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DOE Project: Optimization of Advanced Diesel Engine Combustion Strategies “University Research in Advanced Combustion and Emissions Control”

Office of FreedomCAR and Vehicle Technologies Program

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Program Objectives

Over the three-year duration of the research, fundamental science and engineering concepts and tools have been produced to support the development and commercialization of clean, efficient internal combustion engine powertrains operating on both nonpetroleum- and petroleum-based fuels. The work has developed fundamental knowledge and early applied technology in advanced combustion, efficient emission control, and advanced fuel formulation to help enable the realization of DOE's vehicle efficiency goals. The research projects has contributed to the development of high efficiency IC engines with goals of improving fuel economies by 20-40% in light-duty vehicles and attaining 55% brake thermal efficiency in heavy-duty engines. Increasing the efficiency of internal combustion engines is one of the most promising and cost-effective approaches to increasing vehicle fuel economy in the near- to mid-term.

Program Summary

The goal of the present technology development was to increase the efficiency of internal combustion engines while minimizing the energy penalty of meeting emissions regulations. This objective was achieved through experimentation and the development of advanced combustion regimes and emission control strategies, coupled with advanced petroleum and non-petroleum fuel formulations. To meet the goals of the project, it was necessary to improve the efficiency of expansion work extraction, and this required optimized combustion phasing and minimized in-cylinder heat transfer losses. To minimize fuel used for diesel particulate filter (DPF) regeneration, soot emissions were also minimized. Because of the complex nature of optimizing production engines for real-world variations in fuels, temperatures and pressures, the project applied high-fidelity computing and high-resolution engine experiments synergistically to create and apply advanced tools (i.e., fast, accurate predictive models) developed for low-emission, fuel-efficient engine designs. The companion experiments were conducted using representative single- and multi-cylinder automotive and truck diesel engines.

Approach

The projects focused on advanced combustion research in low-temperature combustion and lean-burn strategies, and on the development of advanced modeling tools. The work was divided into 4 main Tasks with 12 subprojects, featuring experimental and modeling components:

- A.) Combustion strategies for increased thermal efficiency;
- B.) Fuels as an enabler for fuel efficiency improvement;
- C.) Multi-scale predictive tools for understanding combustion & emissions; and
- D.) System-level engine optimization (air, fuel, emissions, after-treatment).

A main focus of Tasks A, B and C was to improve fundamental understanding to overcome technology barriers that control fuel efficiency. The impact of advanced combustion technologies on engine performance linked with the after-treatment system was also considered in Tasks C and D.

Fully instrumented research diesel engines were used to reveal combustion fundamentals and to explore methods of controlling and optimizing fuel efficient combustion under steady-state and transient operation. Information from the engine experiments was incorporated into comprehensive multidimensional Computational Fluid Dynamics (CFD) codes (KIVA3V with large eddy simulation (LES) turbulence models and detailed chemistry using CHEMKIN) and system models (GTPower and WAVE codes and their associated control algorithms). The developed models and experimental methods were used to explore methods to optimize diesel engine fuel efficiency while maintaining low emissions.

Accomplishments

Guidelines were established for significant improvements in engine efficiency for both heavy- and light-duty engines. In particular, low temperature combustion strategies were developed that improve engine fuel efficiency considerably, while controlling NO_x and particulate (soot) emissions in-cylinder, such that SCR and DPF after-treatment would not be required. These include Gasoline Direct-Injection Compression Ignition (GCI) and dual fuel Reactivity Controlled Compression Ignition (RCCI) strategies. Results for each of the four Tasks are summarized as follows:

Task A - Optimum spray and combustion chamber design recommendations were made for improved efficiency of heavy duty (HD) and light duty (LD) diesel engines. Gross Thermal Indicated Efficiencies of ~60% in heavy-duty and ~50% in light-duty engines were demonstrated.

Task B – Guidelines were provided for engine control methodologies under light- and high-load operating conditions with consideration of fuel property and mixture preparation effects,

Task C - Validated predictive combustion and realistic fuel vaporization submodels were developed for science-based engine analysis and optimization and combustion system concept evaluation, and

Task D - Efficient engine system transient control strategies appropriate for engine speed/load mode transitions were developed.

The work commenced July 1, 2009 under the 90-day pre-award provision of the DOE solicitation and concluded September 30, 2012. Quarterly progress reports have been submitted and are available at the DOE EERE project Management Center: <https://www.eere-pmc.energy.gov/SubmitReports.aspx>. In addition, presentations summarizing progress have been presented biannually at DOE AEC meetings, and these presentations are available at: <https://share.sandia.gov/wgs/>.

TASK A: Combustion strategies for increased thermal efficiency

Task objective: Develop guidelines for improved efficiency of HD and LD diesel engines

Subtask A.1 - Optimization of combustion chamber geometry and sprays using advanced CFD - Reitz

The present research has shown that the dual fuel Reactivity Controlled Compression Ignition (RCCI) combustion strategy can achieve high efficiency with low emissions (see, for example, Subtask A.3). However, it has also been revealed that RCCI combustion is difficult at high loads due to its premixed nature. To operate at moderate to high-loads with gasoline/diesel dual fuel, high amounts of EGR or a low compression ratio are required [A.1.1]. Considering that both of these approaches inherently lower thermodynamic efficiency, in this study natural gas and other fuels were explored as a replacement for gasoline as the low reactivity fuel. Due to the lower reactivity (i.e., higher octane number) of natural gas compared to gasoline, it was hypothesized to be a better fuel for RCCI combustion, in which a large reactivity gradient between the two fuels is beneficial in controlling the maximum pressure rise rate.

The multi-dimensional CFD code, KIVA3V, was used in conjunction with the CHEMKIN chemistry tool and a Nondominated Sorting Genetic Algorithm (NSGA-II) to perform optimization for a wide range of engine operating conditions. Engine design parameters that were controlled by the genetic algorithm include the fraction of total fuel that is premixed (methane), the timing of the two diesel injections, the amount of diesel fuel in each injection, the diesel injection pressure, and the EGR percentage. The objective of the optimization was to simultaneously minimize soot, NO_x, CO, and UHC emissions, as well as ISFC and ringing intensity. A broad load/speed range was investigated, including six operating points from 4 to 23 bar IMEP and 800 to 1800 rev/min that were optimized. These load/speed combinations represent typical heavy-duty engine conditions. Using the stock compression ratio of 16.1, it was determined that operation up to 13.5 bar IMEP could be achieved with no EGR, while still maintaining high efficiency and low emissions. The study also examined the sensitivity of RCCI combustion at high load to injection system parameters. The results emphasize that precise injection control is needed for combustion control [A.1.2].

An additional study was conducted to explore the possibility of using ethanol as the low reactivity fuel [A.1.3]. Multidimensional modeling was performed at engine loads from 5 to 17 bars IMEP at 1300 rev/min with various grades of hydrated ethanol and a fixed diesel fraction of the total fuel. The results show that hydrated ethanol can be used in RCCI combustion with gross indicated thermal efficiencies up to 55% and very low emissions. A 70/30 ethanol/water mixture (by mass) was found to yield the best results across the entire load range without the need for EGR.

References

[A.1.1] Dempsey, A.B., and Reitz, R.D., "Computational Optimization of Reactivity Controlled Compression Ignition in a Heavy-Duty Engine with Ultra Low Compression Ratio," SAE Paper 11ICE-0206, 2011-24-0015, 2011.

[A.1.2] Nieman, D.E., Dempsey, A.B., and Reitz, R.D., "Heavy-Duty RCCI Operation Using Natural Gas and Diesel," SAE paper 2012-01-0379, 2012.

[A.1.3] Dempsey, A.B., Adhikary, B. Das, Viswanathan, S., and Reitz, R.D., "Reactivity Controlled Compression Ignition (RCCI) using Premixed Hydrated Ethanol and Direct Injection Diesel," J. Eng. Gas Turbines Power, 134, 082806, 2012.

Subtask A.2 - Modeling combustion control for high power and mode switching - Rutland

Large eddy simulation (LES) was used to study mode transition from a conventional diesel operating condition to a low-temperature combustion operating condition. As part of the project, the LES spray combustion model was improved for better prediction. A mixing controlled direct chemistry (MCDC) model was formulated based on direct chemistry solver (DCS) solution and the local Damköhler number:

$$\dot{\varpi}_i = \frac{1}{1 + Da} \dot{\varpi}_{kinetics,i}, \quad Da = \frac{\tau_{mixing}}{\tau_{kinetics,U}} \quad (A.2.1)$$

Here Da is the Damköhler number, $\dot{\varpi}_{kinetics,i}$ is the DCS reaction rate for species i ; $\tau_{kinetics,U}$ is kinetic time scale based on the change of specific internal energy from DCS; τ_{mixing} is the mixing time scale based on mixture fraction variance and dissipation. The model was validated with engine data from Sandia National Laboratories.

The mode transition studies focused on a rapid change from a conventional operation (Mode 6) to a PCCI operating condition. Mode 6 is at 11.2 bar IMEP and 1737 rev/min, and uses split injection (-57, +12°) with 0% EGR. The PCCI mode is at 10.2 bar IMEP and 1737 rev/min, and uses early injection (-64°) with 64% EGR. This type of transition can occur when changing from a high load to a medium load. The CFD simulates multiple consecutive engine cycles with the mode transition occurring at the third cycle. The focus is on the first cycle after transition so rapid response controls are examined. These include changes to injection schedule, variable valve timing control, and port water injection. In all cases there are tradeoffs between pressure rise rate, maintaining IMEP, and achieving reasonable combustion efficiency. Water vapor injection, by acting like rapid response EGR, was able to achieve reasonable PRR and maintain IMEP, but combustion efficiency suffered. The quantity of water vapor was high (~50% of the charge mass), but it would only be required during mode transients. Table A.2.1 summarizes the results of the project.

Table A.2:1 Results of evaluating different methods for controlling rapid combustion that occurs during mode transition.

Method	Motivation	Result
Retard fuel injection timing.	To control the timing of heat release.	High peak PRR. Gross IMEP below target level. High levels of NOx and soot emission.
Multiple injections	To address high peak PRR and increase ignition delay.	Reduced peak PRR, still much above target. High combustion efficiency. Gross IMEP meets target level. Fuel impingement on piston near TDC.
Late EVO timing with split fuel injection.	To increase internal EGR and meet emission targets of PCCI condition.	Decreased peak PRR close to the target level. High combustion efficiency. Gross IMEP below target level. High levels of CO and HC emissions.
Port water injection with early fuel injection.	To simultaneously decrease peak PRR and increase ignition delay to maintain gross IMEP and low emissions.	Decreased peak PRR to target level. Poor combustion efficiency. Increased gross IMEP to target level. High HC and CO emissions. Near zero NOx and soot emissions. Increased ignition delay and combustion duration.

Subtask A.3 - Experimental investigation of variable injection pressure and dual fuel strategies in a HD engine - Reitz

In this project an experimental investigation of the limits of Reactivity Controlled Compression Ignition (RCCI) engine efficiency was performed. RCCI is a new dual fuel combustion strategy that was developed during the course of the project. It was implemented by introducing low reactivity fuel via port injection, and high reactivity fuel via optimally timed multiple in-cylinder injections. It was found that RCCI combustion is capable of operating over a wide range of engine loads with near zero levels of NO_x and soot, acceptable pressure rise rate and ringing intensity, and with very high indicated efficiency. For example, a peak gross indicated efficiency of 57 per cent was observed with gasoline-diesel dual fuel operation at 9.3 bar IMEP and 1300 rev/min. The comparison between RCCI and conventional diesel showed a reduction in NO_x by 3 orders of magnitude, a reduction in soot by a factor of 6, and an increase in gross indicated efficiency of 18 per cent (i.e., 9 per cent more of the fuel energy was converted to useful work). The simulation results showed that the improvement in fuel conversion efficiency was due both to reductions in heat transfer losses and improved control over the start- and end-of-combustion.

Zero- and multi-dimensional modeling has been used to suggest conditions for the achievement of even higher engine efficiency with RCCI. The modeling and experiments show that reductions in engine heat rejection are a key enabler to increasing engine efficiency. It was found that the piston oil jet gallery cooling in RCCI is unnecessary, and it has a negative impact on efficiency. Without piston oil jet gallery cooling, it was found that RCCI was nearly adiabatic, achieving 95% of the theoretical maximum cycle efficiency (air standard Otto cycle efficiency). The experimental results summarized in Fig. A.3.1 were obtained with a high compression ratio piston (18.7:1) and using a very dilute charge with E85 (low reactivity fuel) and gasoline with 3% ethylhexylnitrate (high reactivity fuel). With reductions in heat transfer and improved combustion, close to 60% gross thermal efficiency has been achieved.

Figure A.3.1 Close to 60% Gross indicated efficiency has been achieved in the ERC Caterpillar HD diesel engine operating with optimized RCCI at 1300 rev/min.

Subtask A.4 - Experimental investigation of chamber design, fuel injection, intake boosting and fuel properties in a LD engine – Foster

The objective of this sub task was to explore interactions between engine operating parameters, including geometry changes, and operational strategies with different fuels in low temperature combustion (LTC) conditions, and evaluate their effects on emissions, efficiency, and noise. Engine operating conditions recommended by the CFD model in subtask A 1 were tested to evaluate emissions and to identify engine control variables to facilitate LTC operation with different fuel characteristics. Bio-fuel blends were also added to the fuel matrix, and combustion chamber geometry assessed by CFD was investigated.

Using a combination of detailed simulation, a derived metric called the Combustion Index, and laboratory exploration was used to demonstrate successful operation of gasoline compression ignition (GCI) in a light duty direct injection engine operating with different fuels, over a wide load/speed range (1500-2500 rev/min, 3-17.8 bar net IMEP), as shown in Fig. A.4.1. The low temperature combustion (LTC) was controlled through variation of multiple injections, variable injection pressure, oxygen concentration (EGR) and boost pressure. Acceptable operation was constrained to have maximum rates of pressure rise, less than 10 bar/deg. NO_x emissions were always less than 1 g/kg-fuel, and particulate matter was significantly less than 0.1 g/kg-fuel. The indicated specific fuel consumption ranged between 175 – 190 g/kW-hr. At the 16 bar IMEP operating point the indicated thermal efficiency was in excess of 47 percent. The synergy between the simulation and the experiments enabled us to determine the optimal injection pressure and robustness for each operating regime in the engine map. It also enabled us to identify the injection logic for achieving high load: an initial injection to establish a premixed base charge, a second injection to manipulate the start of combustion, and a third injection to tailor the load. The results show that gasoline compression ignition (GCI) offers promise for high efficiency and low emissions over a substantial portion of the light duty operating cycle.

Figure A.4.1 Loci of successful Gasoline Direct Injection Compression Ignition operation for an individual cylinder of a 1.9L Engine

With the successful identification of GCI operation over a wide load and speed range, experimental work then focused on GCI sensitivity and robustness in the medium load range (4-7 bar net IMEP). Experiments assessing operating sensitivity within the operating map were done by evaluating load sensitivity due to changes in inlet temperature. Results of these experiments are shown in Figure A.4.2.

Figure A.4.2 Sensitivity of engine load under conditions of constant fueling with changes in inlet temperature

In these experiments, constant fueling was used to achieve operation at a pressure rise rate limit of 8 bar/deg, and then the inlet temperature was reduced and changes in load were observed. For example, at a fuel flow of 0.862 kg/h, 80C, the inlet temperature was reduced to 75C and then 65C, which caused net IMEP to be reduced to 5 bar. This sequence was repeated for different fueling rates and is presented as a super-position on an efficiency color map (i.e., gross ISFC). Iso-lines of NOx and COV of IMEP were added as well. In general, as temperature is reduced, combustion phasing is retarded, which results in a decrease in IMEP. However, at lower fueling rates (and higher inlet temperatures), changes in load with decreasing inlet temperature were not as drastic (compare load vs. inlet temperature curves at 0.945 and 0.862 kg/h). Auto-ignition kinetics at this intermediate operation regime reveal high sensitivity to changes in inlet temperature.

Experiments at 5.5 bar net IMEP using a double injection strategy (first injection during valve overlap; second at -39 dATDC), which resulted in gross ISFC of ~180 g/kWh, NOx<10ppm, and near-smokeless combustion, were chosen as a base condition to evaluate potential control strategies to maintain load during intake temperature fluctuation. Strategies for load control included, increased fueling, varying injection duration and timing, inlet boost, and inlet swirl. The results indicate that fueling rate, injection timing, and injection duration offer promise as control parameters for maintaining stable combustion during fluctuation of intake temperature.

TASK B: Fuels as an enabler for fuel efficiency improvement

Task objective: Explore novel fueling strategies for improved fuel efficiency and combustion control.

Subtask B.1 - Optical engine in-cylinder investigations of gasoline and gasoline/diesel/other fuel mixtures under LTC – Ghandhi

The objective of this project was to investigate the ability of chemical changes, through the fuel composition, to extend the ignition delay to promote volumetric combustion. The focus of the study has been on understanding the role of fuel chemistry on RCCI combustion, and the fundamental mechanism of combustion propagation in RCCI. The experiments were carried out in an optically accessible, single-cylinder engine that has the same geometry as the engine in Subtask A.4, i.e., the 1.9 liter GM HSDI diesel engine. High speed movies of the chemi-luminescence, acquired with an intensified CMOS camera operating at 10 kHz framing rate, were obtained through the piston window. The intensifier extends the camera sensitivity into the ultraviolet, and several filter combinations were investigated to isolate different species.

The comparison of different fuel combinations had to be performed in a consistent manner in order to avoid reaching incorrect conclusions. In this work, prior to performing the optical experiments, an extensive set of firing tests was performed in order to find an optimal set of operating parameters for each fuel combination. The optimal conditions were chosen to give the maximum thermal efficiency with a pressure rise rate less than 5 bar/deg. The independent parameters for optimization were the premixed fuel fraction (based on energy content) and the diesel injection timing. All tests were run at 1200 rev/min with an intake pressure of 160 kPa, but with intake temperature varied. The premixed (low reactivity) fuels investigated were pure isooctane, a PRF 90 blend of *n*-heptane and isooctane, and E85 (an 85% by volume mixture of ethanol and isooctane). The high-reactivity fuel in all cases was low-sulfur diesel fuel. The heat release rate for the optimal conditions is shown in Fig. B.1.1. It can be seen that the heat release duration is a function of the reactivity difference between the two fuels. The PRF90, which has a reactivity closest to diesel fuel, has the highest peak heat release and the shortest overall duration. The E85, which has the largest reactivity difference from diesel fuel, has the lowest peak heat release and the longest overall duration.

Figure B.1.1 Rate of heat release for direct-injected diesel fuel with the premixed fuels identified.

High speed movies were taken and converted to ignition maps, which show the time, in terms of the cumulative heat release, when a pixel exceeds a threshold intensity, i.e., when it ignites. Figure B.1.2 shows the ignition maps at the optimal combustion settings for the three fuel combinations discussed above. The high-speed optical data confirmed that the combustion occurred in a staged manner from the high-reactivity zones, which were located at the periphery of the chamber, to low-reactivity zones in the field of view. Further, the range of ignition timing across the imaged area was found to scale with the difference in the two fuel's reactivity. In cases where there was a small difference in reactivity, the ignition took place in a relatively narrow window within the heat release profile. In cases with large reactivity difference, the progression of the ignition front from high- to low-reactivity regions was found

to occur over an extended part of the heat release duration. Despite the contrast in combustion characteristics and injection timings, similar integrated luminosity levels in the 310 nm range were observed for the tested fuels. The luminosity levels were comparable to HCCI combustion levels and were in excess of two orders of magnitude lower than standard diesel combustion, confirming that low temperature combustion was being observed.

Figure B.1.2 Ignition maps for the (a) Isooctane, (b) PRF90, and (c) E85 optimal cases, respectively.

Subtask B.2 - In-cylinder optical investigation of soot formation during extended lift-off combustion (ELOC) – Rothamer

This task focused on an in-cylinder laser/optical diagnostics-based investigation of extended-liftoff (also called lifted flame, or ELOC) diesel combustion. The body of work conducted over the last three years is divided into three major segments: the design and implementation of the optical engine used in the experiments, data taken exploring the engine parameter space over which ELOC could be achieved and sustained under the given system constraints, and the characterization simultaneously of the in-cylinder temperatures and velocities using simultaneous particle imaging velocimetry and temperature measured with aerosolized thermographic phosphor particles.

The custom-built optically accessible piston and cylinder head of the engine provided for laser sheet access near TDC (allowing for PLIF and PLII measurements), as well as optical access through a window located in the head (to allow for fuel jet-wall and jet-jet interactions to be captured near the cylinder wall) and through a window in the piston. The final head design is shown in figure B.2.1 (a). The cylinder head was also equipped with shrouded valves, allowing for engine swirl to be controlled. This was measured using a Superflow-600 flowbench (results in Figure B.2.1(b)).

Initial experiments using #2 diesel fuel injected from an 8-hole Bosch Crin-2 injector were run under sweeps of intake conditions and injection pressures near the estimated conditions that would give ELOC (using correlations from constant-volume spray chamber experiments). Under these conditions, the long ignition delays (due to relatively low in-cylinder temperatures at SOI, used to increase lift-off lengths and enhance mixing before ignition) result in high maximum pressure rise rates. To mitigate pressure rise rates and temporarily eliminate jet-to-jet interactions, a series of experiments were undertaken with an injector tip with only 2 orifices. Under these conditions, ELOC was achieved for loads of 5 bar IMEP, although combustion was unstable for some injection times. It was also noticed that even for cases for which ELOC was initially produced, the changing pressures and temperatures in the engine due to piston movement, heat transfer, and combustion often caused the combustion to shift back into a sooting mode.

Figure B.2.2 (a-c) summarizes results for soot luminosity measurements as a function of swirl ratio for several start-of-injection times (SOI). The results show a strong influence of swirl ratio on the measured soot luminosity. This is likely the result of increased premixing, however, this may also be influenced by change in in-cylinder temperature distribution. This motivated simultaneous in-cylinder temperature and velocity measurements.

(a)

(b)

Figure B.2.1(a) Image of engine cylinder head developed as part of the project, **(b)** Measured swirl ratio as a function of shrouded valve angle

Figure B.2.2 (a-c) Spatially integrated natural luminosity signal for as a function of swirl ratio and start-of-injection time.

Experiments were performed using a simultaneous velocity and temperature measurement technique. The technique uses seeding of micron sized thermographic phosphor particles (Pr:YAG) into the intake air. A laser emitting 266 nm light co-propagated with 532 nm light was used (through the aforementioned side windows designed into the optical engine). By measuring the luminescence of the particles excited by the 266 nm light and scattering from the 532 nm light, simultaneous characterization of the in-cylinder temperatures and velocities was possible. Measurements were limited to times before -30 CAD before top-dead-center (TDC) due to luminescence interferences from the piston window. Images acquired indicate the presence of significant temperature non-uniformity. This likely plays a critical role in the ELOC combustion process. An image of the experimental setup and a single-shot temperature image taken at -30 CAD BTDC are shown in Figure B.2.3(a) and (b).

In summary, extended lift-off combustion has been investigated in a small bore diesel engine. The results showed the possibility of achieving ELOC for at least limited durations in a small bore engine. The influence of swirl ratio was studied. High swirl ratios were shown to provide a benefit to ELOC due to their ability to increase mixing of the jets before ignition. The influence of swirl is likely related (at least in part) to its influence on the in-cylinder temperature distribution and in-cylinder temperature measurements indicate significant temperature non-uniformities near TDC.

TASK C: Multi-scale predictive tools for understanding combustion and emissions

Task objective: Develop and apply computational and advanced experimental diagnostics for science-based engine analysis and optimization

Subtask C.1 - Develop multi-mode combustion models and reduced chemistry mechanisms – Reitz

An efficient reduced chemistry mechanism, called MultiChem, was developed in this research that can represent realistic fuels by introducing a Physical Surrogate, Group Chemistry Representation (PSGCR) [C1.1]. In the model, a 31 component physical surrogate component data base is used that can account for the major species in most hydrocarbon fuels of interest. Thorough validations of predicted ignition delays have been carried out for each of the fuel components. For example Fig. C.1.1 shows ignition delay times of PRF mixtures in a constant volume ignition process predicted by the present MultiChem mechanism. Prediction performance of the mechanism is seen to be excellent. Similarly, chemistry mechanisms for the other basis chemistry surrogate components have been formulated [C.1.1].

With the mechanisms for basis Chemistry Surrogate Components (CSCs) developed, reaction mechanisms for the Physical Surrogate Components (PSCs) were also formulated. Since generic reactions are employed to model oxidation processes between a PSC and the basis CSCs, reaction rate constants were adjusted to give the good predictions. Figure C1.2 shows ignition delay predictions of n-alkanes and iso-alkanes using the present mechanism. Both trends and values of the ignition delay times are well

captured. In addition, MultiChem includes chemistry mechanisms for biodiesel surrogates [C.1.3]. This enhances its applicability and reliability for engine combustion simulations with multi-component fuels.

Figure C1.1: Predictions of ignition delay times PRF ignition at constant volume using the present MultiChem mechanism. Stoichiometric fuel/air mixtures at 40 bar initial pressure. (a) Results from Ref. [C1.2], (b) results using the present MultiChem mechanism.

Figure C1.2: Predictions of constant volume vessel ignition delay times at using the present MultiChem mechanism. Stoichiometric fuel/air mixtures at 40 bar initial pressure. (a) n-alkanes. (b) iso-alkanes. Numbers in parenthesis are cetane numbers.

References:

- C.1.1. Ra, Y. and Reitz, R. D., "A Chemical Kinetic Model for IC Engine Combustion Simulations with Multi-Component Fuels using Physical Surrogate Group Chemistry Representation," in preparation, 2012.
- C.1.2. Ra, Y. and Reitz, R. D., *Combustion and Flame*, Vol. 155, pp. 713–738, 2008.
- C.1.3. Brakora, J.L., Ra, Y., and Reitz, R.D., "Combustion Model for Biodiesel-Fueled Engine Simulations using Realistic Chemistry and Physical Properties," SAE Paper 2011-01-0831, 2011.

Subtask C.2 - Develop advanced spray and fuel film models for SCR after-treatment – Trujillo

This project focused on the development of advanced modeling techniques for after-treatment systems. The use of urea-water-solution (UWS) sprays has gained considerable popularity over the last few years as an important NO_x elimination procedure for emissions in diesel engines, and is used in combination with Selective-Catalytic Reduction (SCR). Multidimensional CFD models involving urea sprays have also grown in popularity as a means of analyzing the vaporization and subsequent chemical mixing process in the gas phase. In the current work, an investigation of the UWS spray and single droplet vaporization/decomposition was performed. To simulate the process, the chamber upstream of the hydrolysis catalyst was modeled, using $k-\epsilon$ RANS filtering for the Eulerian velocity field, and a Lagrangian spray method for the UWS parcels. The UWS droplets were vaporized using a direct thermolysis model. The results were compared against reported findings from Birkhold et al.[C.2.1] with respect to urea mass fraction for the spray and temperature profiles, and yielded reasonable agreements. Additionally, test cases were performed to study the role of inlet turbulence on the resulting uniformity of the NH_3 distribution.

Several issues became apparent during the analysis; 1.) the direct thermolysis model for urea decomposition disregards urea vaporization [C.2.2], 2.) the rapid mixing model ignores internal species gradients, and 3.) the UWS vaporization takes place in two uncoupled steps, first water then urea. To represent the physics more accurately, a numerical method that fully resolves the mass, chemical species, and thermal transport mechanisms within a UWS (Urea-Water Solution) droplet in both space and time has been developed. The method is based on an interface tracking procedure (Arbitrary-Lagrangian-Eulerian (ALE)) and utilizes a spherically symmetric model by employing the Effective Diffusivity approach to account for internal mixing [C.2.3]. The modified ALE method couples and simultaneously solves for heat transfer, phase change jump conditions, mass conservation, and species diffusion at the surface, and incorporates this solution into solving the internal mass, species, and energy conservation equations. This allows for an important understanding of the internal dynamics of this two-phase, two-component droplet, and a typical modeled spray is shown in Fig. C.2.1.

The validity of the method was verified against an analytical solution, as well as previous numerical results based on work for a melting droplet [C.2.4]. The code was also validated against Vapor-Liquid-Equilibrium calculations and vaporization predictions corresponding to both a water and a C_7H_{16} droplet. Furthermore, the results were compared against UWS experimental data⁵, yielding good agreement. The solver was able to predict accurately both stages of the vaporization process, as shown by direct comparisons to literature [C.2.5], which is initially dominated by the presence of water, and gradually becomes governed by the urea content as the water is depleted from the interfacial region. This can be seen by tracking the thermodynamic state of the interfacial and central regions of the droplet, as mapped on a two-component phase diagram. Additionally, the solver was able to automatically predict the entrapment of water, which results from the rapid enrichment of urea at the gas-liquid interface, as seen in Fig. C.2.2.

In order to verify water entrapment, the internal Reynolds number of the droplet was varied, and internal mixing was found to be limited by the low species diffusion between water and urea. This work, however, is the first to plot the trajectory of the internal and central thermodynamic states of the droplet across the binary phase diagram. It also presents the first fully-coupled interfacial solution of the vapor-phase equilibrium and interfacial constraints for a UWS droplet. Future work will involve implementing this into a complete 3-D solver to accurately calculate the droplet interaction within the exhaust environment. The results have been presented at CLEERS conferences in 2011, 2012, and at ILASS in 2012.

Figure C.2.1 Setup of UWS spray in crossflow, colored by water mole fraction

Figure C.2.2 UWS droplet vaporizing at ambient temperature $T_a=473$ K. Water dominated vaporization in blue, urea dominated in red.

References

- C.2.1. Birkhold et al. (Applied Catalysis B: Environmental 2007);
- C.2.2. Bernhard, A. et al. (The Journal of Physical Chemistry A 2011);
- C.2.3. Abramzon, B. and Sirignano, W. (Int J Heat Mass Transfer 1989);
- C.2.4. Kucera, A. and Hill, J. (Int J Non-Linear Mechanics 1986);
- C.2.5. Wang, T., Baek, S., and S.Y.Lee (AIChE 2009);

Subtask C.3 - Measurement and control of turbulence mixing in engine flows - Ghandhi

The objective of this task was to obtain high-resolution scalar concentration data at crank angles throughout the engine cycle to study the fundamental turbulence and mixing processes in an internal combustion engine. This is needed to improve the fidelity of engine turbulence models, such as the Large Eddy Simulation and combustion models used in Task A.2. The present measurements, which resolve all of the turbulence length scales, were also compared to another, more standard method of evaluating the flowfield, namely particle image velocimetry (PIV). The scalar field measurements were obtained using planar laser-induced fluorescence (PLIF) of a tracer molecule (fluorobenzene) doped into a gas jet. The gas jet was designed to have a very low momentum, and the image timing was delayed until significantly after injection so that the resulting scalar field was dominated by the in-cylinder flow and not the jet momentum. In this way, the scalar field was used as a proxy for the velocity field to measure in-cylinder turbulence. The scalar concentration and velocity field results were analyzed using a spectral fitting procedure. Analysis of the scalar dissipation spectrum provided an estimate of the Batchelor scale, λ_B . Analysis of the turbulent kinetic energy spectrum also provided estimates of the integral length scale and turbulent Reynolds number, from which the Kolmogorov scale, η , could be directly calculated using standard relations from turbulence theory.

The top plot in Figure C.3.1 shows the scalar (red) and kinetic energy dissipation spectra (blue) acquired at a typical operating condition. The scalar and kinetic energy spectra are shown in the lower plot along with a $\kappa^{-5/3}$ line. Both the kinetic energy and scalar energy spectra are seen to exhibit an extended inertial range where the $\kappa^{-5/3}$ dependence of classical turbulence is seen. The scalar energy spectrum, however, begins to roll off from the linear dependence at high wavenumber. This is because the measurements are of sufficient spatial resolution to capture the dissipation phenomena. The scalar dissipation spectrum in Figure C.3.1 is clearly well resolved – the spectrum extends beyond the peak and achieves nearly two orders of magnitude reduction at the high-wavenumber end. In contrast, the kinetic energy dissipation spectrum shown only covers a range up to approximately the peak in the dissipation spectrum. Not shown in the figures is the fact that the measured dissipation and energy spectra match the model spectra very well out to $\kappa \sim 0.04$, where the effects of measurement noise become important. The close correlation between the energy spectra validates the use of the scalar data for investigating the engine flowfield, and moreover, the high spatial resolution that is achievable with PLIF in comparison to PIV allows the Batchelor / Kolmogorov scale to be measured with significantly higher precision than previously possible using estimates from velocity data.

Figure C.3.1 Scalar (in red) and kinetic energy (in blue) dissipation (top) and energy (bottom) spectra acquired at top dead center and 600 rev/min.

Using the present gas jet approach, high resolution scalar measurements were performed through the compression and early part of the expansion strokes, and the resulting measured Batchelor scales are shown with solid symbols in Fig. C.3.2. The results show that there is a reduction in the Batchelor scale as the piston approaches top dead center. This reduction is caused by the confinement of the flow between the head and the piston. On the expansion side, the Batchelor scale is seen to increase again. The Kolmogorov scale estimated from the spectral analysis of the velocity data is shown in the open symbols in Fig. C.3.2. It can be seen that the Kolmogorov scale follows a similar trend as the Batchelor scale. Quantitatively, there is good agreement between these two independent measures of the inner length scale of the flow field, which increases the confidence in the data. These measurements represent the first direct measurement of the dissipation scales of the engine flow at top dead center, and provide new insights into the complicated in-cylinder turbulent flow.

Figure C.3.2 Evolution of the Batchelor (solid) and Kolmogorov (open) scales during a cycle at 1200 RPM. The red symbols are for a shrouded valve, and the blue symbols are for an unshrouded valve.

Subtask C.4 - Crank-angle-resolved species and temperature measurements for improved understanding of chemistry and mixing – Sanders

The goal of this subtask is to characterize in-cylinder gas species composition in fuel-efficient, low-emission combustion regimes. This information is crucial for validating advanced models that can be used to develop concepts that expand homogeneously charged compression ignition (HCCI) operation. The most significant accomplishments over the 3-year project have been:

- Refinement of H₂O sensor systems operating near 1350 nm: incorporation of fused fiber lenses, narrow-linewidth swept-wavelength lasers, and absorption-spectroscopy probes. In-cylinder temperature measurements made using a commercially available instrument that came out of this research are shown in Figure C.4.1.
- Extension of in-cylinder FTIR to allow in-cylinder crank-angle-resolved measurements of major species such as fuel, CO₂, and H₂O in the 2 – 4 μm range, as shown in Figure C.4.2.
- Development of 30 kHz grating spectrometry of OH in the near ultraviolet, as shown in Figure C.4.3.

During the research the FTIR measurement technique was applied in the ERC's Caterpillar HD diesel engine to demonstrate the effectiveness of RCCI by Splitter et al. [C.4.1]. That study showed for the first time that the combustion duration in RCCI is controlled by details of the fuel reactivity gradients in the combustion chamber. In addition, the measurements provided validation data for the CFD modeling.

Figure C.4.1: In-cylinder temperature measured using a 6-mm optical path probe based on absorption spectroscopy. The H₂O absorption spectroscopy-based sensor system used is now commercially available through LaVision GmbH.

Figure C.4.2: In-cylinder FTIR measurements of fuel, H₂O, CO₂ absorption spectra from Splitter et al. [C.4.1].

Figure C.4.3. Measurements of OH absorption spectra and temperature recorded in a flat-flame burner using a 30 kHz grating spectrometer operating near 308 nm.

References

C.4.1 Splitter, D.A., Hanson, R., Kokjohn, S., Rein, K., Sanders, S., and Reitz, R.D., "An Optical Investigation of Ignition Processes in Fuel Reactivity Controlled PCCI Combustion," SAE paper 2010-01-0345, SAE Int. J. Engines, Vol. 3, No.1, pp. 142-162, 2010.

TASK D: System-level engine optimization (air, fuel, emissions, after-treatment)

Task objective: Establish guidelines for efficient transition between LTC and high load combustion

Subtask D.1 - Interactions between high and low pressure EGR systems with mixed-mode operation under load and speed transients – Foster

The objective of this project was to use a commercial multi-cylinder diesel engine to explore transients between LTC and high load operation. Measurements included performance data and cycle-resolved emissions sampling. A low-pressure EGR system was implemented and sub-system response times were assessed and compared between the low-pressure EGR and the high-pressure EGR system. The LTC operating regimes were determined with low-pressure EGR as part of the system, and the potential of higher boosting was evaluated. Activities focused on identifying the fundamental variables that cause differences between actual transient performance and quasi-steady approximations of the transient. Comparisons were performed with the system simulations of subtask D2.

During the course of this research we were able to identify and quantify parametric differences between transient combustion and emission characteristics and values obtained from tests that simulate transient performance via a sequence of steady-state operating conditions. We identified that the O₂ concentration in the cylinder at IVC is a critical parameter. The instantaneous O₂ concentration in cylinder is different from that assessed via the MAF and EGR fraction reported by the ECU. We also found that different combustion strategies were sensitive to different engine parameters during transients. LTC combustion was most affected by inert charge dilution, while more classic diesel combustion was more sensitive to fuel injection characteristics and surface temperature effects.

In an attempt to more accurately capture the in-cylinder conditions during transient operation we devised a test procedure called “Quasi-transient”. The idea of quasi-transient operation was to replicate the speed, injected fuel mass, manifold air pressure, intake O₂, intake temperature and injection rail pressure to the same values actually occurring sequentially in the cylinder during a transient. It was not possible to duplicate the in-cylinder air flow and the O₂ of the transient with a sequence of steady-state operating points. During the transient the intake O₂ changes because of: time delay in the EGR circuit, compositional change of the EGR from combustion changes, and changes in the airflow as commanded by the ECU. That is, during the transient, air flow and O₂ concentration are not directly coupled.

A comparison of different approaches to simulating a transient with a sequence of steady-state operating conditions is shown in Table D1-1. The table lists the control parameters which are duplicated in sequential steady-state operation to approximate the transient.

Table D1-1: Parameters Matched in Steady-State Operation when Approximating Transient for Three Approaches to Simulate Transient Operation.

	Steady State	MAF-MAP*	Quasi-Transient
Speed	X	X	X
Fuel Mass	X	X	X
MAP		X	X
MAF		X	
Intake O2 [%]			X
Intake Temp			X
Rail Pressure			X

*Eastwood et al., SAE 2009-24-0147

Figure D.1.1 shows results of using these approaches as a means of reproducing the transient performance of the engine for a load transition during LTC operation. As seen in the figure, the quasi-steady approximation, which more closely follows the intake O_2 concentration and the intake temperature, also does a superior job reproducing combustion metrics such as CA50, peak heat release rate and ringing index. In terms of emissions it also captures the behavior of NO_x and HC better than the steady state of MAF-MAP approach. Particulate emissions levels were below the measurement resolution of our instruments for LTC combustion so they are not reported.

When a similar comparison was done for a light load transient using standard diesel combustion the results showed an improved prediction of transient emissions for the quasi-steady over the steady-state and MAF-MAP. However, there was not as close a correlation between the quasi-steady and the actual transient, as shown in Figure D.1.1. Reproducing the intake O_2 concentration alone does not account of all of the differences observed between transient and steady state comparisons. Differences in component temperatures, which have a long time constant relative to the transient, were found to have a measurable contribution to the differences in emissions between transient operation and simulated transients using sequences of steady state operation. The standard diesel combustion has a higher sensitivity to these long term thermal transients than does LTC. More detailed discussion of these trends was given in previous quarterly reports.

Figure D.1.1 Comparison of different approaches to simulate transient behavior with a sequence of steady-state tests for an LTC transient load change from 0.5 bar to 2 bar IMEP.

Subtask D.2 - Optimization of engine and after-treatment operation (system modeling) - Rutland

System-level engine after-treatment component models containing diesel oxidation catalyst (DOC), diesel particulate filter (DPF) and advanced controllers, which have been validated individually, were used to explore emissions control. Work focused in three areas: developing improved control models for CA10 and CA50 for transient control, exploring hydrocarbon (HC) slip through a DOC and its impact on DPF performance, and exploration of pulsed regeneration strategies for a DPF.

As part of using the system model to explore transients from conventional diesel operation to LTC operation, control models for CA10 and CA50 were developed. These use inlet manifold conditions and fuel injection parameters as input. They can be used to control pressure rise rate and peak pressure through feedback control of intake valve closure and feed forward control of fuel injection parameters. The combination of the CA10 and CA50 models provide a burn duration estimate. The work shows

promise in controlling pressure rise rate in transitions to LTC during the 10-20 cycles that it takes EGR to adjust to the new operating conditions.

Engine-out HC is normally oxidized in the DOC. However, under some operating conditions or during DPF regeneration by fuel injection, not all of the HC is oxidized and it ‘slips’ through the DOC. A system model was used to predict DPF wall temperature and trapped mass of soot during active regeneration operation. It was found that DPF peak temperature during active regeneration increases with excess HC slip due to oxidation of the HC during DPF regeneration. This occurs for both steady mass and transient conditions. Under low flow rate conditions such as idle, the temperature increase can be significant and could lead to DPF degradation.

Advanced active DPF regeneration strategies were developed using the model. High temperature regeneration leads to high efficient regeneration with less fuel penalty but simultaneously increases the risk of DPF damage or runaway. Pulsed DPF regeneration by multiple hydrocarbon injections upstream of the DOC shows promise in achieving efficient, safe and reliable regeneration performance. Figures D.2.1 and D.2.2 show fuel efficiency and the average DPF wall temperature for various numbers of injections at three regeneration temperatures. It can be seen that multiple injections, especially two or three injections, have higher fuel efficiency and simultaneously lower average wall temperature than single injections. This is because the DPF wall temperature begins to drop right after the end of the first injection, but remains high enough for soot oxidation.

Figure D2.1: Fuel efficiency with respect to number of injections (dwell ratio 50%, initial soot loading 5.65g/L, soot loading at end of regeneration 1.25 g/L)

Figure D2.2: Average DPF wall temperature with respect to number of injections

Publications:

Hanson, R., Reitz, R.D., Splitter, D., and Kokjohn, S., "An Experimental Investigation of Fuel Reactivity Controlled PCCI Combustion in a Heavy-Duty Engine," SAE paper 2010-01-0864, SP-2279, SAE Int. J. Engines, Vol. 3, No.1, pp. 700-716, 2010.

Brakora, J., and Reitz, R.D., "Investigation of emissions predictions from biodiesel-fueled engine simulations using a reduced chemical kinetic mechanism," SAE paper 2010-01-0577, 2010.

Splitter, D.A., Hanson, R., Kokjohn, S., Rein, K., Sanders, S., and Reitz, R.D., "An Optical Investigation of Ignition Processes in Fuel Reactivity Controlled PCCI Combustion," SAE paper 2010-01-0345, SAE Int. J. Engines, Vol. 3, No.1, pp. 142-162, 2010.

Shi, Y., Ge, H.-W., Brakora, J., and Reitz, R.D., "Automatic Chemistry Mechanism Reduction of Hydrocarbon Fuels for HCCI Engines based on DRGEP and PCA Methods with Error Control," Energy and Fuels, Vol. 24, Issue 3, pp 1646–1654, DOI:10.1021/ef901469p, 2010.

Shi, Y., and Reitz, R.D., "Optimization of a heavy-duty compression-ignition engine fueled with diesel and gasoline-like fuels," Fuel, <http://dx.doi.org/10.1016/j.fuel.2010.02.023> , 2010.

Ra, Y., and Reitz, R.D., "A Combustion Model for IC Engine Combustion Simulations with Multi-component Fuels," Combustion & Flame, Vol. 158, pp. 69-90, 2011.
doi:10.1016/j.combustflame.2010.07.019

Shi, Y., Wang, Y., and Reitz, R.D., "CFD modeling a heavy-duty compression-ignition engine fueled with diesel and gasoline-like fuels," International Journal of Engine Research, Vol. 11, No. 5, pp. 355-374, DOI: 10.1243/14680874JER537, 2010.

Curran, S., Prikhodko, V., Wagner, R., Cho, K., Sluder, C., Kokjohn, S., and Reitz, R.D., "In-Cylinder Fuel Blending of Gasoline/Diesel for Improved Efficiency and Lowest Possible Emissions on a Multi-Cylinder Engine," SAE Paper 2010-01-2206, 2010.

Splitter, D.A., Hanson, R., and Reitz, R.D., "High Efficiency, Low Emissions Reactivity Controlled Combustion through use of a Fuel Additive," SAE paper 2010-01-2167, SAE International Journal of Fuels and Lubricants, Vol. 3, no. 2, pp. 742-756, 2010. This paper was named SAE **Horning Award** winner for 2010.

Kokjohn, S.L., Hanson, R.M., Splitter, D.A., and Reitz, R.D., "Fuel Reactivity Controlled Compression Ignition (RCCI): A Pathway to Controlled High-Efficiency Clean Combustion," International Journal of Engine Research, Special Issue on Fuel Efficiency, Vol. 12, pp. 209-226, <http://jer.sagepub.com/content/12/3/209.full.pdf+html> doi:10.1177/1468087411401548, 2011.

Dempsey, A.B., and Reitz, R.D., "Computational Optimization of a Heavy-Duty Compression Ignition Engine Fueled with Conventional Gasoline," SAE Paper 2011-01-0356, 2011.

Brakora, J.L., Ra, Y., and Reitz, R.D., "Combustion Model for Biodiesel-Fueled Engine Simulations using Realistic Chemistry and Physical Properties," SAE Paper 2011-01-0831, 2011.

Kokjohn, S.L., Hanson, R.M., Splitter, D.A., Kaddatz, J., and Reitz, R.D., "Fuel Reactivity Controlled Compression Ignition (RCCI) Combustion in Light- and Heavy-duty Engines," SAE Paper 2011-01-0357, SAE International Journal of Engines, 2011.

Hanson, R.M., Kokjohn, S.L., Splitter, D.A., and Reitz, R.D., "Fuel Effects on Reactivity Controlled Compression Ignition (RCCI) Combustion at Low Load," SAE Paper 2011-01-0361, 2011.

Kokjohn, S.L., Splitter, D.A., Hanson, R.M., Reitz, R.D., Manente, V. and Johansson, B., "Modeling Charge Preparation and Combustion in Diesel Fuel, Ethanol, and Dual Fuel PCCI Engines," Atomization and Sprays, Vol. 21, No. 2, DOI:10.1615/AtomizSpr.2011002836, pp. 107-119, 2011.

Shi, Y., Ge, H.-W., and Reitz, R.D., "Computational Optimization of Internal Combustion Engines," ISBN 978-0-85729-618-4, Springer book, 2011
<http://www.springer.com/engineering/mechanical+eng/book/978-0-85729-618-4>

Splitter, D.A., Hanson, R.M., Kokjohn, S.L., and Reitz, R.D., "Reactivity Controlled Compression Ignition (RCCI) Heavy-Duty Engine Operation at Mid-and High-Loads with Conventional and Alternative Fuels," SAE Paper 2011-01-0363, 2011.

Dempsey, A.B., and Reitz, R.D., "Computational Optimization of Reactivity Controlled Compression Ignition in a Heavy-Duty Engine with Ultra Low Compression Ratio," SAE Paper 11ICE-0206, 2011-24-0015, 2011.

Splitter, D.A., Hanson, R.M., Kokjohn, S.L., Wissink, M., and Reitz, R.D., "Injection Effects in Low Load RCCI Dual-Fuel Combustion," SAE Paper 11ICE-0154, 2011-24-0047, 2011.

Kokjohn, S.L., Reitz, R.D., Splitter, D.A., and Musculus, M.P.B., "Investigation of Fuel Reactivity Stratification for Controlling PCI Heat-Release Rates Using High-Speed Chemiluminescence Imaging and Fuel Tracer Fluorescence," SAE paper 2012-01-0375, 2012.

Splitter, D.A., Wissink, M., Kokjohn, S.L., and Reitz, R.D., "Effect of Compression Ratio and Piston Geometry on RCCI Load Limits and Efficiency," SAE paper 2012-01-0383, 2012.

Hanson, R.M., Curran, S., Wagner, R., Kokjohn, S.L., Splitter, D.A., and Reitz, R.D., "Piston Bowl Optimization for RCCI Combustion in a Light-Duty Multi-Cylinder Engine," SAE paper 2012-01-0380, 2012.

Kaddatz, J., Andrie, M.J., Reitz, R.D., and Kokjohn, S.L., "Light-duty Reactivity Controlled Compression Ignition Combustion using a Cetane Improver," SAE Paper 2012-01-1110, 2012.

Nieman, D.E., Dempsey, A.B., and Reitz, R.D., "Heavy-Duty RCCI Operation Using Natural Gas and Diesel," SAE paper 2012-01-0379, 2012.

Dempsey, A.B., Adhikary, B. Das, Viswanathan, S., and Reitz, R.D., "Reactivity Controlled Compression Ignition (RCCI) using Premixed Hydrated Ethanol and Direct Injection Diesel," J. Eng. Gas Turbines Power, 134, 082806, 2012.

Ra, Y., Loeper, P., Reitz, R.D., Krieger, R.B., Foster, D.E., Durrett, R.P., Gopalakrishnan, V., Plazas, A., Peterson, R., and Szymkowicz, P., "Study of high speed gasoline DICI engine operation in the LTC regime," SAE Paper 2011-01-1182, 2011. This paper was named SAE **Horning Award** winner for 2011

Ra, Y., Loeper, C.P., Andrie, M.J., Krieger, R.B., Foster, D.E., Reitz, R.D., and Durrett, R., "Gasoline DICI Engine Operation in the LTC Regime using Triple-Pulse Injection," SAE Paper 2012-01-1131, 2012.

Burton, J., Williams, D., Glewen, W., Andrie, M., Krieger, R., "*Investigation of Transient Emissions and Mixed Mode Combustion for a Light Duty Diesel Engine*," SAE Technical Paper 2009-01-1347, 2009, doi:10.4271/2009-01-1347.

Glewen, W., Meyer, C., Foster, D., Andrie, M., Krieger, R., "*Sources and Tradeoffs for Transient NO and UHC Emissions with Low Temperature Diesel Combustion*," SAE Technical Paper 2011-01-1356, 2011, doi:10.4271/2011-01-1356.

Heuwerker, D., Glewen, W., Meyer, C., Foster, D., Andrie, M., Krieger, R., "*Effects of Low Pressure EGR on Transient Air System Performance and Emissions for Low Temperature Diesel Combustion*," SAE Technical Paper 2011-24-0062, 2011, doi:10.4271/2011-24-0062.

Glewen, W., Heuwerker, D., Foster, D., Andrie, M., Krieger, R., "*Analysis of Deviations from Steady State Performance During Transient Operation of a Light Duty Diesel Engine*," SAE Int. J. Engines 5(3):909-922, 2012, doi:10.4271/2012-01-1067.

Paper Draft In Submission: Heuwerker, Glewen, Andrie, Krieger and Foster, "*Transient Comparison of High Pressure and Hybrid EGR Strategies on a Light Duty Diesel Engine Using Low Temperature Combustion*," to be submitted for SAE 2013 International Congress.

Blessinger, M.K. and Ghandhi, J.B., "Initial Optical Investigation of Reactivity Controlled Combustion in an HSDI Engine," 7th US National Technical Meeting of the Combustion Institute., Atlanta, GA, March 20-23, 2011.

Blessinger, M., Stein, J. and Ghandhi, J.B., "An Optical Investigation of Fuel Composition Effects in a Reactivity Controlled HSDI Engine," SAE Int. J. Engines 5(2):2012, doi:10.4271/2012-01-0691. Also published as SAE Paper 2012-01-0829, 2012.

Zhang, Y., Jesch, D., Oakley, J., and Ghandhi, J.B., "High Resolution Flowfield Measurements during the Compression and Expansion Strokes," paper to be submitted to the 2013 SAE World Congress.

S. Deshpande, J. Gao, and M.F. Trujillo (2011) "Characteristics of hollow cone sprays in crossflow," 23rd Annual Conference on Liquid Atomization and Spray Systems, May, Ventura, CA.

J. Gao, M. F. Trujillo, and S. S. Deshpande (2011) "Numerical Simulation of Hollow-Cone Sprays Interacting with Uniform Crossflow for Gasoline Direct Injection Engines," SAE Int. J. Engines, 4:2207-2221.

D.T. Ryddner and M.F. Trujillo (2012) "A Fully Resolved UWS Droplet Simulation," 24th Annual Conference on Liquid Atomization and Spray Systems, May, San Antonio, TX.

S. Deshpande, J. Gao, and M. F. Trujillo (2011) "Characteristics of Hollow Cone Sprays in Crossflow," Atomization and Sprays, 21:349-361

D.T. Ryddner and M.F. Trujillo (2012) "UWS Droplet Vaporization," (to be submitted to Int. J. Heat and Mass Transfer).

Zhang, Y., Ghandhi, J., Petersen, B., and Rutland, C.J., 2010, Large Eddy Simulation of Scalar Dissipation Rate in an Internal Combustion Engine, SAE 2010-01-0625, SAE Congress, Detroit, MI, April 13-15, 2010.

Rutland, C.J., 2011 “Large Eddy Simulations for Internal Combustion Engines – A Review,” Int. J. of Engine Research, Vol. 12 (5), pp 421-451, DOI: 10.1177/1468087411407248.

Banerjee, S. and Rutland, C.J., “Numerical Study of Diesel Combustion Regimes”, SAE 2011-01-0823, SAE World Congress, Detroit, MI April 2011.

Zhang, Y. and Rutland, C.J. 2012, “A Mixing Controlled Direct Chemistry (MCDC) Model for Diesel Engine Combustion Modeling using Large Eddy Simulation,” Combustion Theory and Modelling, Vol.16, Issue.3, pp.571-588. DOI:10.1080/13647830.2011.642819.

Banerjee, S. and Rutland, C.J., “Numerical Investigation of High Powered Diesel Mode Transition Using Large Eddy Simulations”, SAE 2012-01-0693, SAE World Congress, Detroit, MI April 2012.