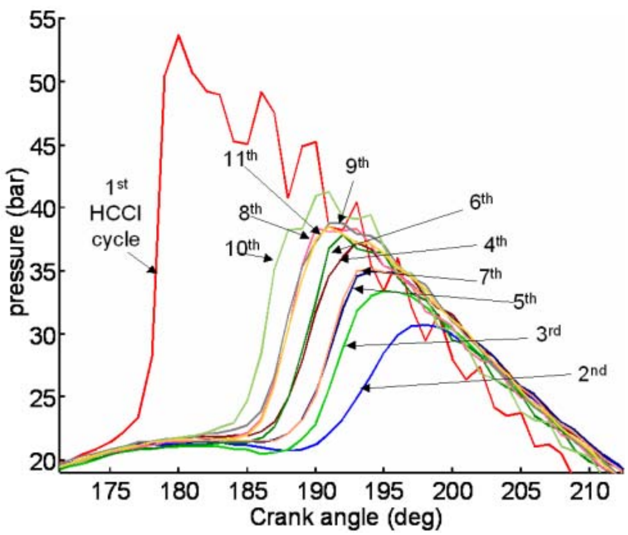


Figure 1. Pressure Traces of the First 10 Cycles During an SI-HCCI Transition (MIT)

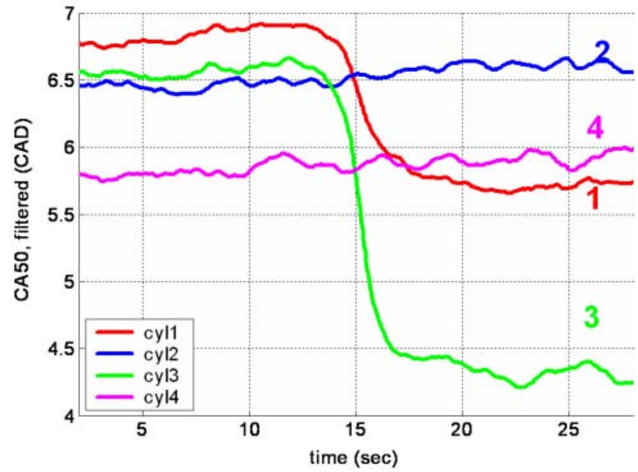


Figure 2. Cylinder-to-Cylinder Cross Talk Observed at UCB (Adjusting combustion phasing by exhaust throttle in Cylinder 1 affects phasing of Cylinder 4.)

inlet heaters, and variable valve actuation (VVA). Figure 1 shows the first HCCI cycle in a SI-HCCI transition using VVA, as well as the following 10 cycles. From this work, the time required for mode and load changes was found to be on the order of ten cycles and is related to prior cycle residual carryover effects. In a multi-cylinder setup at UCB, significant crosstalk was observed between cylinders when exhaust pressure was used for HCCI control (Figure 2). This is expected to present challenges for real-world control, especially for engines that rely on internal EGR for HCCI initiation. Experiments on thermal management at UM determined sensitivities to wall and intake temperature, intake manifold pressure, backpressure, and internal/external EGR. Most significant is the finding that wall temperature is as critical a variable as intake temperature in determining combustion phasing. Work is underway at MIT, Stanford, and UCB to develop controls-oriented models and controller algorithms and to test them in engine experiments. An example of such a control strategy is shown in Figure 3 where Stanford researchers employed a linear reduced-order controller strategy to control peak pressure to desired values.

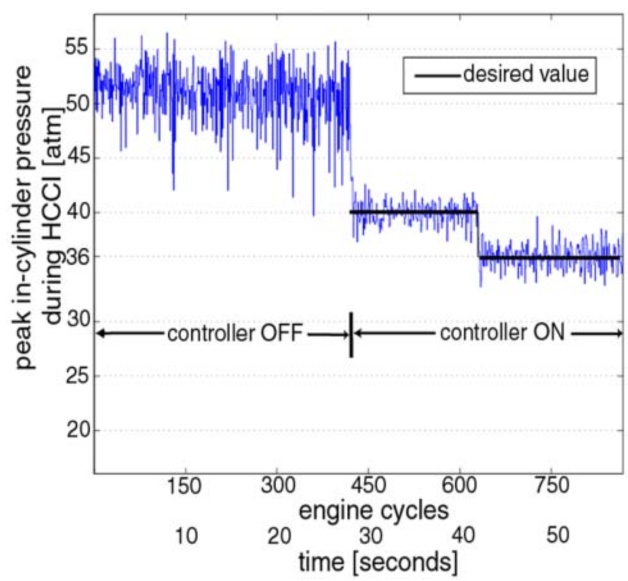


Figure 3. Demonstration of the Effect of a Linear Controller in Combustion Phasing and Load Control Using VVA (Stanford)

Full cycle and system modeling tools

A combined CFD-multizone model was developed at UM and used to explore effects of in-cylinder EGR mixing with different valve strategies. A comparison of negative overlap vs. rebreathing valve profiles showed that the rebreathing strategy provided better EGR mixing, which may be desirable under certain conditions. This approach has been extended with a new integrated CFD-kinetic model developed in collaboration with Lawrence Livermore National Laboratory (LLNL). This allows the CFD computation to be carried out throughout the

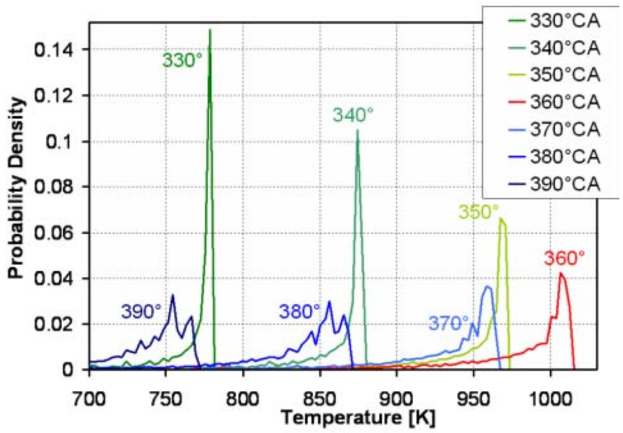


Figure 4. KIVA Results Showing the Broadening of the Probability Density of the Unburned Charge Temperature in the Crank Angle Range 330 - 390°CA (UM-LLNL)

combustion phase. The results in Figure 4 show significant broadening of the temperature profile with crank angle as the piston passes through top dead center and are consistent with the well-known increase in burn duration with later combustion phasing.

A new heat transfer correlation for HCCI was developed at UM based on measured instantaneous heat fluxes. A method was also developed for normalizing kinetic mechanisms for isooctane in order to represent "gasoline" in engine models. Also, a single-zone thermo-kinetic model and an auto-ignition integral model for HCCI combustion were developed.

For the first time, these submodels were incorporated into a GT-Power system environment. The combined system model has been exercised to simulate VVA mode transitions in the MIT experiments. The model results successfully demonstrated the same 10-cycle timescale noted earlier for engine cycle stabilization. Figure 5 shows the experimental SI-HCCI transition achieved by the MIT team compared to the UM modeled results. The system modeling tool was then used in the context of a thermal network of piston, head and cylinder liner to characterize in-vehicle thermal transients for speed and load changes. These transients were found to have timescales on the order of hundreds of engine cycles and will have a major influence on control strategies. Validation work on the model is

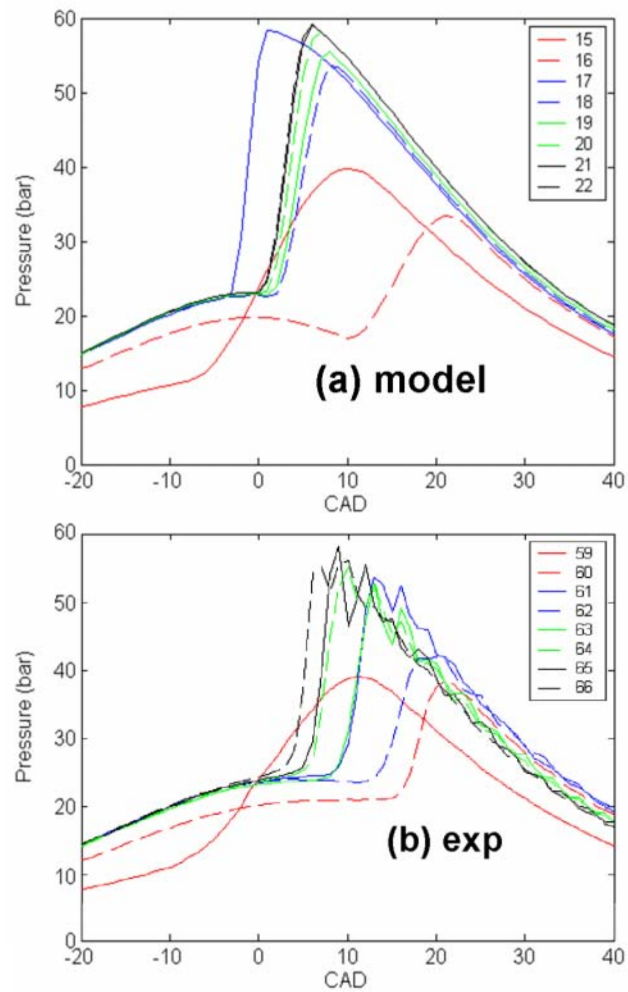


Figure 5. SI-HCCI Transition Simulated by UM System Model (a), and Corresponding Experimental Results from MIT (b)

continuing in preparation for application to a full engine control system simulation.

Investigation of chemical kinetics for gasoline HCCI

Experiments in the UM Rapid Compression Facility (RCF) and shock tube experiments at Stanford have been focused on measuring ignition delay in isooctane air/diluent mixtures. Based on these results, an ignition time correlation was developed quantifying the role of temperature (T), pressure (P), fuel-oxygen equivalence ratio (ϕ_{FO}), oxygen-to-diluent ratio, and EGR on ignition delay. Figure 6 shows the experimental data and the line representing the correlation. The correlation has been successfully used in the engine system

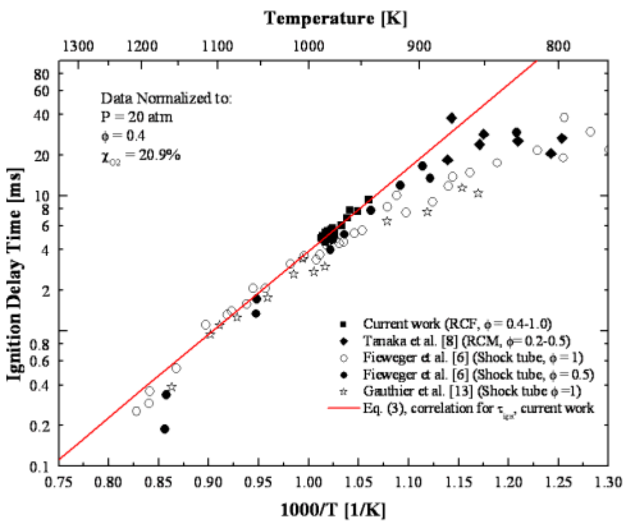


Figure 6. Ignition Delay Data from UM (RCF) and Stanford (shock tube) Along with Correlation Line Developed for Use in Engine System Models

modeling work at UM and has been validated against isooctane engine data and, with a calibration factor, for gasoline data.

On the modeling front, a 258-species skeletal mechanism for isooctane was developed at UCB based on the detailed 857 Curran mechanism. When this mechanism was benchmarked against the data, it was found to perform well near stoichiometric conditions. Under lean conditions, the 84-species reaction scheme of Golovitchev et al. performed better. Both mechanisms significantly reduce the time required for detailed kinetics calculations. At MIT, two software packages have been developed: one automatically constructs detailed chemistry models for any fuel, while the other produces reduced mechanisms from a given detailed mechanism, based on required accuracy over a specified thermodynamic path. Validation is continuing.

Detailed modeling of reaction, mixing and spray dynamics using CFD

Optical engine experiments provided instantaneous and average imaging of fuel disappearance, yielding information about the instantaneous and average mixture inhomogeneities within the engine. The effects of swirl and residual levels on mixture inhomogeneity and combustion phasing have also been investigated. Zero- and one-dimensional counterflow simulations were performed to identify fundamental mixing criterion for different ignition regimes. The parameterization of ignition regimes in terms of mixedness (mixture fraction) and rate of mixing (scalar dissipation rate) was performed to guide an advanced multi-zone modeling effort. KIVA-3V was integrated with a representative interactive flamelet model as an advanced full-cycle simulation strategy. The code integration is complete, and test simulations are currently in progress.

Conclusions

Significant accomplishments have been achieved in FY 2004 through the linked efforts of the multi-university research team:

Control of HCCI operation has been demonstrated on three engines in the consortium, each with a different strategy. Both static (low speed) and dynamic (high speed mode change) control have been achieved. A fourth engine provided detailed heat transfer data and determined sensitivities of combustion to thermal variables. Initial controller algorithms have been developed and tested.

A new heat transfer correlation for HCCI was developed at UM based on measured heat fluxes which were found to be different from gasoline engines. Fundamental combustion data obtained in a rapid compression facility and in shock tube experiments have been used to test available chemical mechanisms for describing HCCI ignition and combustion with isooctane as a surrogate for gasoline. A simple auto-ignition integral correlation with a calibration factor for gasoline was developed for use in engine system models.

These submodels were incorporated into a GT-Power system environment modeling tool. The combined system model has been exercised to simulate VVA experiments and successfully demonstrated the same 10-cycle timescale noted in the experiments for engine cycle stabilization. The system modeling tool was also used in the context of a thermal network to characterize in-vehicle thermal transients for speed and load changes, which were found to have timescales on the order of hundreds of engine cycles and will have a major influence on control strategies. Validation work on the model is continuing in preparation for application to a full engine control system simulation.

References and FY 2004 Publications/ Presentations

1. Babajimopoulos, A., Lavoie, G.A., and Assanis, D.A. (2003), "Modeling HCCI Combustion with High Levels of Residual Gas Fraction – A Comparison of Two VVA Strategies," SAE Paper 2003-01-3220.
2. Chang, J., et al. (2004), "New Heat Transfer Correlation for an HCCI Engine Derived From Measurements of Instantaneous Surface Heat Flux," SAE Paper No. 2004-01-2996.
3. Chen, J.-Y., Kolbu, J., Homma, R., and Dibble, R.W. (2003), "Optimization of Homogeneous Charge Compression Ignition with Genetic Algorithms," *Combustion Science and Technology*, 175, 373-392, 2003.
4. Chen, J.H., Hawkes, E., Hewson, J.C., Sankaran, R., and Im, H.G. (2003), "The Effect of Turbulent Mixing on Compression Ignition of a Lean Hydrogen/ Air Premixture," Fall Meeting of the Western States Section, The Combustion Institute, University of California, Los Angeles, CA, October 20-21.
5. Choi, Y. and Chen, J.-Y. (2003), "Numerical Modeling of Start-of-Combustion (SOC) in HCCI Engine with Artificial Neural Network (ANN)," Presented at the 2003 Fall Western States Meeting of The Combustion Institute, WSSCI paper 03F-69.
6. Choi, Y. and Chen, J.-Y. (2004), "Fast Prediction of Start-of-Combustion in HCCI with Combined Artificial Neural Networks and Ignition Delay Model," Presented at the 30th Symposium on Combustion, July 2004.
7. Davidson, D.F., Gauthier, B.M., Hanson, R.K. (2004), "Shock Tube Ignition Measurements of Iso-Octane/Air and Toluene/Air at High Pressures," Proceedings of the Combustion Institute 30: in press (2004).
8. Filipi, Z. (2004), "Experimental Insight into Heat Transfer in a Gasoline HCCI Engine," Presented at the SAE Symposium on HCCI, Berkeley, CA, August 10-11, 2004.
9. Flowers, D., Aceves, S., Martinez-Frias, J., Hessel, R., and Dibble, R.W. (2003), "Effect of Mixing on Hydrocarbon and Carbon Monoxide Emissions Prediction for Isooctane HCCI Engine Combustion Using a Multi-Zone Detailed Kinetics Solver," SAE Paper No. 2003-01-1821.
10. Gauthier, B.M., Davidson, D.F., Hanson, R.K., "Shock Tube Ignition Measurements of Iso-Octane and Toluene Ignition at High Pressures," Paper 03F-26, Western States Section/ Combustion Institute Fall Meeting, Los Angeles (2003).
11. Green, W.H., Wijaya, C.D., Yelvington, P.E., and Sumathi, R., "Predicting Chemical Kinetics with Computational Chemistry: Is QOOH = HOQO Important in Fuel Ignition?" *Molecular Physics* 102, 371–380 (2004).
12. Green, W.H., "Computer-Aided Construction of Chemical Kinetic Models," 25th Annual US DOE BES Combustion Research Conference, Airlie, VA, June 2004.
13. Mathews, J., Santoso, H. and Cheng, W.K. (2005), "Load Control for an HCCI Engine," to be presented at SAE Congress, Detroit, MI.
14. Oehlschlaeger, M.A., Davidson, D.F., and Hanson, R.K. (2004), "High-Temperature Thermal Decomposition and Iso-Butane and n-Butane Behind Shock Waves," Journal of Physical Chemistry A108: 4247-4253 (2004).
15. Sankaran, R., Im, H.G., Hawkes, E.R., and Chen, J.H. (2004), "The Effects of Nonuniform Temperature Distribution on the Ignition of a Lean Homogeneous Hydrogen-Air Mixture," Proceedings of The Combustion Institute 30, in press.
16. Sankaran, R. and Im, H.G. (2004), "Characteristics of Auto-Ignition in a Stratified Iso-Octane Mixture with Exhaust Gases under HCCI Conditions," Combustion Theory and Modelling, submitted.
17. Sankaran, R., Oh, T.K., and Im, H.G. (2003), "Ignition and Front Propagation in a Stratified Methane-Air Mixture with Exhaust Gases," Technical Meeting of the Eastern States Section, The Combustion Institute, Pennsylvania State University, University Park, PA, October 27-29.
18. Sankaran, R. and Im, H.G. (2004), "Effects of Mixture Inhomogeneity on the Auto-Ignition of Reactants under HCCI Environment," 42nd Aerospace Sciences Meeting & Exhibit, Paper No. 2004-1328, Reno, NV, January 5-8.
19. Sankaran, R., Im, H.G., Hawkes, E.R., and Chen, J.H. (2004), "A Computational Study on the Ignition of a Lean Hydrogen-Air Mixture with Non-Uniform Temperature Distribution," Spring Technical Meeting of the Central States Section, The Combustion Institute, University of Texas at Austin, Austin, Texas, March 21-23.
20. Santoso, H., Mathews, J. and Cheng, W.K. (2005), "Managing SI/HCCI Dual-Mode Engine Operation," to be presented at SAE Congress, Detroit, MI.

21. Sjöberg M., Dec, J.E., Babajimopoulos, A., and Assanis, D. (2004), "Comparing Enhanced Natural Thermal Stratification against Retarded Combustion Phasing for Smoothing of HCCI Heat-Release Rates," SAE paper 2004-01-2994.
22. Song, J., Sumathi, R., Yu, J., and Green, W.H., "Next Generation Model Construction Software, & New Approaches to Estimating Rates and Thermochemistry for Combustion," American Chemical Society National Meeting (Fuels Division), Philadelphia, PA, August 2004.
23. Tham, Y.F. and Chen, J.-Y. (2003), "Recent Advancement on Automatic Generation of Simplified Mechanisms," Presented at the 2003 Fall Western States Meeting of The Combustion Institute, WSS-CI paper 03F-49.
24. Yelvington, P.E., Bernat i Rollo, M., Liput, S., Tester, J.W., Green, W.H., and Yang, J. (2004), "Predicting Performance Maps for HCCI Engines," *Combustion Science & Technology* 176, 1243-1282.

II.A.14 Diesel HCCI Development

Kevin Duffy (Primary Contact), Gerald Coleman, and George Donaldson
Caterpillar Inc.
PO Box 1875
Peoria, IL 61552-1875

DOE Technology Development Manager: John Fairbanks

Objectives

- Identify a cost-effective engine technology strategy to meet the stringent 2010 heavy-duty and 2014 off-road emissions standards.
- Develop enabling technology to implement the engine technology strategy.

Approach

This research effort focuses on the development of an advanced combustion regime called homogeneous charge compression ignition (HCCI). HCCI holds the potential of meeting future emissions regulatory challenges for internal combustion engines while satisfying the needs of the marketplace. The multi-year development project focuses on the key challenges associated with implementing this technology. Specifically, the challenges are:

- Air-Fuel Mixture Preparation – To date, HCCI using diesel fuel has been largely unsuccessful due to the difficulty of achieving the proper air-fuel mixture. The Caterpillar project has evaluated a number a technical approaches to achieve appropriate mixing.
- Power Density – To date, HCCI demonstrations have been limited to relatively low power density (circa 500 kPa BMEP). Higher power density (1500+ kPa BMEP) is required for a commercially viable technology. The Caterpillar project has evaluated a number of options to increase power density.
- Combustion Phasing and Control – With HCCI, direct control of the combustion event is lost. The Caterpillar project will investigate the parameters that influence the control and identify a means to actively control combustion.

Accomplishments

Caterpillar's project has made significant progress in each of the key technical challenges associated with this technology.

- Caterpillar developed a novel engine system that successfully achieves the proper air-fuel mixture using conventional diesel fuel. This novel engine system overcomes many of the barriers associated with the mixture preparation challenge of diesel HCCI, thereby facilitating the demonstration of engines that achieve future emissions standards. A novel mixed mode injector has been developed and tested which allows for engine operation with unique injection strategies.
- Caterpillar achieved 2100+ kPa BMEP while meeting future emissions standards. This achievement is the highest known power density in the world achieved using any form of HCCI, and specifically diesel-fuelled HCCI. This achievement advances HCCI as a potentially viable approach to meeting future regulatory and marketplace requirements.
- Caterpillar has completed a comprehensive engine test stand evaluation of key performance parameters (boost level, injection event, intake manifold temperature, etc.) to better understand the parameters that impact and control combustion. A novel neural network controls approach has been explored which offers an alternative closed loop feedback controls approach to HCCI combustion phasing control.

Future Directions

The Caterpillar team will utilize best-in-class design practices, advanced combustion modeling techniques, single-cylinder engine testing and multi-cylinder engine testing to advance the technology. Technology development continues in the following key areas:

- With the advent of the novel engine system, the air-fuel mixture issue is largely resolved. Future work will focus on identifying and developing a cost-effective method of manufacturing the engine system.
- Caterpillar will continue to focus on the power density issue to achieve additional breakthrough results. The team will focus on achieving the results with improved engine structure, enhanced air system capabilities, and improved combustion control.
- Additional test stand evaluation, sensor development, and algorithm development are needed to address the challenges associated with controlling this novel combustion approach. Rapid control algorithm development tools will be utilized to expedite the development of this technology. In addition, novel combustion control mechanisms will be designed, analyzed and, if appropriate, evaluated on the engine test stand.

Introduction

Increasingly stringent air quality standards have driven the need for cleaner-burning internal combustion engines. Many emissions reduction technologies adversely affect fuel consumption (and subsequently U.S. dependence on foreign oil). Homogeneous charge compression ignition fundamentally shifts the traditional emissions and fuel consumption trade-off. This breakthrough emissions technology may enable compression ignition engines to compete cost-effectively in the automotive and heavy- duty truck markets, resulting in a dramatic improvement in fuel economy for that market segment. Additionally, this advanced combustion technology will reduce (or eliminate) the need for expensive NO_x aftertreatment devices which rely heavily upon imported precious metals.

Approach

The development team is utilizing a multi-disciplinary approach to resolve this complex engineering challenge. The development team has a unique mix of technical experts from the fields of controls, combustion fundamentals, engine design, engine development, fuel systems development and manufacturing. The team is concurrently developing the analytical tools to model and understand the fundamentals of combustion while delivering novel hardware to the test stand to validate the models, improve our understanding and advance the technology. The unique team is utilizing best-in-class design practices, advanced combustion and engine system modeling techniques, rapid control strategy development tools, single-cylinder engine testing, multi-cylinder engine testing and over 70 years of experience delivering successful compression ignition engine technology to the marketplace.

Results

As stated above, Caterpillar has made significant progress in each of the key technical challenges associated with this technology. Figure 1 shows a prototype fuel system called a mixed mode injector which allows for dual mode operation. The injector can be run in pure HCCI mode, conventional combustion mode or a combination mode. This injector has proven to be a valuable tool for exploring alternative low-temperature combustion modes. Figure 2 shows the power density achieved with HCCI. Caterpillar has made significant progress toward achieving the power levels required for a commercially viable technology. Across the speed range of the engine, over 2000 kPa BMEP was

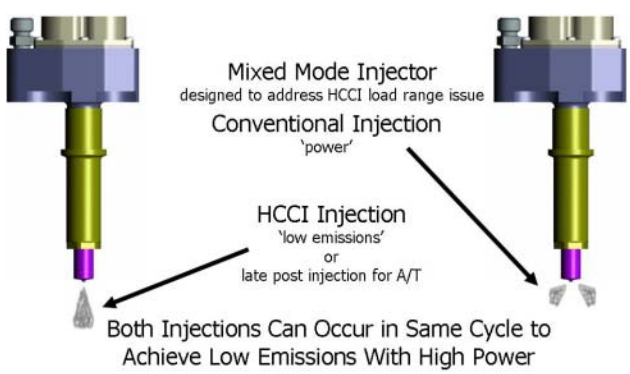


Figure 1. Flexible Injection System

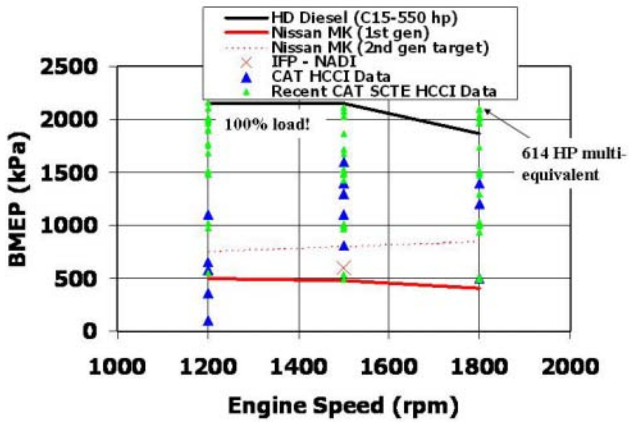


Figure 2. High Power Density

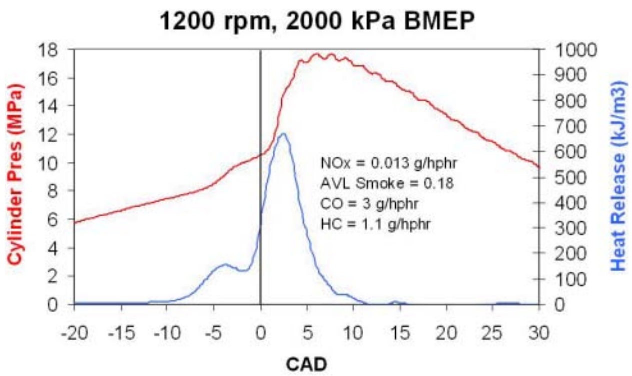


Figure 3. Full Load Diesel HCCI Operation

realized on a single-cylinder test engine. Additional work is needed to translate these results to multi-cylinder platforms; however, the progress to date illustrates the exciting promise that this technology holds. Figure 3 shows the cylinder pressure and heat release curves for a high-load operation point. The cylinder pressure rise rate is significantly higher for HCCI combustion compared to conventional combustion, which suggests engine structural issues cannot be ignored for this concept. NO_x and smoke emissions are very low for this engine operation point. Hydrocarbon (HC) levels at over 1 g/hphr will require the use of an oxidation catalyst to lower them to the 2010 required level of 0.14 g/hphr. Figures 4-6 illustrate the remaining control challenges associated with the combustion process. Figure 4 shows the general effects of injection timing on emissions for diesel HCCI. Both early and late

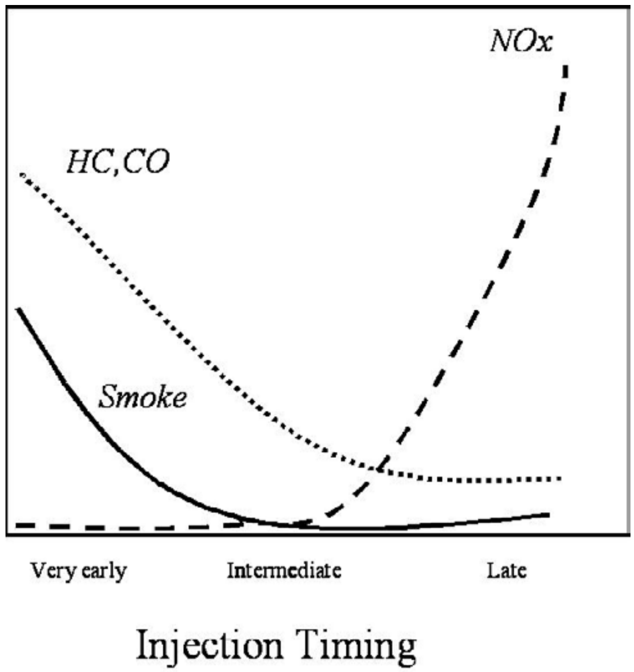


Figure 4. Effect of Injection Timing

injection timings lead to excessive levels of either NO_x, smoke, CO, or HC. An optimum mid-range worktiming exists where NO_x and smoke are low and HC/CO are at moderate levels. As Figures 5-6 illustrate, relatively minor changes in the injection timing and boost level will influence the combustion event, which subsequently affects the fuel consumption and emissions. The combustion phasing must be monitored and a closed loop algorithm used to adjust the appropriate control inputs to arrive at the desired combustion phasing.

Conclusions

Caterpillar's aggressive diesel HCCI development has resulted in significant technical progress against each of the key technical challenges. The progress made by this project has clearly positioned this advanced combustion technology as a potentially viable approach to meeting the regulatory and marketplace challenges of the future. This technology holds the promise of reducing the U.S. dependence on foreign oil and improving the trade balance.

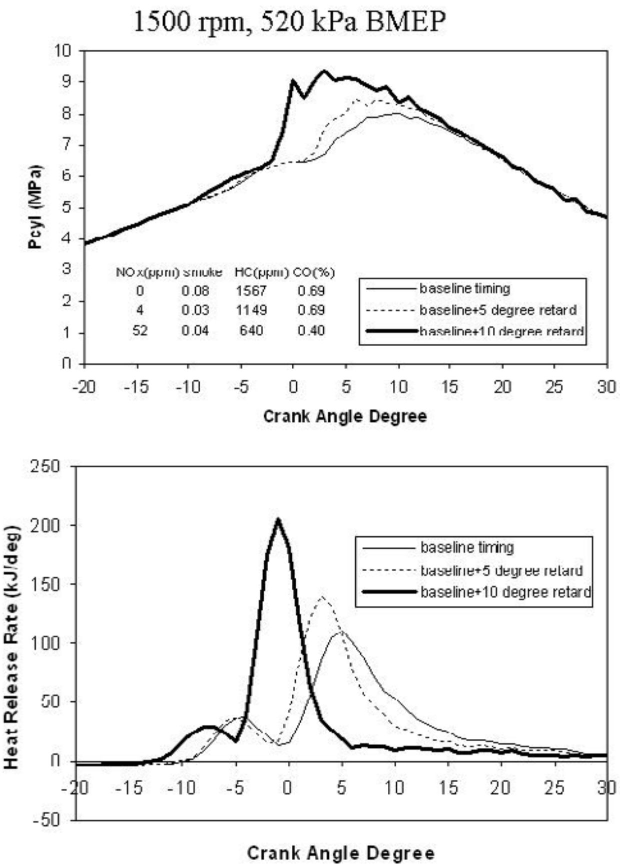
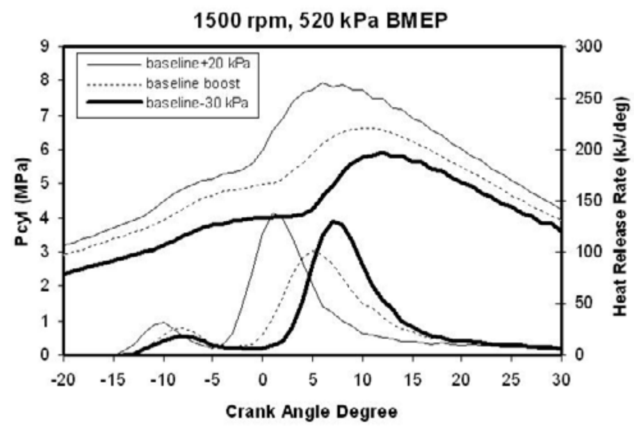


Figure 5. Effect of Injection Timing



	BL+20kPa	Baseline	BL-30kPa
NO_x (ppm)	1	0	13
Smoke (AVL)	0.01	0.06	0.4
HC (ppm)	890	1605	1514
BSFC (% change)	+5%	baseline	+6%

Figure 6. Effect of Boost

FY 2004 Presentations

1. Duffy, K. "HCCI for Heavy Duty Engines," SAE Powertrain & Fluids Meeting, Pittsburgh, PA, October 2003.
2. Duffy, K. "HCCI for Heavy Duty Diesel Engines," SAE Government-Industry Meeting, Washington, DC, May 2004.
3. Duffy, K. "High Load Diesel HCCI Research,HiH" SAE Homogeneous Charge Compression Ignition Symposium, Berkeley, CA, August 2004.
4. Duffy, K., Fluga, E., Kieser, A. "Heavy Duty HCCI Development Activities," DOE DEER Conference, Coronado, CA, August 2004.
5. Duffy, K., Fluga, E., Faulkner, S., Heaton, D., Schleyer, C., and Sobotowski, "Latest Development in Heavy Duty Diesel HCCI," IFP International Conference on Which Fuels for Low CO_2?, Paris, France, September 2004.

FY 2004 Publications

1. Duffy, K., Fluga, E., Faulkner, S., Heaton, D., Schleyer, C., and Sobotowski, "Latest Development in Heavy Duty Diesel HCCI," IFP International Conference on Which Fuels for Low CO_2?, Paris, France, September 2004.

II.A.15 Spark Augmentation for HCCI Control

Bruce G. Bunting
Oak Ridge National Laboratory
2360 Cherahala Blvd.
Knoxville, TN 37932

DOE Technology Development Manager: Kevin Stork

Subcontractor:
AVL Powertrain, Inc, Plymouth, MI

Objectives

- Demonstrate the effects of spark augmentation for the control of homogeneous charge compression ignition (HCCI) combustion.
- Quantify benefits of HCCI combustion over conventional combustion.
- Determine performance of a rotating arc sparkplug (RASP) compared to a conventional sparkplug for HCCI control.

Approach

- Develop research relationship with subcontractor for access to existing HCCI engine.
- Design test plan and manage test project to achieve research objectives.
- Analyze data obtained relative to HCCI combustion and HCCI combustion control.

Accomplishments

- Demonstrated that HCCI combustion in a gasoline engine could improve fuel economy by an average of 12% while reducing NO_x emissions by 95% compared to conventional combustion.
- Showed that spark augmentation was necessary for successful transition to HCCI and quantified effect of spark after HCCI was achieved.
- Demonstrated that low NO_x is achieved by charge dilution and that HCCI combustion allows the engine to operate in a stable manner at very high exhaust gas recirculation (EGR) rates. This opens the door for combining conventional and HCCI combustion for low NO_x providing good combustion stability can be achieved.
- Compared HCCI control and performance using a conventional sparkplug and the Oak Ridge National Laboratory (ORNL) RASP and found that the conventional sparkplug performed as well or better than the RASP for the conditions tested.

Future Directions

- Continue to evaluate and quantify the use of spark augmentation for HCCI control and transition to HCCI combustion.
- Evaluate the use of combined HCCI and spark augmentation with various fuels and HCCI combustion strategies.

Introduction

In HCCI, fuel and air are pre-mixed prior to combustion and ignition is initiated by kinetic reactions which occur during the compression stroke. Ignition occurs when a threshold temperature is reached, and the timing of ignition is controlled by setting the cylinder conditions at the start of the compression stroke. The cylinder charge of fuel and air is diluted with excess air or with exhaust gas. The purpose of this dilution is to lower the peak flame temperature to reduce NO_x and to regulate the rate of burning after combustion begins. Although HCCI holds the promise of reduced NO_x and smoke emissions combined with improved fuel economy, HCCI stability and control continue to be major barriers to the implementation of HCCI. In addition, HCCI may not be achievable over the entire range of engine operation; conventional operation may be needed at high or light loads, under cold operating conditions, or during transient operation. Spark ignition is often present in gasoline-engine-derived HCCI engines and can be used for engine starting or to assist the transition to HCCI. Results of using the spark during HCCI have been mixed, and various studies have shown different effects. In this study, we explore the use of spark assist during HCCI operation and show the use of spark assist in transitions from conventional to HCCI combustion. In addition, the engine platform is used to evaluate the effect of motor octane number on HCCI combustion characteristics.

Table 1. Specifications for AVL Research Engine as Configured for HCCI Operation

Capable of HCCI, mixed mode, and conventional operation
500 cc, 11.34 C/R
2 valves, naturally aspirated
Gasoline port fuel injection
Spark ignition
Fully variable valve actuation
HCCI currently initiated by early exhaust valve closing
- "negative overlap"
- Retains heat in cylinder
- Retains internal EGR
- Typically operates at > 50% EGR

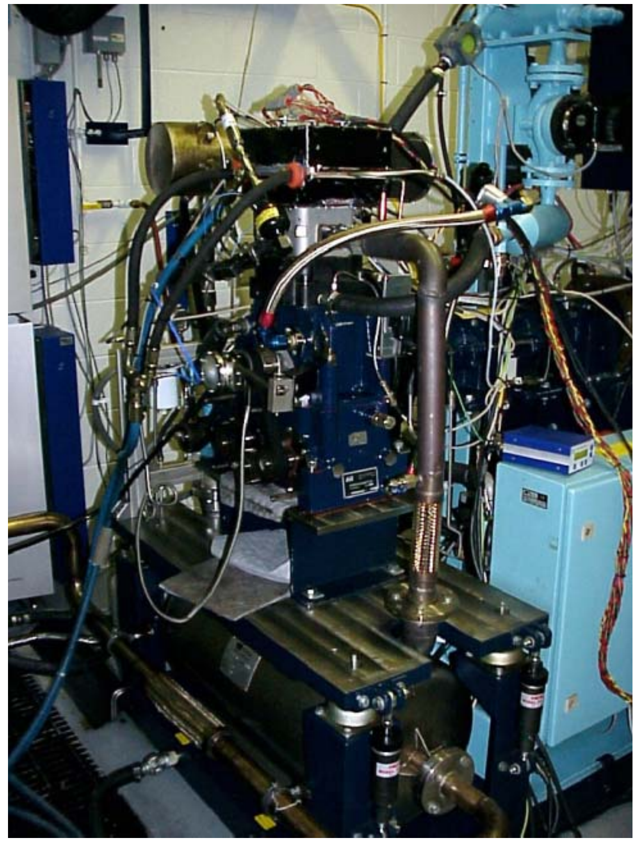


Figure 1. AVL Single-Cylinder Research Engine

Approach

This research was subcontracted to AVL Powertrain in Plymouth, MI, since they already had an existing single-cylinder research engine mapped for HCCI operation. The engine is set up as a 2-valve, naturally aspirated, port fuel injected gasoline engine with 500 cc displacement. HCCI is achieved by a combination of increased compression ratio (11.34:1) and negative valve overlap (early exhaust valve closing). By closing the exhaust valve early, a high residual fraction of the exhaust is retained in the cylinder, which raises compression pressure and temperature to achieve HCCI ignition conditions. Figure 1 shows the engine installed in the lab, and Table 1 lists the important specifications of the engine. A variety of speed-load conditions were run in HCCI with and without spark, and these conditions were also repeated with conventional combustion. Engine operation was compared based on combustion stability, emissions, fuel efficiency, and ability to operate and transition to other combustion modes.

Results

In a comparison of conventional and HCCI combustion, HCCI combustion has higher peak cylinder pressure and higher rate of cylinder pressure rise but also lower peak combustion temperature. These effects are due to the large amount of exhaust gas retained in the cylinder from the previous cycle due to the valve timing strategy. On the average, retained exhaust was 55% of the cylinder charge in HCCI compared to 12% for the baseline engine configuration. Overall, HCCI operation resulted in a 12% fuel economy gain and a 95% reduction in NO_x compared to conventional combustion. Table 2 compares engine performance in HCCI operation with and without spark and in conventional spark-ignited operation over the range of 1200 to 2400 rpm and 2.0 to 4.5 bar indicated mean effective pressure (IMEP). It is apparent from this data that the spark still exerts an influence on HCCI operation, as indicated by a resulting increase in NO_x. Most probably, the spark initiates a flame kernel which helps pull the remainder of the combustion chamber into HCCI combustion, resulting in earlier or more rapid ignition. In HCCI, the spark can be turned off and the engine will continue to run. If the spark remains on, its influence can be varied by changing the relative timings of exhaust valve closing (% retained exhaust) and spark timing.

Table 2. Comparison of Engine Performance in HCCI and Conventional Combustion

	HCCI no spark high EGR	Spark assisted HCCI high EGR	Conventional throttled low EGR
indicated specific fuel consumption, gm/kw-hr	244	242	277
NOx output, ppm	63	91	1967
coeff of variation of IMEP, %	2.71	2.64	0.98

The engine can be transitioned from conventional to HCCI combustion by progressively earlier closing of the exhaust valve until the pre-flame reaction-initiated combustion preceeds the spark-ignited combustion. This transition is indicated by an improvement in combustion variability (compared to the transition zone), a rise in peak cylinder pressure by up to double, and a shortening of combustion duration from about 20 degrees crank angle (CA) to less than 10 degrees CA. Interestingly, NO_x decreases before this transition to HCCI due to the increasingly large charge dilution from internal EGR. This indicates that low NO_x can be achieved before transition to HCCI and that the main benefit of HCCI is to stabilize combustion with EGR levels above 50%. This finding opens the way to combined combustion modes of conventional and HCCI ignition which may also show acceptable combustion stability while exhibiting low NO_x. Figure 2 shows the transition from conventional ignition to HCCI at 1600 rpm, 3.0 bar IMEP.

The RASP was tested in the engine using a modified cylinder head and compared to a conventional sparkplug for conventional and HCCI combustion behavior. The RASP is an ORNL invention for lean-burn natural gas engines. The plug design imposes a fixed magnetic field on the plug gap area, which causes the spark discharge to rotate. Benefits are a larger spark volume and the continual movement of the spark to new locations on the plug to reduce erosion of the electrodes. Three engine conditions were evaluated for transition from conventional to HCCI combustion. At 1200 rpm, 2.5

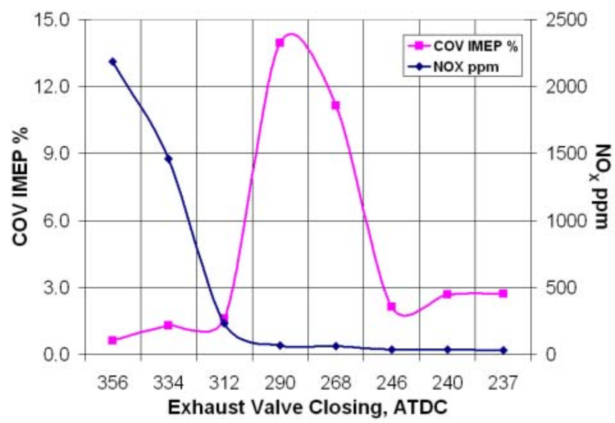


Figure 2. Transition from Conventional to HCCI Combustion at 1600 rpm, 3.0 bar IMEP

bar IMEP, the engine ran with the conventional plug but would not run at all with the RASP plug. At 1600 rpm, 3.0 bar IMEP, the engine ran with both plugs, but the RASP plug showed higher combustion variability. At 2400 rpm, 4.5 bar IMEP, the engine ran with both spark plugs and transitioned to HCCI combustion. Engine performance relative to NO_x emissions, fuel consumption, and combustion variability was about equivalent. Further optimization of the RASP sparkplug is probably needed relative to ignition duration and tip design. The RASP plug has no protrusion into the combustion chamber and may not be reaching a good pocket of fuel/air mixture.

Conclusions

- HCCI combustion provided a 12% fuel economy improvement and 95% NO_x reduction compared to conventional spark ignition in the engine tested.
- The spark addition was needed for transition from conventional to HCCI ignition and was also shown to have an effect on HCCI combustion. This effect could be varied with spark and exhaust valve timing.
- Low NO_x was achieved by charge dilution, and HCCI allowed the engine to operate in a stable manner at EGR rates greater than 50%.
- The RASP did not provide an expected benefit compared to a conventional sparkplug, probably because the RASP ignition system and plug tip configuration were not optimized for the engine.

FY 2004 Publications/Presentations

1. Bruce G. Bunting, COMBUSTION, EFFICIENCY, AND FUEL EFFECTS IN A SPARK-ASSISTED HCCI GASOLINE ENGINE, presented at 2004 DOE DEER Conference, August 31, 2004.
2. Bruce G. Bunting, FUEL EFFECTS ON SPARK ASSISTED HCCI COMBUSTION IN A GASOLINE ENGINE, presented at 2005 annual meeting, American Chemical Society, August, 2004.

II.A.16 Real-Time Control of Diesel Combustion Quality (CRADA with Detroit Diesel Corporation)

Robert M. Wagner (Primary Contact), Eric J. Nafziger
Oak Ridge National Laboratory
2360 Cherahala Blvd.
Knoxville, TN 37932

Craig Savonen (Primary CRADA Contact), He Jiang
Detroit Diesel Corporation (CRADA No. ORNL00-0609)
13400 Outer Drive
Detroit, MI 48239

DOE Technology Development Manager: Kevin Stork

Objectives

- Commission prototype Detroit Diesel Corporation (DDC) heavy-duty diesel engine at Oak Ridge National Laboratory (ORNL).
- Explore operational range of high-efficiency clean combustion (HECC) on DDC engine.
- Perform detailed emissions characterization for improved understanding of the combustion process.

Approach

- Install prototype DDC heavy-duty diesel engine and develop supporting data acquisition and measurement systems at ORNL.
- Determine boundaries of HECC operation on DDC-supplied heavy-duty engine with detailed combustion and emissions characterization.
- Begin construction of physical and statistical-based models for use in evaluating potential control approaches for expanding operational range of HECC.

Accomplishments

- Commissioned DDC engine and supporting infrastructure at ORNL.
- Performed extensive experiments under low and medium load conditions to characterize effects of exhaust gas recirculation (EGR) rate, rail pressure, and injection timing on achieving HECC operation.
- Selected commercially available software package and began development of low-order combustion model for engine simulations.

Future Directions

- Continue analysis and interpretation of recent data.
- Continue model development for multi-cylinder simulations and control.
- Explore potential of achieving homogeneous charge compression ignition (HCCI)-like operation and further expanding HECC operating range on heavy-duty multi-cylinder platform.

Introduction

This CRADA focuses on expanding the operational range of HECC through improved simulation and control with emphasis on the unique dynamics of multi-cylinder engines. Expansion of the stable HECC speed-load range is a key step to operating advanced diesel engines at the regulated emissions levels of 2010 and beyond. Achieving HECC in a diesel multi-cylinder engine requires operation under conditions which are often inherently unstable. These instabilities result in the occurrence of poor or marginal combustion events which cause excessive hydrocarbon and particulate emissions. Practical solutions to the problem are especially difficult to achieve because of the extreme sensitivity of combustion and after-treatment performance to engine parameters as well as "communication" between cylinders on multi-cylinder platforms. The experimental setup has been commissioned this year, and extensive experiments have been performed to understand the potential of achieving HECC operation on the DDC multi-cylinder engine. We have also begun the selection and development of models for future simulations of engine operation and evaluations of potential control approaches.

Approach

The overall objective of this work is to expand the operational range of HECC through improved simulation and control with emphasis on the unique dynamics of multi-cylinder engines. Achieving this objective requires extensive experimentation as well as the development of new low-order models and control strategies. A key target in satisfying this objective will be to minimize the addition of new engine hardware and rely as much as possible on existing actuators, sensors, and signal processors.

The objective is being pursued utilizing a unique multi-cylinder engine provided by DDC to ORNL. The research engine is sized for Class 7-8 heavy trucks, is fully operational, and is installed in a transient-capable dynamometer cell with full instrumentation. The engine is equipped with an electronic control package, exhaust gas recirculation, and other features that are essential for this type of research.

Results

Extensive experiments have been performed to determine the "natural" boundaries of HECC operation in the DDC engine. Engine parameter ranges for these experiments are summarized in Table 1. Note that all of these experiments were carried out using a single injection event to keep the parameter space reasonable for this stage of experiments. The frequency and timing of multiple injection events will be included in the next round of experiments.

The initial exploratory experiments performed on this engine involved studying the effects of load and EGR on emissions and efficiency. Specifically, the purpose of these experiments was to determine whether high EGR is sufficient to cause a simultaneous reduction in oxides of nitrogen (NO_x) and particulate matter (PM), as has been observed on some light-duty diesel engines. An EGR level sweep was performed for the three loads at 1500 rpm with all other engine parameters held constant. The results in Figure 1 show a significant decrease in NO_x and a significant increase in smoke number with increasing EGR level for all three engine loads. The increase in EGR level also results in a decrease in efficiency (increase in brake specific fuel consumption, BSFC) and a significant increase in CO emissions. Although not shown, the 10-50% and 50-90% heat release (HR) intervals increased with EGR level, and the coefficient of variation (COV) in indicated mean effective pressure (IMEP) was relatively constant in the 1-2% range for all conditions.

The effects of beginning of injection (BOI) and fuel pressure were investigated at 20% and 50% load for a fixed speed of 1500 rpm. A summary of the

Table 1. Engine Parameter Ranges Investigated in Recent Experiments

Parameter	Range
Speed, rpm	1500 (fixed)
Torque, % full load	10, 20, 50
EGR rate, %	0 to 65
BOI, deg BTDC	17.5 to 0
Fuel Pressure, bar	600 to 1600

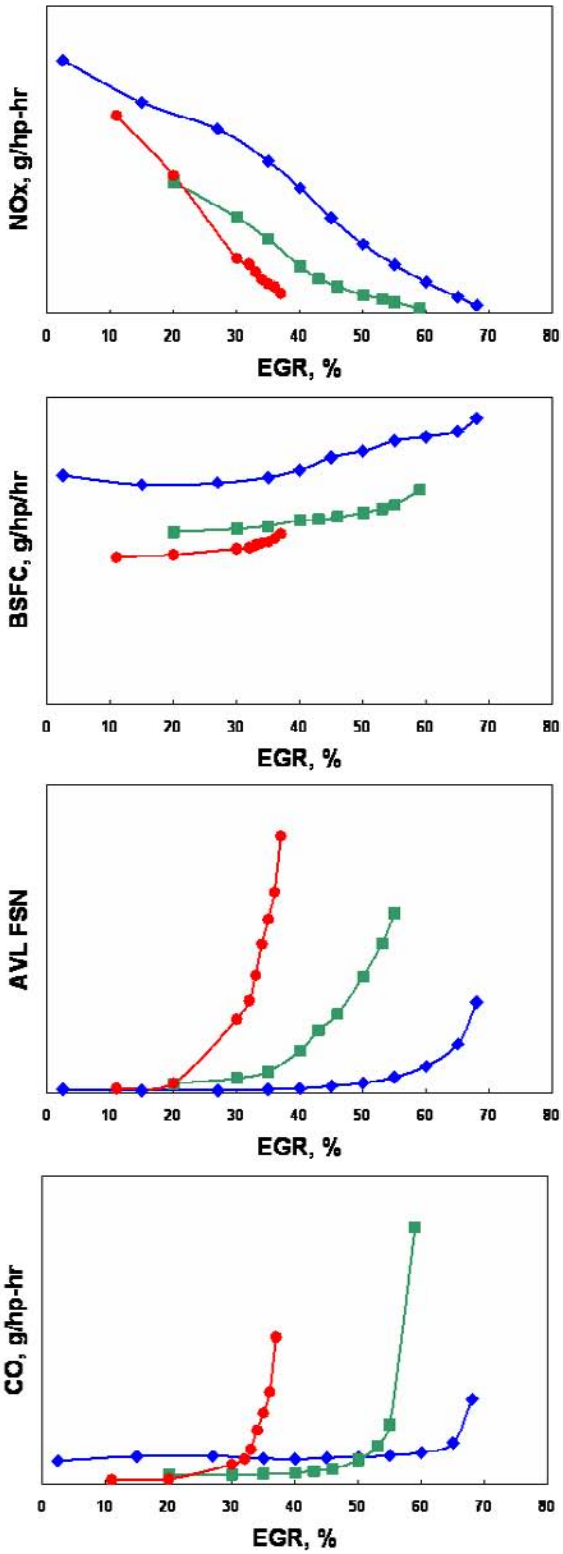


Figure 1. EGR rate sweep at 1500 rpm and 10% (blue diamonds), 20% (green squared), and 50% (red circles) load. All other engine parameters are held constant.

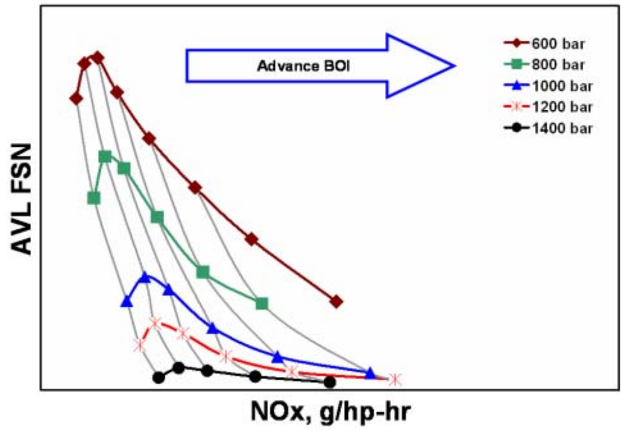


Figure 2. Fuel pressure and injection timing sweep at 1500 rpm, 20% load, and 39% EGR rate. Shaded lines correspond to fixed injection timings.

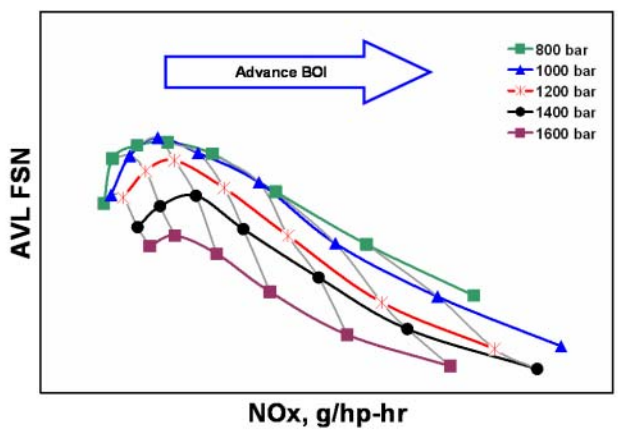


Figure 3. Fuel pressure and injection timing sweep at 1500 rpm, 50% load and 29% EGR rate. Shaded lines correspond to fixed injection timings.

results is shown in Figures 2 and 3 for 20% and 50% load, respectively. EGR rate was held fixed at a slightly elevated level to improve NO_x suppression. In general, smoke number decreased and NO_x increased with increasing fuel pressure. Note that the scales are the same in Figures 2 and 3, and the effect of rail pressure on PM was much stronger for the lower loads. Constant injection timing lines are also shown in Figures 2 and 3 and indicate a decrease in NO_x as injection timing is retarded toward top dead center (TDC). Although not shown, BSFC increased with the later injection timings. Also note that a simultaneous reduction in NO_x and smoke number was observed for later injection timings. This is opposite of the classic NO_x-PM tradeoff typically observed under conventional operating conditions (see Figure 1). Although not shown, the 10-50% HR interval decreased with fuel pressure, and the 50-90% HR interval decreased with retarding injection. All parameters investigated had little to no effect on stability as indicated by COV in IMEP.

Parameter effects are summarized for the above experiments in Table 2. Note that the effect of each parameter is influenced by a variety of engine conditions including speed and load. For example, the effect of fuel pressure on smoke number appears weaker at high loads. Trends summarized in Table 2 are only for the evaluated parameter combinations.

Table 2. Summar of Parameter Effects Observed in Recent Experiments

Parameter	NOx (g/hp-hr)	PM (g/hp-hr)	BSFC (g/hp-hr)	10-50% HR (deg)	50-90% HR (deg)
EGR Increase	↓	↑	↑	↑	↑
Fuel Pressure Increase	↑	↓	—	↓	
BOI retard	↓	↓↑	↑	–↓	↓

Conclusions

A simultaneous reduction in NO_x and PM emissions was observed with retarded (later) injection timings. A simultaneous reduction was not observed for elevated EGR levels for the conditions investigated in this study but may be possible depending on the settings of other operational parameters such as fuel injection rate and timing. This will be investigated in more detail in the next phase of this study. Increasing fuel pressure appeared to be most effective at reducing PM while maintaining efficiency, particularly at lower loads. This study indicates simultaneous reductions of NO_x and PM emissions (as compared to baseline) are possible with single-injection approaches. More advanced injection strategies involving multiple injections and early injection are expected to provide greater emissions reductions with the ability to maintain efficiency. More advanced injection strategies and their effects on engine emissions and stability will be investigated in the next phase of this activity.

FY 2004 Publications/Presentations

1. CRADA review meeting at ORNL on September 30, 2004.

II.A.17 KIVA-4 Development

David J. Torres
Group T-3, MS B216
Los Alamos National Laboratory
Los Alamos, NM 87544

DOE Technology Development Manager: Kevin Stork

Objectives

- Modify the remaining subroutines in KIVA-3V to accommodate unstructured grids, and call the unstructured version KIVA-4.
- Simulate 3D engines with KIVA-4.
- Distribute KIVA-4 to interested industry and university parties to gain feedback.

Approach

- Implement and validate changes to KIVA-3V subroutines.
- Construct 3D structured and unstructured grids for 3D engine geometries. Compare KIVA-3V results with KIVA-4.
- Perform classification review for KIVA-4. Issue non-commercial licenses to universities interested in KIVA-4.

Accomplishments

- All subroutines of KIVA-3V have been modified to accommodate unstructured grids.
- Calculations have been performed on 3D engines, sector meshes, and a fully tetrahedral mesh. A version of KIVA-4 without allocatable memory is no more than 10% slower than KIVA-3V. A version of KIVA-4 with allocatable memory is about 20% slower.
- A beta version of KIVA-4 has been distributed to the following industry Memorandum of Understanding (MOU) participants: Ford, Caterpillar, Detroit Diesel, and International Truck. Noncommercial licenses have been issued and the code has been distributed to the University of Wisconsin and the University of California at Berkeley. Noncommercial licenses are currently being developed for Massachusetts Institute of Technology (MIT) and Wayne State University.

Future Directions

- Provide support services to KIVA-4 users after its initial distribution in late August 2004.
- Assemble a KIVA-4 manual.
- Develop a KIVA-3V mesh converter which will convert KIVA-3V meshes to KIVA-4 format.
- Continue validation of KIVA-4 by adding to the existing test suite of engine problems.
- Begin parallelization of KIVA-4.
- Develop and begin implementing a grid-generation strategy for KIVA-4 that incorporates commercial grid-generation packages.

Introduction and Approach

Computational fluid dynamics (CFD) computations of engines are increasingly being used as a tool to guide engine design. Most commercial CFD packages use unstructured meshes to grid complex engine geometries because unstructured grids tend to be easier to build and of better quality for complex geometries. Unstructured meshes can use a variety of element types (hexahedra, prisms, tetrahedra and pyramids) to fill up the interior of an engine. Structured meshes generally use only hexahedra. KIVA-3V and all prior versions of KIVA have only accommodated structured meshes. Our objective is to enable KIVA to compute with unstructured as well as structured meshes and to make the grid-generation process easier for KIVA users by developing a new version of KIVA called KIVA-4. KIVA-4 will remain an open source code and thus enable universities and users to interact directly with the code and conduct fundamental research and submodel development.

Results

In FY 2004, Los Alamos National Laboratory finished development of KIVA-4, an unstructured version of KIVA-3V. Simulations were performed on structured and unstructured 3D engine meshes. Simulations were compared with KIVA-3V results to validate the code.

Figure 1 and Figure 2 show vapor fuel (iso-octane) mass fraction contours in a 3D engine simulation with vertical valves performed with KIVA-3V and KIVA-4, respectively. Figure 1 uses a structured grid and Figure 2 uses an unstructured grid. Figure 3 and Figure 4 both show fuel (iso-octane) vapor mass fraction contours in a box with fuel particles currently being compressed by a rising bottom moving surface. Figure 3 only uses hexahedra while Figure 4 only uses tetrahedra. Despite differences in the grids, Figures 1-4 show that KIVA-4 is capable of computing with unstructured grids and producing reliable results.

A beta version of KIVA-4 was distributed in late August, 2004, to interested industry and university parties which included Ford, Detroit Diesel, Caterpillar, General Electric, International Truck,

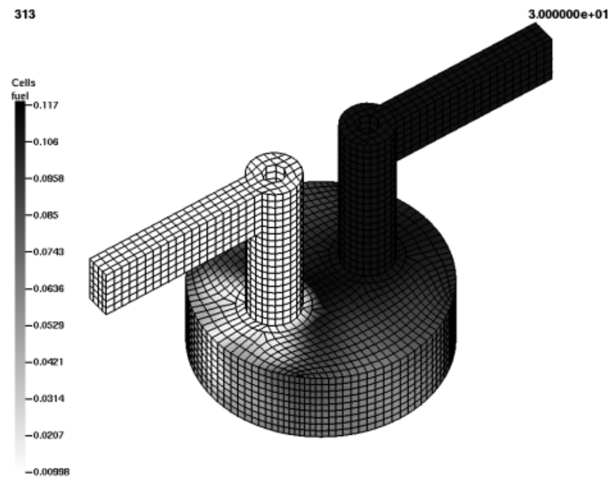


Figure 1. Iso-octane mass fraction vapor contours in a structured mesh. Calculation performed with KIVA-3V.

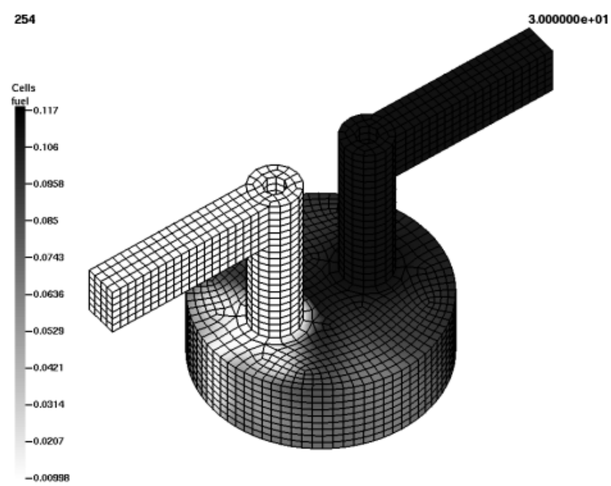


Figure 2. Iso-octane mass fraction vapor contours in an unstructured mesh. Calculation performed with KIVA-4.

University of Wisconsin and the University of California at Berkeley. Noncommercial licenses are being drafted for Wayne State University and MIT.

Conclusions

KIVA-4 (an unstructured version of KIVA-3V) has been developed and tested in several engine geometries. A beta version of KIVA-4 has been distributed to interested industrial members of the MOU and interested university parties. Los Alamos will provide support services for the new KIVA-4

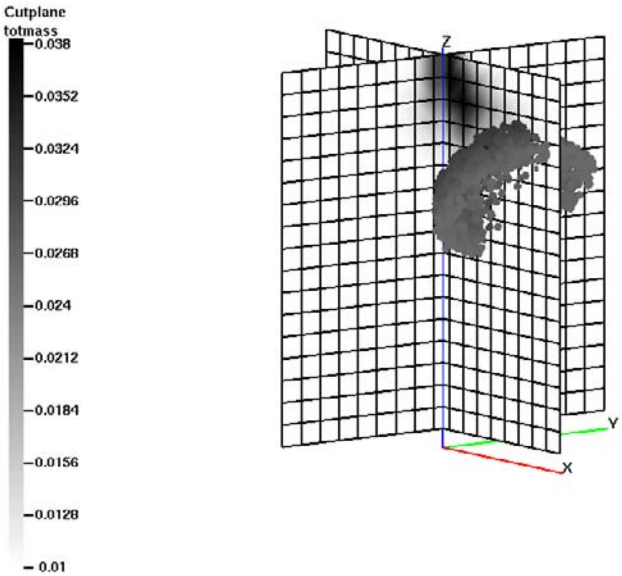


Figure 3. Iso-octane vapor mass fraction contours and particles in a hexahedral structured mesh. Particles are colored according to their temperature (358K- 362K), where the lighter colors designate the cooler particles. Calculation performed with KIVA-4.

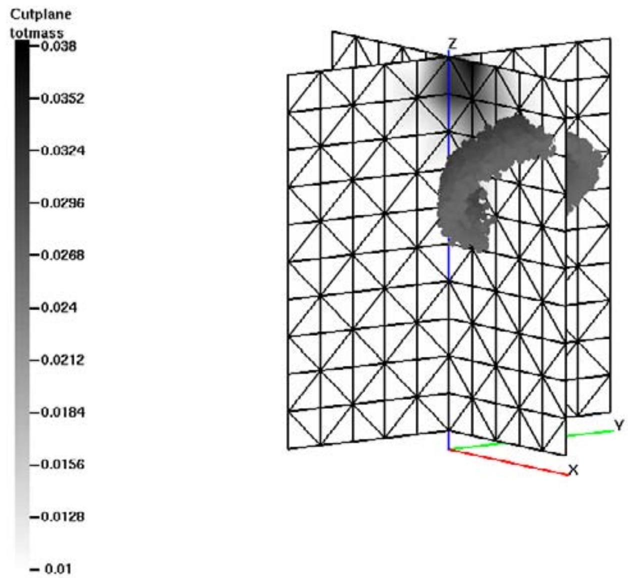


Figure 4. Iso-octane vapor mass fraction contours and particles in a tetrahedral unstructured mesh. Particles are colored according to their temperature (358K- 362K), where the lighter colors designate the cooler particles. Calculation performed with KIVA-4.

code by resolving compiler and run-time issues. We believe the code will be more easily adopted if users can rely on assistance in transitioning from KIVA-3V to KIVA-4. Feedback from users will be incorporated in an updated version of KIVA-4 that will be released after this testing period.

Los Alamos will continue to develop KIVA-4 by beginning to parallelize the code and will use commercial grid packages to create grids for KIVA-4 simulations.

FY 2004 Presentations

1. D. J. Torres, "KIVA-4," Advanced Engine Combustion Meeting, Detroit, MI, June 2004.
2. D. J. Torres, "KIVA-4 Development," DOE National Laboratory Advanced Combustion Engine R&D, Merit Review and Peer Evaluation, Argonne, IL, May 2004.
3. D.J. Torres, "KIVA-4," *International Multidimensional Engine Modeling User's Group Meeting at SAE Congress*, Detroit, MI, March 2004.
4. D. J. Torres, "Unstructured KIVA (KIVA-4)," Advanced Engine Combustion meeting, Livermore, CA, January 2004.

FY 2004 Publications

1. D. J. Torres and P.J. O'Rourke, "KIVA-4," *International Multidimensional Engine Modeling User's Group Meeting Proceedings at SAE Congress*, March 2004.
2. M. F. Trujillo, D. J. Torres and P.J. O'Rourke, "High-pressure multicomponent liquid sprays: departure from ideal behaviour," Int. J. Engine Res., **5**:229-246, October 2003.

II.A.18 Chemical Kinetic Modeling of Combustion of Automotive Fuels

Charles K. Westbrook (Primary Contact), William J. Pitz
Lawrence Livermore National Laboratory
P. O. Box 808, L-091
Livermore, CA 94551

DOE Technology Development Manager: Kevin Stork

Objectives

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

Approach

- Identify individual fuel components and their molecular structures
- Develop kinetic reaction mechanisms for fuel components and additives
- Compute ignition and flame structure for mixtures of fuel components under diesel, spark-ignition and HCCI conditions
- Compute ignition and flame structure for mixtures of surrogate fuel components under diesel, spark-ignition and HCCI conditions

Accomplishments

- Developed models for chemical kinetics of combustion of two major fuel components, toluene and methyl cyclohexane, and for an oxygenated diesel fuel additive, dimethyl carbonate
- Combined various amounts of fuel components and constructed three distinct surrogate mixtures to describe HCCI ignition
- Compared calculated ignition delays under HCCI conditions using surrogate mixtures with experimental results, to provide optimal surrogate
- Continued past studies of mechanisms by which oxygenated diesel fuel components reduce soot production

Future Directions

- Extend model capabilities to additional classes of fuel components
- Continue development of increasingly complex surrogate fuel mixtures
- Increase collaborations with programs outside Lawrence Livermore National Laboratory (LLNL) dealing with automotive fuel issues

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Introduction

Automotive hydrocarbon fuels consist of complex mixtures of hundreds or even thousands of different components. These components fall largely into a number of rather distinct classes, consisting of n-paraffins, branched paraffins, cyclic and branched cyclic paraffins, olefins, oxygenates, and aromatics (Figure 1). The fractional amounts of these components are quite different in gasoline, diesel

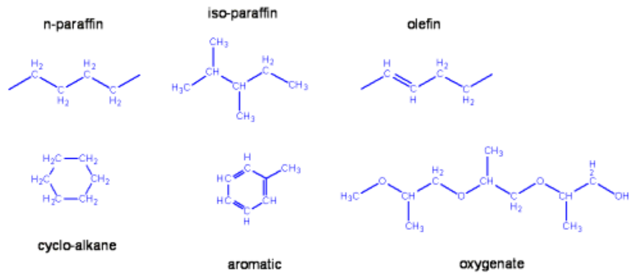

Figure 1. Examples of the major classes of hydrocarbon species present in practical transportation fuels. These specific examples are n-hexane, 2,3-dimethyl pentane, 2-hexene, cyclo-hexane, toluene, and tri-propylene glycol monomethyl ether (TPGME).

fuel and jet fuels, contributing to the very different combustion characteristics of each different type of combustion system.

In order to support large-scale computer simulations of each kind of engine combustion system, there is a need to provide reliable chemical kinetic models for each of the types of fuels. Unfortunately, very few specific hydrocarbon components of these fuels have been modeled, although a few representative components of each type have been simulated. For example, models for benzene and toluene have been developed, although models for few if any larger aromatic compounds currently exist. Similarly, detailed models for small n-paraffins such as propane, n-heptane and n-octane have been developed, but detailed models do not exist for the much larger versions characteristic of diesel fuels, such as n-hexadecane. One solution for this dilemma is to construct a fairly large fuel model, combining one or more representatives of each class of components but not all such components that exist in the real fuels, to serve as a surrogate mixture for which kinetic submodels exist for all of the components. This high-level approach can create realistic substitutes for gasoline or diesel fuel that reproduce experimental behavior of the practical real fuels, and these substitutes, or surrogates, will also then be reproducible in both experiments and modeling studies.

Our recent studies continue our efforts to understand the soot-producing characteristics of diesel fuels. Understanding the kinetics of oxygenated chemical species and their effects on sooting remains a major goal, and we have added several new species to the list of available chemicals, but our current focus is to understand and calculate the separate contributions of the major constituent chemical species on sooting by regular diesel fuels. This will lead to improved understanding of the effects of these diesel fuel components on engine performance and pollutant formation and to development of efficient simplified chemical models for diesel fuel for use in multidimensional computational fluid dynamics (CFD) models of engine combustion. Other applications to ignition and pollutant formation in HCCI engines have also been pursued using a multi-zone spatial model for this type of engine and using suitable surrogates for both diesel fuel and gasoline.

Approach

Chemical kinetic modeling has been developed uniquely at LLNL to investigate combustion of hydrocarbon fuels in practical combustion systems such as diesel and HCCI engines. The basic approach is to integrate chemical rate equations for chemical systems of interest, within boundary conditions related to the specific system of importance. This approach has been used extensively [1-4] for diesel and HCCI engine combustion, providing better understanding of ignition, soot production, and NO_x emissions from these engines in fundamental chemical terms.

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

Kinetic reaction models were developed for the oxygenated additives proposed by a DOE/industry panel of experts. We then computed diesel ignition and combustion using heptane [5] as a reasonable diesel fuel surrogate model, mixed with oxygenated additives. The impact of the additive on predicted levels of soot-producing chemical species can then be assessed.

Ignition under HCCI engine conditions is closely related to that in diesel engines since both are initiated by compression ignition of the fuel/air mixtures. Our recent kinetic modeling studies [6] have in fact demonstrated that diesel ignition, HCCI ignition, and spark-ignition gasoline engine knocking are the result of thermal decomposition of the exact same chemical compound, hydrogen peroxide (H_2O_2). However, in very fuel-lean HCCI ignition, the premixing of fuel and air in the gaseous state results in no soot and extremely low NO_x production. Kinetic modeling has proven to be exceedingly valuable in predicting not only the time of ignition in HCCI engines, but also the duration of burn and the emissions of unburned hydrocarbons, CO, NO_x and soot [7].

Results

Our kinetic models assume that soot production in diesel combustion occurs from reactions of chemical species created in fuel-rich ignition near the fuel injection location. Because there is insufficient oxygen in this region to burn the fuel completely, the hydrocarbon species remaining there react instead to produce soot. Our kinetics calculations show that when the fuel itself contains some oxygen, that oxygen helps convert more of the ignition products into chemical species that do not contribute to soot production.

During the past year, the LLNL project has examined additional oxygenated hydrocarbon species that have been proposed as possible diesel fuels or additives, specifically dimethyl carbonate, which includes significant amounts of oxygen imbedded in the primarily hydrocarbon fuel molecule. A detailed chemical kinetic reaction mechanism has been developed for this fuel [8], and the resulting model was used to assess its sooting tendency. The computed soot precursor evolution for this new oxygenated compound was entirely consistent with our previous findings, confirming again that the kinetic analysis of soot production is becoming more and more consistent and reliable.

Our recent publication [9] summarizing several years of experimental and kinetic modeling work describes the mechanisms by which oxygenated additives influenced sooting and was just selected as a winner of the Society of Automotive Engineers Arch Colwell Award of Merit for 2005, a prestigious recognition that we previously had received for an earlier (1999) study of diesel engine combustion [3]. We also presented the plenary paper on Computational Combustion [10] at the most recent international Symposium on Combustion.

In addition to the study of oxygenates, we continued numerical studies of soot growth [11-13] from tiny precursors into macroscopic soot particles. The power of this modeling capability is able to relate the chemical properties of these soot particles based on very elementary physical principles.

Basic chemical kinetic studies developing detailed mechanisms for iso-octane [14] and dimethyl ether [15] have been completed recently. The iso-octane model has become an important tool for chemical studies of gasoline in spark-ignition and HCCI engines, and the dimethyl ether (DME) model is a refinement of a previous model that has become heavily used in many studies of DME combustion. DME appears to be a potentially attractive fuel for use in diesel engines and in other applications, since it can be produced relatively inexpensively from natural gas to convert a gaseous fuel to a more convenient liquid fuel.

Finally, we have continued computational studies of HCCI ignition. The multi-zone model [16] has been shown to reproduce nearly all of the important features of engine performance and emissions characteristics when the engines are operated in the normal, fuel-lean regime. We are using the same approach to examine other operating regimes, such as operation with extensive amounts of exhaust gas recirculation or other forms of dilution but with richer fuel/air mixtures. In collaboration with the Combustion Research Facility at Sandia National Laboratories in California, we developed several surrogate gasoline mixtures using representative fuel components from Figure 1 in proportions summarized in Table 1, and compared computationally predicted times of ignition to

Table 1. Three different compositions used as surrogate mixtures for gasoline. Research (RON) and motored (MON) octane numbers for each blend are included for reference.

% Composition	Mix 1	Mix 2	Mix 3
iso-Octane	60	40	40
n-Heptane	8	10	20
Toluene	20	10	10
Methyl Cyclohexane	8	40	30
1-Pentene	4	0	0
RON (blend)	99.2	94	87.6
MON (blend)	94.5	84.8	82

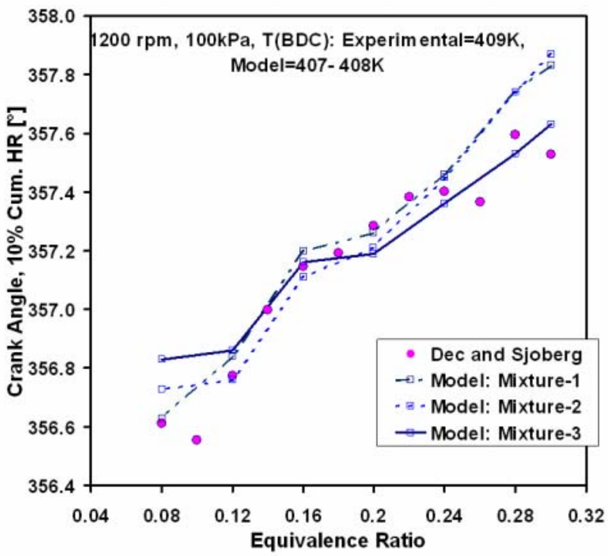

Figure 2. Multicomponent kinetic model for gasoline predictions of ignition timing in Sandia HCCI combustion experiments. Three different multicomponent mixtures with compositions summarized in Table 1.

experimentally measured values under HCCI conditions, as shown in Figure 2.

Conclusions

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

References and Publications

1. Fisher, E. M., Pitz, W. J., Curran, H. J., and Westbrook, C. K., "Detailed Chemical Kinetic Mechanisms for Combustion of Oxygenated Fuels," **Proc. Combust. Inst. 28:** 1579-1586 (2001).
2. Curran, H. J., Fisher, E. M., Glaude, P.-A., Marinov, N. M., Pitz, W. J., Westbrook, C. K., Layton, D. W., Flynn, P. F., Durrett, R. P., zur Loye, A. O., Akinyemi, O. C., and Dryer, F. L., "Detailed Chemical Kinetic Modeling of Diesel Combustion with Oxygenated Fuels," Society of Automotive Engineers paper SAE-2001-01-0653 (2001).
3. Flynn, P. F., Durrett, R. P., Hunter, G. L., zur Loye, A. O., Akinyemi, O. C., Dec, J. E., and Westbrook, C. K., "Diesel Combustion: An Integrated View Combining Laser Diagnostics, Chemical Kinetics, and Empirical Validation," Society of Automotive Engineers paper SAE-1999-01-0509 (1999).
4. Curran, H. J., Fisher, E. M., Glaude, P.-A., Marinov, N. M., Pitz, W. J., Westbrook, C. K., Layton, D. W., Flynn, P. F., Durrett, R. P., zur Loye, A. O., Akinyemi, O. C., and Dryer, F. L., "Detailed Chemical Kinetic Modeling of Diesel Combustion with Oxygenated Fuels," Society of Automotive Engineers paper SAE-2001-01-0653 (2001).
5. Curran, H. J., Gaffuri, P., Pitz, W. J., and Westbrook, C. K., "A Comprehensive Modeling Study of n-Heptane Oxidation," **Combustion and Flame 114**, 149-177 (1998).
6. Westbrook, C. K., "Chemical Kinetics of Hydrocarbon Ignition in Practical Combustion Systems," **Proc. Combust. Inst. 28**, 1563-1577 (2001).
7. Flowers, D., Aceves, S., Westbrook, C. K., Smith, J. R., and Dibble, R., "Detailed Chemical Kinetic Simulation of Natural Gas HCCI Combustion: Gas Composition Effects and Investigation of Control Strategies," **ASME Journal of Engineering for Gas Turbines and Power 123**, 433-439 (2001).
8. Glaude, P.-A., Pitz, W. J., and Thomson, M. J., "Chemical Kinetic Modeling of Dimethyl Carbonate in an Opposed-Flow Diffusion Flame," **Proc. Combust. Inst. 30**, 1111-1118 (2004).

9. Mueller, C. J., Pitz, W. J., Pickett, L. M., Martin, G. C., Siebers, D. L., and Westbrook, C. K., "Effects of Oxygenates on Soot Processes in DI Diesel Engines: Experiments and Numerical Simulations," Society of Automotive Engineers paper SAE 2003-01-1791 and Japan Society of Automotive Engineers paper JSAE 20030193.
10. Westbrook, C. K., Mizobuchi, Y., Poinsot, T. J., Smith, P. J., and Warnatz, J., "Computational Combustion," **Proc. Combust. Inst. 30**, 125-157 (2004).
11. Violi, A., Kubota, A., Truong, T. N., Pitz, W., Westbrook, C. K., and Sarofim, A. F., "A Fully Integrated Kinetic Monte Carlo/Molecular Dynamics Approach for the Simulation of Soot Precursor Growth," **Proc. Combust. Inst. 29,** 2343-2349 (2003).
12. Kubota, A., Mundy, C. J., Pitz, W. J., Melius, C., Westbrook, C. K., and Caturla, M.-J., "Massively Parallel Combined Monte Carlo and Molecular Dynamics Methods to Study the Long-Time-Scale Evolution of Particulate Matter and Molecular Structures Under Reactive Flow Conditions," Proceedings of the Third Joint Meeting of the US Sections of The Combustion Institute, Chicago, March 2003.
13. Kubota, A., Harris, L., Mundy, C. J., Pitz, W. J., Melius, C., Westbrook, C. K, and Caturla, M.-J., "Combined Monte Carlo and Molecular Dynamics Methods to Study the Long-Time-Scale Evolution of Particulate Matter and Molecular Structures Under Reactive Flow Conditions: Hydrocarbon Soot Nanoparticulate Matter Inception, Growth and Aging," Nineteenth International Colloquium on the Dynamics of Explosions and Reactive Systems, Hakone, Japan, July 2003.
14. Curran, H. J., Gaffuri, P., Pitz, W. J. and Westbrook, C. K., "A Comprehensive Modeling Study of iso-Octane Oxidation," **Combustion and Flame 129**, 253-280 (2002).
15. Zheng, X., Lu, T. F., Law, C. K., and Westbrook, C. K., "Experimental and Computational Study of Non-Premixed Ignition of Dimethyl Ether," **Proc. Combust. Inst. 30** (2004).
16. Aceves, S. M., Flowers, D. L., Westbrook, C. K., Smith, J. R., Pitz, W. J., Dibble, R., Christensen, M., and Johansson, B., "A Multi-Zone Model for Prediction of HCCI Combustions and Emissions," Society of Automotive Engineers publication SAE 2000-01-0327, February, 2000. **SAE Transactions**, Section 3, Volume 109, pp. 431-441 (2000).