High load (21 bar IMEP) dual fuel RCCI combustion optimization

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ABSTRACT

Dual-fuel reactivity controlled compression ignition (RCCI) combustion has shown high thermal efficiency and superior controllability with low engine-out NOx and soot emissions. However, as in other low temperature (LTC) combustion strategies, the combustion control using low EGR or high compression ratio at high load conditions has been a challenge. The objective of this work was to find an optimum injection strategy utilizing dual direct injectors that enabled high load RCCI operation. The present computational work employed KIVA3V-Release2 code that had a discrete multi-component fuel evaporation model. The chemical reaction calculation was done using a sparse analytical Jacobian approach solving the chemistry of two fuels (iso-octane and n-heptane). Compared to the KIVA-CHEMKIN code, the calculation time was about three times faster with a new chemistry solver. In order to find an optimum injection strategy the KIVA code was coupled with Nondominated Sorting Genetic Algorithm (NSGA II), which is a multi-objective genetic algorithm. The resulting optimum injection strategy demonstrates that 21bar IMEP RCCI combustion is achievable with low engine-out NOx, soot, and carbon monoxide (CO) emissions. The simulations were performed for a heavy-duty engine of 2.44 liter displacement and 15:1 compression ratio. The resulting optimum strategy yields 12.6bar/deg peak pressure rise rate, 158bar maximum pressure, and 48.7% gross thermal efficiency. The engine performance and emission results between CHEMKIN solver and a sparse analytical Jacobian solver were also compared.

INTRODUCTION

In recent years dual-fuel reactivity controlled compression ignition (RCCI) combustion has shown superior combustion phasing control while retaining the benefit of homogeneous charge compression ignition (HCCI) combustion – high thermal efficiency and low engine-out nitrogen oxide (NOx) and soot emissions. However, high load operation still remains as an important hurdle to overcome. The target load of the present work is 21bar gross IMEP, and this was achieved using two independent direct-injectors. The fuels used for this study were iso-octane and n-heptane, which are surrogate fuels for gasoline and diesel, respectively. The required fuel mass to achieve this load was estimated to be 245mg/cycle. The IVC condition was set at 363K (90°C) and 3.42bar with 46%EGR. The engine speed and the compression ratio were maintained at 1800rev/min and 15.0:1, respectively.



Figure 1. HCCI combustion of port-injected fuel and schematic representation of the injection strategy

Figure 1 shows results of the port-injected iso-octane method. The two pressure traces are HCCI combustion of 240mg and 230mg of iso-octane with the abovementioned IVC conditions. This charge was not supposed to combust since it lacks the n-heptane injection. This demonstrates that a different approach in low-reactivity fuel delivery is necessary. Therefore, the idea of utilizing two independent direct injectors to deliver fuels after IVC was explored. A combustion chamber of an engine using a re-entrant bowl type piston can be divided into two regions –

bowl and squish. Unlike the bowl, the squish region typically has higher surface-to-volume ratio. This high surfaceto-volume ratio allows higher heat transfer from the charge to the surfaces. With two independent direct-injectors low-reactivity fuel (i.e., iso-octane or gasoline) can be placed in the squish region. Thus, the goal of the present work is to find an optimum injection strategy with reasonable pressure rise rates and maximum pressures as well as reasonable emissions.

COMPUTATIONAL TOOLS

The computations were performed using the KIVA3v-release2 code with a discrete multi-component fuel vaporization model, which is capable of calculating the evaporation of a droplet when it is composed of more than one species [1]. As mentioned earlier, in the present study iso-octane and n-heptane were used as surrogates for low-reactivity fuel (i.e., gasoline) and high-reactivity fuel (i.e., diesel), respectively, in the chemistry calculations. For the physical properties of the fuel, iso-octane and tetradecane were used to represent the low-reactivity fuel and high-reactivity fuel, respectively.

The chemical reaction calculations used a reduced PRF mechanism consisting of 46 species and 142 reactions including NOx chemistry [2]. Soot emissions were calculated using a phenomenological soot model [3]. The KIVA code was coupled with a sparse analytical Jacobian solver, called SpeedChem, for the chemistry calculation [4]. Compared to the set up where the code was coupled with Chemkin II, the SpeedChem solver reduced the CPU time by 3-4 times without noticeable changes in pressure trace, heat release rate, or emissions. Typical calculation time was 10-15 hours.

Engine Specifications				
Displacement [L]	2.44			
Bore x Stroke [mm]	137 x 165			
Connecting Rod [mm]	261.6			
Compression Ratio [-]	15.0:1			
Swirl Ratio [-]	0.7			
IVC [°ATDC]	-143			
EVO [°ATDC]	130			
Speed [rev/min]	1800			
High pressure injector (for iso-octane)				
Number of holes	6			
Hole Diameter [mm]	0.250			
Included Spray Angle [°]	145			
Injection Pressure [bar]	1400			
Low pressure injector (for n-heptane)				
Number of holes	6			
Hole Diameter [mm]	0.170			
Included Spray Angle [°]	145			
Injection Pressure [bar]	100			

Computational grid		
Cells at BDC	6750	
Cells at TDC	2790	
Average cell size	~3.4mm	
Azimuthal resolution	4°	
Run time	10-15 hr	



Figure 2. Engine, injectors, and computational grid specifications

The spray model used in the present study employed the Lagrangian-drop and Eulerian-fluid approach. In order to reduce the grid size dependency of the spray and to use a relatively coarse mesh, the Gasjet model was used. The Kelvin Helmholtz-Rayleigh Taylor (KH-RT) model was used to calculate the spray break-up. The Re-Normalization Group (RNG) k- ε model was used for the turbulent flow calculation.

The simulations were based on the 2.44L, Single Cylinder Oil Test Engine (SCOTE) of Caterpillar, Inc. However, unlike the stock piston configuration, the squish height was increased by 0.859mm in order to reduce the compression ratio (15.0:1 instead of 16.1:1). Details of engine specifications along with the injector characteristics, as well as the computational grid specifications, are shown in Figure 2. Although there are 2 independent injectors delivering iso-octane and n-heptane, both injectors were assumed to be at the axis of the cylinder. This assumption allowed the use of a 60° sector mesh, reducing the computational burden. This assumption regarding the injector location was tested in a previous study, and experimental data verified the validity of this assumption [5].

GENETIC ALGORITHM OPTIMIZATION

In this work the genetic algorithm (GA) based optimization tool was used. In the present work 6 design parameters were used to minimize 6 objectives. The 6 objectives to be minimized were: soot, NOx, CO, UHC emissions, indicated specific fuel consumption (ISFC), and ringing intensity (β =0.05). There are different types of Multi-Objective Genetic Algorithms for different optimization tasks; however, Shi and Reitz [6] showed the Nondominated Sorting Genetic Algorithm II (NSGA II) suggested by Deb et al. [7] with a large population was most suitable in searching for a true Pareto front.

The 6 design parameters for the present study are shown in Table 1. Total fuel mass was 245mg/cycle. There are two iso-octane injections. One injection targets the squish region earlier in the compression stroke, and the other injection targets the bowl. A single n-heptane injection is supplied closer to TDC providing an ignition source for the rest of the charge. Each generation had 32 cases (they are called citizens).

Design Parameters	Range
n-heptane mass [mg]	0 to 20
n-heptane SOI [ATDC]	-40 to 0
Premixed iso-octane [%]	0 to 60
Iso-octane in 1 st inj. [%]	0 to 50
DI Iso-octane SOI #1 [ATDC]	-143 to -50
DI Iso-octane SOI #2 [ATDC]	-50 to 0

Table 1. Design parameters for the NSGA optimization

RESULTS

In order to check if the optimization has converged, a convergence metric suggested by Deb and Jain [8] was used. The optimization process produces a number of solutions filling up the Pareto front, and it must be decided which ones are more feasible than other Pareto solutions. Therefore, one design was chosen to be the optimum solution out of all the designs that produced equally low emissions, low ISFC, and low ringing intensity. This design was chosen because it produced the lowest maximum in-cylinder pressure. A summary of the optimum design is shown in Figure 3.



Optimum Design Parameters			
Premixed iso-octane mass [mg]	2.8		
DI Iso-octane mass #1 [mg]	118.8		
DI Iso-octane mass #2 [mg]	115.0		
n-heptane mass [mg]	8.4		
DI Iso-octane SOI #1 [ATDC]	-126.8		
DI Iso-octane SOI #2 [ATDC]	-49.7		
n-heptane SOI [ATDC]	-16.7		

Figure 3. Optimum injection strategy

Before further analysis, it was of interest to examine the effect of the small premixed mass. Since the premixed fuel mass was very small compared to the total fuel mass (2.8mg out of 245mg), a case was set up in which no fuel was premixed at IVC. For this condition the premixed iso-octane was divided equally and given to the two direct-injections of iso-octane. Furthermore, as mentioned earlier the n-heptane injection is the ignition source. In other words, without the n-heptane injection the charge should misfire. A case with no n-heptane injection was tested in order to verify the role of the n-heptane injection. The pressure traces and HRR of these cases are shown in Figure 3. As seen in Figure 3, the case where no iso-octane was premixed at IVC does not show a significant change in

combustion phasing, and the peak pressure is decreased by 7bar. On the contrary, the lack of n-heptane injection caused misfire, proving the role of n-heptane was indeed an ignition source. The combustion phasing control mechanism is further explained in Figure 4 and Figure 5.

Figure 4 shows the in-cylinder Φ evolution up to 20°BTDC. The three iso-surfaces represent the three equivalence ratios of Φ =0.90, 0.80, and 0.50, as shown in the legend on the right. At 110°BTDC the first iso-octane injection ends. This early injection results in a high iso-octane region in squish region. The background temperature and density were high enough to evaporate the iso-octane droplets, preventing wall wetting. At 40°BTDC the second isooctane injection is about half-way finished. This injection supplies additional iso-octane in the bowl region. It appears as if the new iso-octane jet could penetrate all the way into the squish region; however, the background density is even higher at this point, preventing deep penetration of this jet. Therefore, as shown at 20°BTDC, there form 2 distinctive high Φ regions – one in the squish and the other in the bowl.

Figure 5 shows the in-cylinder temperature evolution from 20°BTDC to 20°ATDC. Each of the 5 pictures in this figure contains iso-surfaces of different temperatures. The temperatures of the three iso-surfaces being traced are the ones shown in red boxes in the legend. At 20°BTDC it can be seen the low temperature region develops near the lip of the piston because of the second iso-octane injection. Compared to this low temperature region the lower part of the bowl develops a higher temperature pocket because it has not been exposed to an iso-octane injection and the subsequent evaporation. At 15°BTDC the thermal stratification is increased. Unlike the bowl region, there is no 800K or higher temperature present in the squish. At TDC the n-heptane injection is complete and the initial reaction starts near the injector, and the squish region still remains cooler than in the bowl. At 15°ATDC the combustion is about half-complete. A high temperature region in the bowl is fully developed, while the squish region still remains cooler, only showing a slight sign of initial reactions. The small reaction site at the lip of the piston is where the second injection did not reach. Note that an initial swirl ratio of 0.7 was applied to this simulation; therefore, the gas rotates in the clockwise direction over time. At 20°ATDC, when approximately 80% of chemical energy has been released, more extensive squish combustion is observed.



The sources of the 4 key emissions – soot, NOx, CO, and UHC – are shown in Figure 6. As shown in this figure NOx is mainly from the 2 ignition sources shown in Figure 5 previously. UHC is caused by the first iso-octane injection targeting the squish region. Some of this fuel ended up in the ring-pack crevice during the compression stroke, becoming the main source of UHC emissions. The emission and the overall performance parameters are shown in Table 2. The gross thermal efficiency of this optimum strategy was 48.7%.



Emissions and Performance					
	SpeedChem	CHEMKIN2	Relative error [%]		
Soot [g/kW-hr]	0.015	0.015	0		
NOx [g/kW-hr]	0.058	0.055	+5.5		
CO [g/kW-hr]	0.73	0.78	-6.4		
UHC [g/kW-hr]	1.13	1.14	-0.9		
ISFC [g/kW-hr, IVC→EVO]	174.7	175.1	-0.2		
PPRR [bar/deg]	12.6	12.3	2.4		
Run time [hrs]	9.1	23.3	-61		

Table 2. Difference between SpeedChem and CHEMKIN2



ERC PRF mechanism [2].

Earlier it was mentioned that a sparse analytical Jacobian solver (called SpeedCHEM) was used instead of CHEMKIN2 in chemistry calculations. The code [4] is a Fortran 2003 library developed for the integration of chemical kinetics in gaseous mixtures. Computational efficiency is achieved by exploiting the sparsity of the reaction mechanism, where typically every species interacts with few other species (the reduced PRF mechanism, as shown in Figure 7, is 61.2% sparse) and adopting sparse linear algebra for all the matrix computations. Furthermore, an analytical formulation is provided for all the functions related to the ODE system, including the Jacobian matrix. A high-degree interpolation approach to thermodynamic functions is eventually used to substitute computationally expensive exponentials and logarithm evaluations. The differences in emission and performance estimates are shown in Table 2. As seen in this table, the differences in 4 key emissions are small enough to disregard. However, the calculation time decreased drastically when SpeedChem was coupled with KIVA3v code. As seen in Figure 8, the pressure traces, HRR, combustion phasing, and combustion duration were nearly identical between the two chemistry solvers.

CONCLUSIONS

In this study an injection strategy was optimized for a heavy-duty compression ignition engine for high load RCCI operation. The optimum injection strategy was identified using computational tools – KIVA3v-Release2, sparse analytical Jacobian solver, and the multi-objective genetic algorithm NSGA II. The main objective of the work was to examine the effectiveness of utilizing piston geometry for combustion control. After examining the results, the following conclusions were drawn.

- 1. Even with the relatively high compression ratio (15:1) piston, it was possible to achieve high load (21bar gross IMEP) RCCI combustion. The IVC conditions were: 3.42bar, 90°C, and 46%EGR. The engine speed was 1800rev/min. The optimum injection strategy resulted in 158bar maximum in-cylinder pressure, 12.6bar/deg peak pressure rise rate, and 48.7% gross thermal efficiency.
- 2. This high load operation was possible because the piston geometry and the regions with different surfaceto-volume ratios were utilized by the dual direct-injectors. There were two iso-octane injections – one targeting the squish region and the other targeting the bowl. The single n-heptane injection was the ignition source for the entire charge.
- 3. The sparse analytical Jacobian solver, called SpeedCHEM, showed good agreement with CHEMKIN2. The calculation time decreased by more than 60% compared to CHEMKIN2, enabling faster turn-out time for KIVA3v calculations.
- 4. For future study, it is of interest to understand the effect of increased squish land length on the combustion control. With increased squish land length, more iso-octane can be placed in the squish region. Along with the increased squish land length, the effect of smaller n-heptane spray included angle must be examined. With smaller n-heptane spray included angle, the PRF stratification can be increased. The effect of this smaller included angle on combustion control and emissions will be the subject of future research.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge financial support from Caterpillar and the Sandia National Laboratories.

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