Final Close-out Report: January-September, 2009

DOE Project: Optimizing Low Temperature Diesel Combustion (LTC-D)
"FreedomCAR and Vehicle Technologies Program Solicitation for University Research and Graduate Automotive Technology Education (GATE) Centers of Excellence"
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Program Objectives

The engine industry is currently facing severe emissions mandates. Pollutant emissions from mobile sources are a major source of concern. For example, US EPA mandates require emissions of particulate and nitrogen oxides (NOx) from heavy-duty diesel engine exhaust to drop at least 90 percent between 1998 and 2010. Effective analysis of the combustion process is required to guide the selection of technologies for future development since exhaust after-treatment solutions are not currently available that can meet the required emission reduction goals. The goal of this project is to develop methods to optimize and control Low Temperature Combustion Diesel technologies (LTC-D) that offers the potential of nearly eliminating engine NOx and particulate emissions at reduced cost over traditional methods by controlling pollutant emissions in-cylinder.

The work was divided into 5 Tasks, featuring experimental and modeling components:
1.) Fundamental understanding of LTC-D and advanced model development,
2.) Experimental investigation of LTC-D combustion control concepts,
3.) Application of detailed models for optimization of LTC-D combustion and emissions,

4.) Impact of heat transfer and spray impingement on LTC-D combustion, and
5.) Transient engine control with mixed-mode combustion.

As described in the final report (December 2008), outcomes from the research included providing guidelines to the engine and energy industries for achieving optimal low temperature combustion operation through using advanced fuel injection strategies, and the potential to extend low temperature operation through manipulation of fuel characteristics. In addition, recommendations were made for improved combustion chamber geometries that are matched to injection sprays and that minimize wall fuel films. The role of fuel-air mixing, fuel characteristics, fuel spray/wall impingement and heat transfer on LTC-D engine control were revealed. Methods were proposed for transient engine operation during load and speed changes to extend LTC-D engine operating limits, power density and fuel economy. Low emissions engine design concepts were proposed and evaluated.

Program Summary

As summarized above, the research activities included five integrated tasks to develop methods to optimize and control Low Temperature Diesel Combustion (LTC-D) for improved fuel efficiency and low emissions. This report represents final close-out reporting for the work completed under the no-cost extension for the period January to September 2009. The report documents the final activities under the grant.

Approach

The Tasks develop and apply novel diagnostics, fuel-types, injection concepts, optimized piston geometry with advanced CFD models and coordinated engine experiments.

Major Accomplishments

- Reduced chemistry mechanisms for petroleum and non-petroleum fuels have been formulated for use in advanced CFD and engine system combustion models.
- Efficient chemistry solvers have been developed to allow comprehensive simulations.
- New high resolution optical diagnostics have been developed for in-cylinder chemical species measurement, and the measurements have been used for combustion model validation.
- Grid-independent spray models have been developed to improve the accuracy of CFD model predictions.
- Improved accuracy turbulence models based on Large Eddy Simulation (LES) have been developed and applied to LTC-D analysis.
- Advanced fuel injection concepts have been proposed and explored, and group-hole and transient VCO/Sac injector models have been formulated.
- The utility of variable pressure injection for minimizing spray impingement has been demonstrated using CFD modeling.
- Practical implementation of a variable injection pressure system has been demonstrated in the laboratory.
- LTC-D engine performance has been characterized in the ERC's light-duty and heavy-duty diesel engine laboratories with a wide variety of fuels, with emphasis on fuel property effects such as Cetane Number, aromatic content and volatility.
- Ultra-low emissions and improved fuel efficiency have been demonstrated when operating a LTC-D diesel engine on gasoline fuel.

- Component heat transfer models have been developed for improved thermal analysis modeling.
- Advanced optimization tools have been developed and applied to recommend optimal piston bowl geometries.
- Mixed-mode combustion regime transitions have been explored in multi-cylinder engine tests and system models.

No-Cost Extension Activities

Work conducted under the no-cost extension reported here continued to develop and apply tools to explore methods to reduce emissions and increase fuel efficiency in the following areas:

- Exploring effect of piston-liner crevice geometry effects on emissions
- Optimized combustion chamber piston geometries.
- Exploration of dual fuel (gasoline/diesel) LTC operation.

Current Progress

Task 1: Fundamental understanding of LTC-D and advanced model development

<u>1.1a LTC-D and premixed combustion modeling - Reitz</u>

At high-load operating conditions in diesel engines, NOx and soot are the primary emissions of concern, since they are strictly regulated in emission standards and can also limit the engine's operation range. In terms of modeling, accurate prediction of emissions requires accurate prediction of the thermodynamic conditions in the combustion chamber. Since diesel engine operation is usually overall lean, CO is often neglected, particularly under high-load conditions. However, due to its relatively low threshold reaction temperature, CO emissions serve as an indicator of inadequate mixing in the combustion chamber.

Accordingly, Computational Fluid Dynamics predictions of the flow field and pollutant emissions in a diesel engine operating at high load and rated speed were explored. Piston-liner crevice flows during the expansion stroke can give rise to vortex motion, as shown in Fig. 1, whose characteristics depend on the piston crevice configuration. Both a realistic and a simplified crevice volume that consists of a neck area and a reservoir to keep the surface to volume ratio realistic were considered. In the simplified crevice approach, with moderate intensity of the crevice flow the in-cylinder flow vortex enhances mixing and engine-out CO (carbon monoxide) emissions are reduced. However, when the crevice flow vortex strength is above a certain level, a strong tumble motion was created in the bulk mixture in the squish area, which isolates the region of high CO concentration and prevented oxidation.

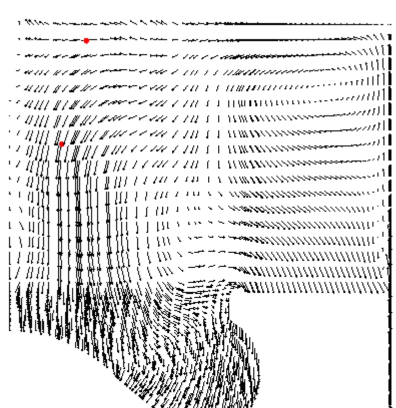

Figure 1: Predicted flow field in the engine showing vortex in upper right-hand corner of the combustion chamber generated by piston-liner crevice flow.

The results also showed that proper timing of the crevice flow into the combustion chamber lowers the mixture temperature and reduces NOx (nitrogen oxide) emissions. Calculation with the realistic crevice flow geometry captured the vortex motion at milder level, predicting more CO and less NOx emissions. Further details are described in a paper accepted for publication in the International Journal of Engine Research.

1.1b Experimental verification measurements of species composition in an optical LTC-D engine - Sanders

Task completed, as described in Final report, December 2008.

1.2 Formulation of turbulence and mixing models for LTC-D

1.2a Large Eddy Simulation Models for Mixing in Engine Applications – Rutland

Task completed, as described in Final report, December 2008.

1.2b Fine-scale Mixing Measurements of Gas and Spray Jets in Engines - Ghandhi

Task completed, as described in Final report, December 2008.

Task 2: Experimental investigation of LTC-D combustion control concepts

2.1 Use of Variable Valve Timing and Variable Geometry Sprays for mixing and combustion control in a Heavy Duty LTC-D engine – Reitz

As described in previous quarterly reports, a Variable Geometry Spray (VGS) experiment has been conducted and was demonstrated to produce low NOx and HC emissions, but with relatively high PM emissions. The VGS experiment used two injectors, a low pressure GDI injector and a high pressure common rail injector in the Caterpillar heavy-duty diesel engine. In the last report, the use of different fuels helped show that PM from the main high-pressure injection was due to the high temperatures from the first combustion event. In the present tests, a Bosch diesel injector with a 250 micron hole diameter and 154 deg spray angle was installed, along with a low pressure intake port injector to allow dual-fuel operation.

In the no-cost extension activity, the Caterpillar lab continued to explore Partially Premixed Combustion with dual-fueled engine operation. The engine was fueled using commercially available gasoline (PON 91.6) and ULSD diesel delivered through the separate port and direct injection systems, respectively. Engine experiments were conducted at a steady-state engine load of 9 bar IMEP and speed of 1300 rev/min. In-cylinder optical measurements focused on understanding the fuel decomposition and formation of low temperature combustion precursors in the engine.

The measurement technique utilized a modified cylinder head to allow optical access through a sapphire fiber-optic probe. The probe was integrated with a specially configured Fourier Transform Infra-Red (FTIR) system, previously developed under Task 1.1b, operating in the 2-4.5 μm spectral region. Measured spectra such as those shown in Fig. 2 were indexed to engine crank-angle thus enabling cycle-averaged, crank-angle-resolved in-cylinder spectroscopy. The measured spectra were compared to fitted spectra from the HITRAN database to monitor fuel decomposition and the formation of formaldehyde, water, and carbon dioxide. These results are exciting because they demonstrate the possibility of monitoring the evolution of numerous species in-cylinder, including intermediates such as formaldehyde.

CFD modeling, using the KIVA 3v Release 2 code coupled with the CHEMKIN II solver and the reduced PRF mechanism, previously developed under Task 1.1a, was used to further explain the observed results. Comparison of experimental and the CFD modeling results such as those shown in Fig. 3 demonstrated good agreement of measured species both spatially and temporally. Further research results are documented in a paper that has been submitted for the 2010 SAE Congress.

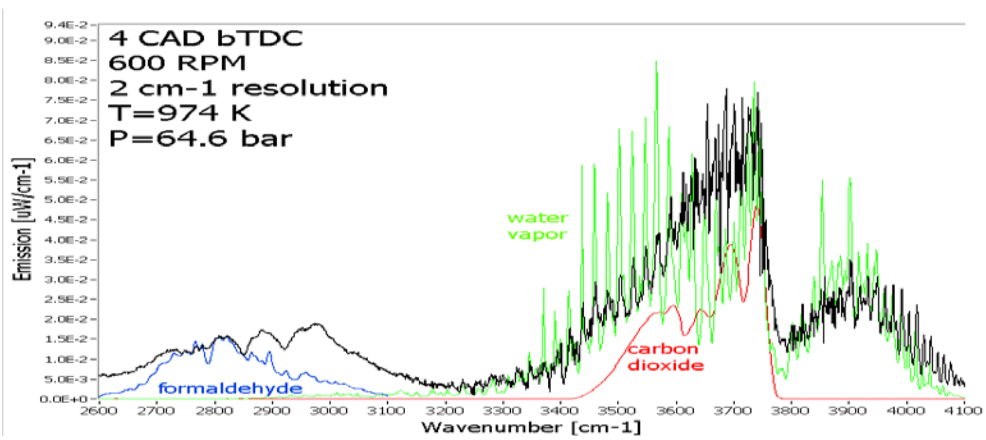

Figure 2: Measured emission spectra in the ERC Caterpillar SCOTE engine

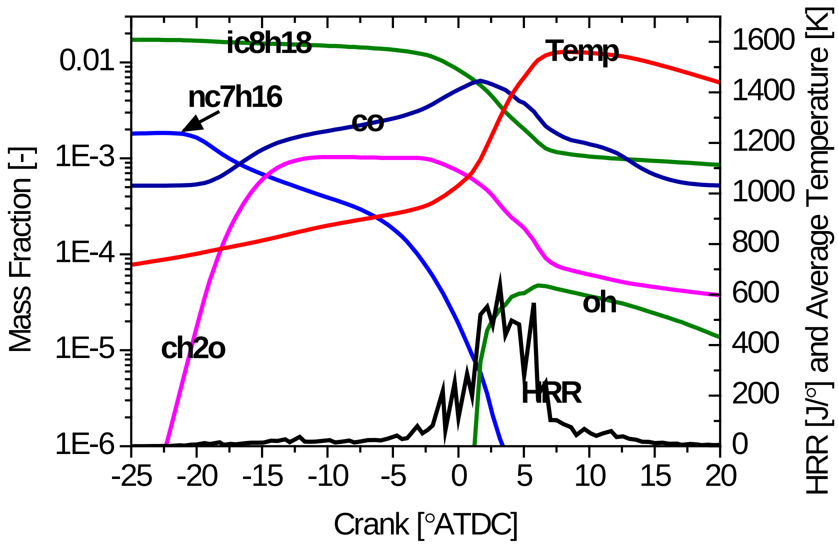

Figure 3: Predicted fuel and major species histories as a function of time for dual fuel operation at 9 bar IMEP with 89% gasoline (iso-octane), 11% diesel (n-heptane) fuel split.

Task 3: Application of detailed models for Optimization of LTC-D combustion and emissions

3.1 Optimization of HD engine piston bowl geometry using GA-CFD with detailed chemistry and experimental validation – Reitz

An investigation was conducted to optimize a light-duty diesel engine in order to minimize soot, NOx, carbon monoxide (CO), unburned hydrocarbon (UHC) emissions and peak pressure rise rate (PPRR) while improving fuel economy in a low oxygen environment. The variables considered are the injection timings, fractional amount of fuel per injection, half included spray angle, swirl and a stepped-bowl piston geometry. The KIVA-CHEMKIN code with detailed chemistry, developed in Task 1.1a, was used and was coupled to a multi-objective genetic algorithm (MOGA) along with an automated grid generator.

A stepped-piston bowl configuration was explored since it allows more options for spray targeting and improved charge preparation. The results show that optimal combinations of the above variables exist to simultaneously reduce emissions and fuel consumption. Details of the spray targeting were found to have a major impact on the combustion process. With the stepped-bowl and split injection strategy, combustion can occur in two distinctly different regions of the bowl. When the first injection targeted the top portion and second injection targeted the bottom portion of the stepped-bowl a low emission combustion process with improved fuel economy resulted. This is because combustion takes place in two different areas, allowing better use of the oxygen, thus limiting the production of soot. The stepped-bowl has less surface area than the conventional reentrant bowl resulting in less heat transfer out causing the fuel consumption to be lower in the stepped-bowl. Swirl, and spray angle along with the bowl geometry details affected the pre-combustion mixing process. Second injection timing and amount of exhaust gas recirculation (EGR) affected the objectives as well.

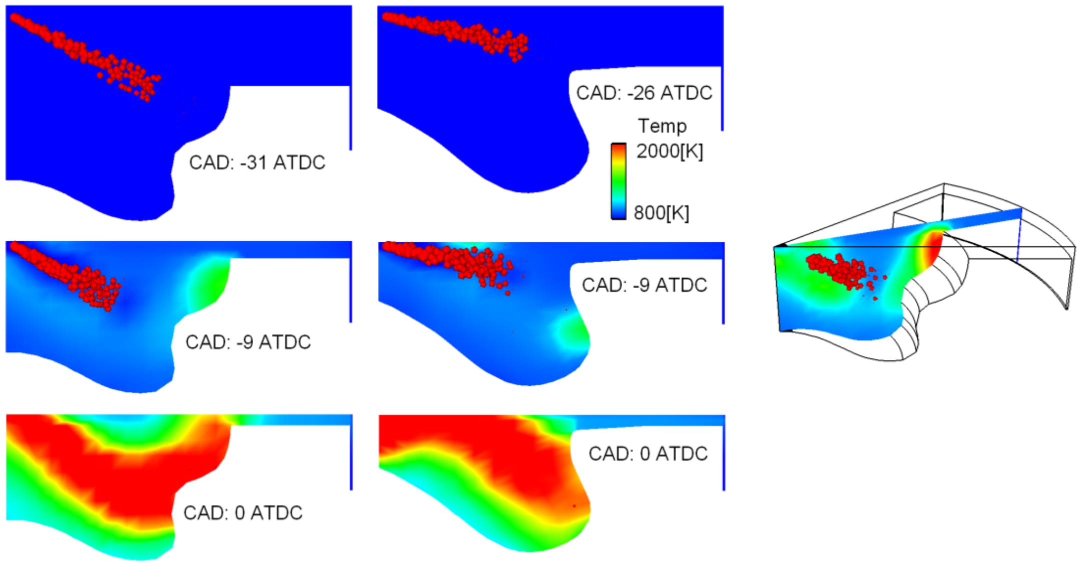

Figure 4: Temperature contours for the stepped-bowl and conventional pistons

Figure 4 shows for the stepped-bowl, the first injection targets the upper portion of the bowl and the second targets the lower. This allows fuel from the first injection to combust away from the second injection. At nine degrees BTDC one can see combustion starting in both the stepped and conventional bowls. This is indicated by the green area. In the stepped-bowl the fuel in the second pulse targets another area of the bowl, and this explains why soot emissions are reduced by over a factor of two, as shown in Fig. 5, when compared to the conventional bowl at a similar operating condition. In the conventional bowl, fuel from the first injection combusts in the same area as where the second injection is placed. Further research results are documented in a paper that has been submitted for the 2010 SAE Congress.

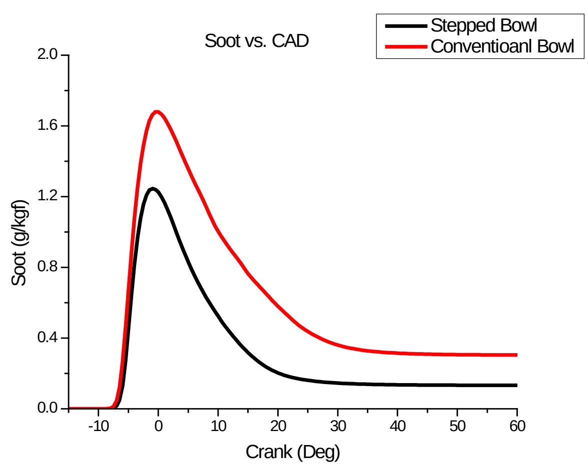

Figure 5: Predicted total in-cylinder soot history for the stepped and conventional bowls

<u>3.2 Investigation of optimal spray characteristics for HSDI LTC-D combustion – Reitz</u>

Task completed, as described in Final report, December 2008.

3.3 Investigation of improved mixing strategies using early injection and LES - Rutland

Task completed, as described in Final report, December 2008.

Task 4: Impact of heat transfer and spray impingement on LTC-D combustion

4.1 Thermal analysis of LTC-D engines using detailed CFD coupled with 3-D metal component heat conduction – Reitz

Task completed, as described in Final report, December 2008.

4.2 Experimental measurements of piston temperature and heat flux for LTC-D combustion analysis - Ghandhi

Task completed, as described in Final report, December 2008.

Task 5: Transient engine control with mixed-mode combustion

5.1 Multi-cylinder HSDI engine control strategies with mixed-mode combustion regime transitions – Foster

Task completed, as described in Final report, December 2008.

5.2 Engine system analysis and optimization with mixed-mode combustion regime transitions – Rutland

Task completed, as described in Final report, December 2008.

Papers submitted and/or published:

Lee, C.-W and Reitz, R.D., “Predictions of the effects of piston-liner crevices on flow motion and emissions in 3-D diesel engine simulations,” Accepted, International Journal of Engine Research, August, 2009.

Splitter, D.A.,, Hanson, R., Kokjohn, S., Rein, K., Sanders, S., and Rolf Reitz, R.D., "An Optical Investigation of Ignition Process in Fuel Reactivity Controlled PCCI Combustion," 10PFL-0879, SAE Congress, 2010.

Dolak, J., Shi, Y., and Reitz, "A Computational Investigation of a Stepped-Bowl Piston Geometry for a Light Duty Engine Operating at Low Load," Paper Offer/Number: 10PFL-0127, SAE Congress, 2010.