

An Optical Investigation of Ignition Processes in Fuel Reactivity Controlled PCCI Combustion

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ABSTRACT

The ignition process of fuel reactivity controlled PCCI combustion was investigated using engine experiments and detailed CFD modeling. The experiments were performed using a modified all metal heavy-duty, compression-ignition engine. The engine was fueled using commercially available gasoline (PON 91.6) and ULSD diesel delivered through separate port and direct injection systems, respectively. Experiments were conducted at a steady state-engine load of 4.5 bar IMEP and speed of 1300 rev/min. In-cylinder optical measurements focused on understanding the fuel decomposition and fuel reactivity stratification provided through the charge preparation. The measurement technique utilized point location optical access through a modified cylinder head with two access points in the firedeck. Optical measurements of natural thermal emission were performed with an FTIR operating in the 2-4.5 μm spectral region. Measured spectra were indexed to engine crank-angle, thus enabling cycle-averaged, crank-angle-resolved in-cylinder spectroscopy. The measured spectra were compared to emission spectra from the HITRAN database for qualitative species formation. Experimentally measured spectra of fuel decomposition and the formation of aldehydes, water, and carbon dioxide were observed. The reaction extent of the measurements was calculated and compared to that of predictions from the CFD modeling. The modeling predictions used the KIVA 3v Release 2 code coupled with the CHEMKIN II solver and a reduced primary reference fuel mechanism. Comparison of the experimental and CFD modeling results showed good agreement of measured species both spatially and temporally. Reaction extent comparisons were used to provide quantitative evidence for spatially and temporally staged combustion established via in-cylinder reactivity blended charge preparation. The results demonstrated that, at the tested conditions, the charge preparation strategy delayed combustion by approximately

4-5 CAD in areas of lower fuel reactivity as compared to areas of higher fuel reactivity, thus extending the combustion duration. This establishes the well controlled ultra-low emission, high efficiency PCCI-type combustion with reasonable pressure rise rates described by [references \[14 and 15\]](#).

INTRODUCTION

Rising fuel costs and a focus on the reduction of greenhouse gases has necessitated increased efficiency from the internal combustion engine, thereby increasing interest in the diesel engine due to its high efficiency. Furthermore, current and future legislation place stringent standards on the exhaust emissions. These demands require the development of advanced engine technology, which can simultaneously yield high efficiency and low emissions.

Many strategies have been investigated to meet the future requirements of clean, efficient diesel engines. Most of the current strategies utilize low temperature premixed combustion. Lower combustion temperatures result in NO_x reduction due to the high activation energy of NO formation reactions [1]. In addition, utilizing long ignition delay allows adequate time for mixing prior to the start of combustion; thus, rich regions are reduced and soot formation is inhibited. Many researchers have shown Homogeneous Charge Compression Ignition (HCCI) and Premixed Charge Compression Ignition (PCCI) concepts to be promising techniques for simultaneous NO_x and soot reduction [2,3,4,5]. Sun [6] indicated the PCCI, HCCI, and traditional diesel operating regimes on an equivalence ratio-temperature diagram, see [Figure 1](#). This diagram was originally presented by Kamimoto [7] and has been extensively discussed by Pickett et al. [8] and Akihama et al. [9]

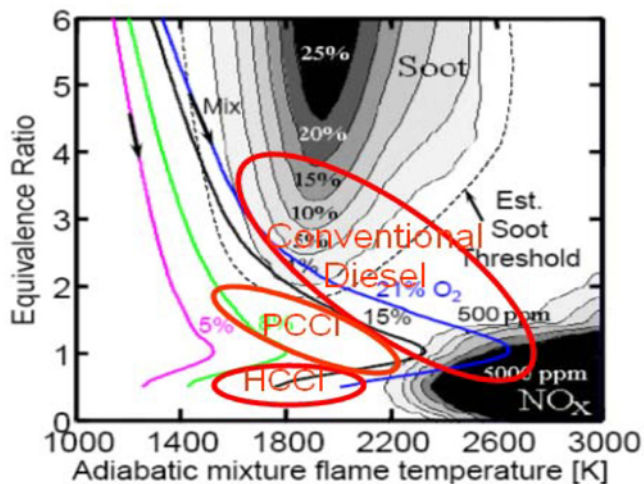


Figure 1. PCCI, HCCI, and conventional diesel operating regimes shown in $T-\Phi$ space [6].

Due to the existing fuel infrastructure, most HCCI and PCCI research has been conducted using strictly either gasoline or diesel fuel. However, in their neat forms, each fuel has both specific advantages and shortcomings for premixed compression ignition (PCI) operation. Gasoline has a high volatility; thus, evaporation is rapid enabling a premixed charge to be obtained using port fuel injection. However, because the autoignition qualities of gasoline are poor, it becomes difficult to achieve combustion at low-load conditions (e.g., [10, 11]). Conversely, diesel fuel has superior auto-ignition qualities; however, this, in turn, can lead to difficulty controlling the combustion phasing as engine load is increased. Therefore, when neat diesel fuel is used in a PCI strategy, high levels of exhaust gas recirculation (EGR) are required to phase combustion appropriately. Opat et al. [4] showed high efficiency, clean PCCI combustion at 5.5 bar IMEP using diesel fuel and ~67% EGR. However, such high levels of EGR restrict high load operation due to reduced air flow. Furthermore, combustion phasing control during transient operation may be difficult when only EGR is used to control combustion phasing [12] due to the long EGR response times.

Recent experiments performed by Bessonette et al. [13] have suggested that the best fuel for HCCI operation may have autoignition qualities between those of diesel fuel and gasoline. Using a compression ratio of 12:1 and a fuel with a derived cetane number of ~27 (i.e., a gasoline boiling range fuel with an octane number of 80.7), they were able to extend the HCCI operating range to 16 bar BMEP - a 60% increase in the maximum achievable load compared to operation using traditional diesel fuel. Furthermore, their results showed low load operation, below 2 bar BMEP, required a derived cetane number of ~45 (i.e., traditional diesel fuel). Thus, it may be beneficial to explore HCCI operation using fuel blends optimized for specific operating conditions.

Inagaki et al. [12] investigated dual-fuel PCI operation as means for reducing the EGR requirements of PCI strategies. Using premixed iso-octane and direct-injection diesel fuel, they were able to operate in PCI mode at 12 bar IMEP. Furthermore, they showed that stratification of fuel reactivity (rather than only equivalence ratio) resulted in reduced rates of heat release and reasonable combustion noise.

Based on the work of Bessonette et al. [13] and Inagaki et al. [12], it is likely that different fuel blends will be required at different operating conditions (e.g., a high cetane fuel at light load and a low cetane fuel at high load). Thus, it is desirable to have the capability to operate with fuel blends covering the spectrum from neat gasoline to neat diesel fuel depending on the operating regime.

Kokjohn et al. [14] and Hanson et al. [15] have demonstrated that fuel reactivity stratification can be used as a strategy for efficient control and operation of premixed combustion. These studies utilized port fuel injection of gasoline and early-cycle, direct-injection of diesel fuel for in-cylinder blending and fuel reactivity stratification. In these studies the authors demonstrated that the use of fuel reactivity stratification aided in extending the combustion duration, lowered pressure rise rates, allowed 11 bar IMEP operation, and were able to obtain indicated thermal efficiencies up to 53 (%) with NO_x and PM emissions below EPA 2010 heavy duty regulation without aftertreatment. However, [References \[14 and 15\]](#) did not provide experimental evidence to quantify the nature of the fuel reactivity stratification. Although the authors suggested that the combustion process was aided through the progression from more to less-reactive fuel species, additional experimental evidence was desired.

SCOPE AND OBJECTIVES

The objective of this study was to experimentally investigate the fuel decomposition process and operational benefits of in-cylinder blended dual-fuel PCCI combustion. Natural thermal emission of formaldehyde, water, carbon dioxide, and fuel spectra between 2-4.5 (μm) wavelengths were measured and compared to multidimensional modeling results. The presented comparisons demonstrate the achievement of fuel reactivity stratification, nearly simultaneous global NTC behavior, and spatially staged transition into thermal ignition through cycle resolved spectra measurements.

EXPERIMENTAL SETUP

ENGINE

A heavy-duty 2.44 L Caterpillar 3401 Single-Cylinder, Oil-Test Engine (SCOTE) was used for all the engine tests. The specific engine lab setup is given in [Figure 2](#), and the engine geometry and configuration are given in [Table 1](#).

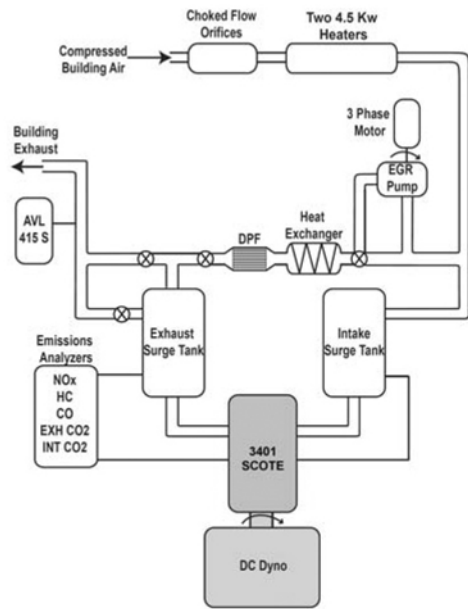


Figure 2. Diagram of the engine lab

Table 1. Test engine geometry

Base engine type	Caterpillar SCOTE
Bore x stroke	13.72 x 16.51cm
Connecting Rod Length	21.16 cm
Squish height	0.157 cm
Displacement	2.44 L
Geometric compression ratio	16.1:1
Effective compression ratio	15.1:1
Swirl ratio	0.7
Bowl type	Stock (wide diameter open chamber)
Number of valves	4
Intake valve opening	-335° ATDC Firing
Intake valve closing	-143° ATDC Firing
Exhaust valve opening	130° ATDC Firing
Exhaust valve closing	-355° ATDC Firing

INJECTION SYSTEM

Dual-fuel PCCI engine experiments were performed using port fuel injection of gasoline and early direct-injection of diesel fuel using a conventional (i.e., wide angle, large nozzle hole) high-pressure, common-rail injector. The specifications for the port fuel injector and common rail injector are given in Tables 2 and 3, respectively.

Table 2. Port fuel injector specifications

Steady flow rate @ 3 bar	750 cc/min
Included spray angle	15°
Fuel pressure	5.17 bar

Table 3. Common rail injector specifications

Number of holes	6
Hole Diameter	250 µm
Included spray angle	145°
Injection pressure	800 bar

DATA ACQUISITION AND LABORATORY HARDWARE

Cylinder pressure was measured with a Kistler model 6067C1 water-cooled pressure transducer in conjunction with a Kistler model 510 charge amplifier. Acquired cylinder pressure traces were averaged for 500 cycles to help smooth pressure data due to the ringing experienced from PPC combustion. Intake air flow was measured using choked flow orifices. In order to get choked flow for a variety of engine operating conditions, combinations of 6 different sized orifices were used to obtain the desired intake air flow rate. Intake air was heated with two immersion style heaters and PID control to $\pm 1^\circ\text{C}$. Both the intake and exhaust system surge tank pressures were equipped with PID control to ± 0.7 kPa. PM measurements were performed with an AVL model 415s smoke meter. PM measurements of filter smoke number (FSN), mass per volume ($\text{mg}/\text{m}^{3\text{sup}}$) and specific emissions (g/kWh) were related with the factory AVL calibration and averaged between 5 samples of a 2 L volume each with paper-saving mode off. All gaseous emissions measurements were performed with a 5 gas emissions bench. EGR rate was determined through the ratio of intake CO_2 to exhaust CO_2 levels. Gaseous emissions were averaged for 30 seconds after attaining steady-state for several minutes.

FUEL PROPERTIES

Commercially available 91 pump octane number ($\text{PON}^\dagger$) gasoline and USLD were used for all tests. Tables 4 and 5 show the fuels properties obtained from an independent lab analysis.

$^\dagger \text{PON} = (\text{RON} + \text{MON})/2$

Table 4. Gasoline fuel properties

Distillation Curve	ASTM D86
Initial Boiling Point	38.9 °C
Temperature 10% evaporated	69.4 °C
Temperature 50% evaporated	105.0 °C
Temperature 90% evaporated	160.6 °C
Final Boiling Point	215.6 °C
Lower Heating Value	43.2 MJ/kg
MON	87.8
RON	95.6
(R+M)/2	91.6
Ethanol Content	0 %
H/C ratio	1.88
Specific Gravity (@ 15.6°C)	0.737
Sulfur (ASTM D5453)	4.6 ppm

Table 5. Diesel fuel properties

Specific Gravity (@ 15.5 °C)	0.856
Viscosity (@ 40 °C)	2.71 °C
Surface Tension (@ 25 °C)	30.0 dyne/cm
Lower Heating Value	42.526 MJ/kg
Cetane Number	46.1
H/C ratio	1.74

OPTICAL ACCESS

To gain optical access, a modified cylinder head with two optical access points was used. The optical access points were at Locations A (bowl) and B (squish) as shown in [Figures 3 and 4](#).

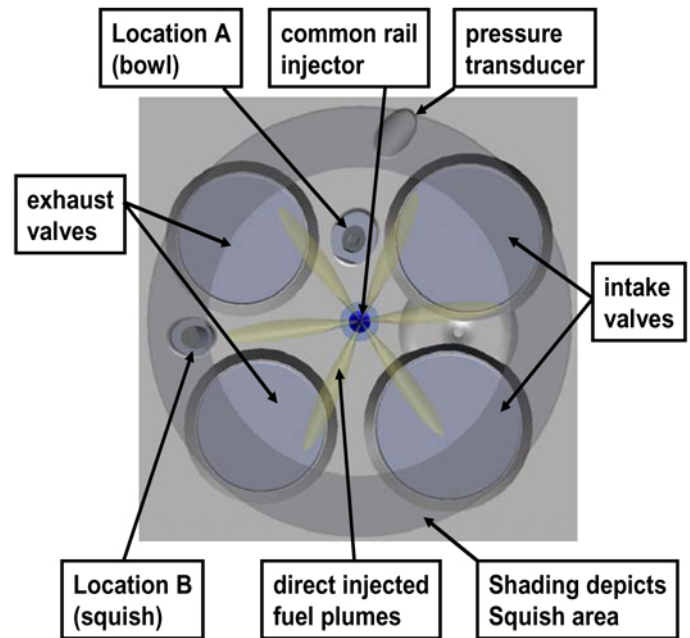


Figure 3. Bottom view of optical access

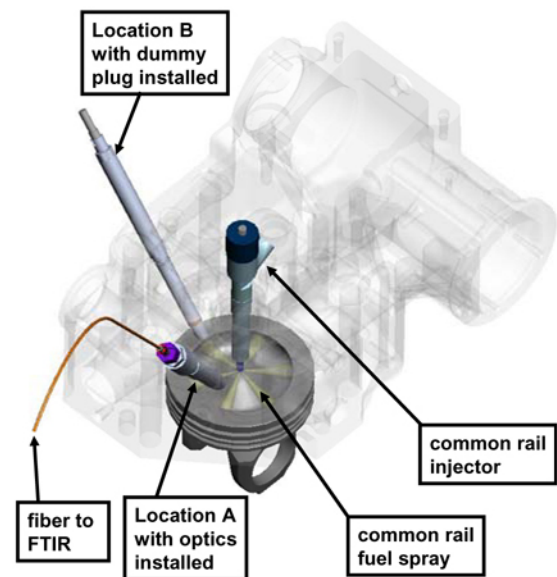


Figure 4. Isometric view of optical access

Optical access Location A (bowl) and Location B (squish) are at respective angles of 36 and 37 degrees from the bore centerline, with both locations flush cut to the cylinder head firedeck. As diagramed in [Figures 3 and 4](#), the field of view from Location A was near the center of the bowl while location B provides access to the squish near the squish/bowl interface. By using two separate optical access locations, a degree of spatial resolution was introduced into the point measurement technique used in the present study. The spatial resolution helped to further research the ignition behavior of in-cylinder blended fuel reactivity stratification.

OPTICAL DIAGNOSTIC TECHNIQUE

The optical diagnostic technique enabled cycle-resolved spectral measurements of natural thermal emission using a standard Fourier-transform infrared spectrometer (FTIR). The technique was initially demonstrated in [References \[16 and 17\]](#), where measurements of natural thermal emission water spectra were conducted with an optical spark plug on a small-displacement, spark-ignition engine. A complete explanation of Fourier-transform spectroscopy can be found in [Reference \[18\]](#). The technique has been adapted to this research through the implementation of a novel fabricated optical instrument. The instrument consisted of a 3.25 (mm) diameter by 210 (mm) long sapphire rod, jacketed in a 9 (mm) outer diameter Kovar housing. The instrument was installed in one of the two available optical access holes in the cylinder head as seen in [Figures 3 and 4](#).

The instrument was coupled to a 550 μm core diameter sulfide fiber (As_2S_3), which pitched light collected by the optical instrument into a standard Nexus 670 FTIR manufactured by Thermo Fisher Scientific. Two additional photodiodes (PDs) and a beamsplitter were introduced into the FTIR to provide easy access to the relevant interferometric signals. These modifications are not required; the signals could also be obtained from the original PDs in the FTIR, provided one has the means to access these signals without disturbing interlocks integrated into the FTIR. The beamsplitter (S1 in [Figure 5](#)) was placed in the beam path of the HeNe laser in the FTIR. The light reflected by the beamsplitter was focused onto a PD (Thorlabs PDA55, silicon) (B in [Figure 5](#)) and was used to monitor FTIR mirror position. The standard interferogram detector in the FTIR was also replaced by a different PD (Kolmar Technologies KISDP-1-J2, InSb) (C in [Figure 5](#)) and was amplified with a Stanford Research Systems SR570 current amplifier. All open optical paths and fiber connections were continuously purged with zero-grade nitrogen gas. The engine crankshaft encoder A and Z (A in [Figure 5](#)) pulses were continuously recorded. [Figure 5](#) shows the optical setup for the measurement.

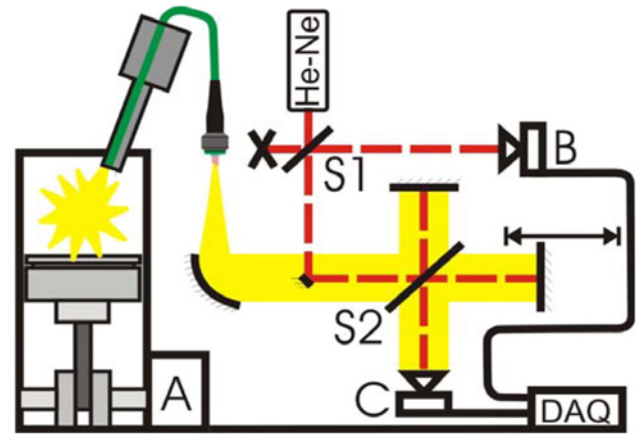


Figure 5. Diagram of optical setup

The translating mirror in the FTIR was continuously scanned at a frequency, independent of and unrelated to the engine speed. The mirror position, interferometer, and crank shaft encoder signals were simultaneously recorded at 500 kS/s using a LabVIEW based DAQ device (National Instruments PCI-6123, LabVIEW 8.5). In post processing, a low-pass filter was applied to the interferometer signal to remove the frequency modulation induced by the Michelson interferometer. The original interferometer signal was then divided by this filtered signal to reduce sensitivity to imperfect repeatability of the combustion event. Without this step, noise that was attributed to cycle-by-cycle fluctuations in gas temperature was observed. It is believed that these variations, although small enough to modify the spectral shapes only slightly on a cycle-by-cycle basis, were associated with large enough variations in total emitted power to contaminate the interferogram. Next, the data were sorted by engine crank-angle. For each crank-angle, different engine cycles populated different regions of the interferogram, according to the location of the translating mirror. The superposition of the interferometer signals from many engine cycles resulted in a composite interferogram for a given engine crank-angle. Overlapping sections in each interferogram were averaged and gaps in the interferogram were filled using a 1D spline interpolation function to ensure constant spacing between points in the interferogram. The interferogram was then phase-corrected to remove any phase errors caused by imperfect optical alignment or nonlinearities in the detection system. A Flat Top windowing function and zero-padding were then applied before performing a fast-Fourier-transform (FFT) on the interferogram, yielding a spectrum for each crank-angle. These measured spectra were in turn corrected for the spectral response of the system. Corrections for optical depth of field within the combustion chamber were not considered due to the unknowns of the measured gasses. Corrections for piston face and optical path induced emission were not performed because no observed underlying continuum or emission from these sources was observed under hot (post fired) motored or fired operation.

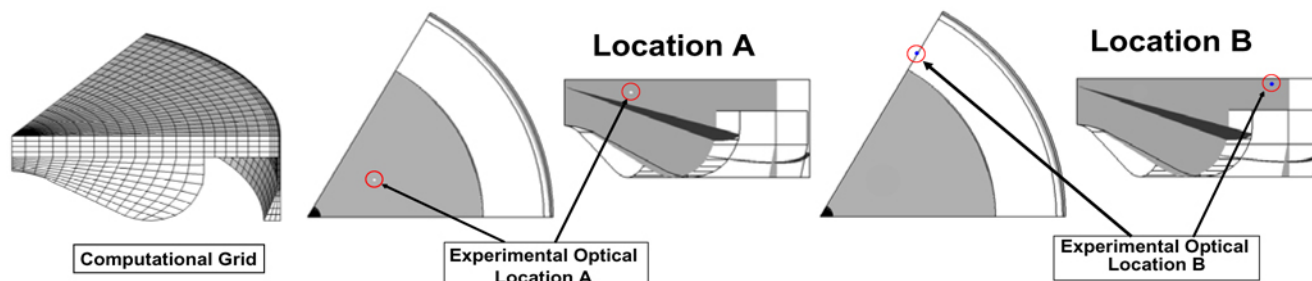


Figure 6. Computational grid with 8500 cells at BDC, crevice volume, shown at 16 °BTDC. Experimental measurement Locations A (bowl) and B (squish) depicted as dots relative to computational mesh

Also, corrections for residual trapped EGR and ambient humidity and carbon dioxide emission were not preformed because they were minimal, and concentration based measurements were not preformed in this study.

COMPUTATIONAL MODEL

Computations were performed using the KIVA-3v release 2 code [19] with improvements to many physical and chemistry models developed at the Engine Research Center ERC [20,21,22]. The KIVA-3v code was coupled with the CHEMKIN II solver for detailed chemistry calculations. A 39 species and 131 reaction mechanism for n-heptane [23] was used to simulate diesel fuel chemistry. Soot was predicted using a phenomenological soot model [24], based on the approach of Hiroyasu [25]. The soot model used in the present study used acetylene as an inception species, which allows the soot model to be coupled to the chemistry solver through the addition of 13 reactions involving acetylene. NO_x emissions were predicted using a reduced NO mechanism [6] consisting of 4 additional species and 12 reactions. The reduced NO mechanism is based on the Gas Research Institute (GRI) NO mechanism [26].

The spray model employed in this study uses the Lagrangian-Drop and Eulerian-Fluid (LDEF) approach. Because a detailed chemistry model is used, it is desirable to use a relatively coarse computational mesh; however, severe grid-size dependency has been observed in the LDEF spray models. This problem is most severe in the near nozzle region where the droplets are very close together and occupy only a small portion of the Eulerian mesh. Abraham [27] showed that accurate modeling of the near nozzle region required grid resolution on the order of the orifice diameter. However, it is not feasible from a computational time standpoint to solve engine problems on such a fine mesh. Furthermore, a fundamental assumption of the LDEF approach is that the volume fraction of droplets in each cell is small, that is, the void fraction is near one. Thus, if the mesh size is overly refined (i.e., mesh size equal to the droplet size) this assumption may be violated. In order to reduce the grid size dependency of the LDEF spray model and allow accurate spray simulation on a relatively coarse grid, the Gasjet model

of Abani et al. [21] was employed to model the relative velocity between the droplets and gas phase in the near nozzle region. Their approach assumes that the relative velocity between a droplet and the gas phase is equal to that between the droplet and a turbulent gas-jet with the same mass and momentum of that of the injected fuel.

Droplet breakup was modeled using the hybrid Kelvin Helmholtz (KH) - Rayleigh Taylor (RT) model described by Beale and Reitz [29]. The droplet collision model is based on O'Rourke's model; however, a radius of influence method was used to determine the possible collision partners to further reduce mesh dependency [21]. In addition, the collision model was expanded by Munnannur [30] to include a more comprehensive range of collision outcomes. The current implementation of the droplet collision model considers bounce, coalescence, and fragmenting and non-fragmenting separations. Droplet interactions with the wall are considered through a wall film submodel [31, 32], which includes the effects associated with splash, film spreading, and motion due to inertia.

A three dimensional computational grid with the crevice volume resolved was used, as shown in Figure 6. To reduce computational burden, a 60 degree sector mesh (corresponding to a single nozzle hole of the six hole injector of this study) with periodic boundaries was used for spray simulations and a 0.5 degree sector with periodic boundaries was used for HCCI simulations. The crevice above the top piston ring (between the piston and liner) was resolved and the region behind the ring was represented as an additional volume attached to the top ring crevice. Furthermore, the volumes associated with the head gasket, valve pockets, and pressure transducer crevices were added to the volume attached to the top ring crevice in order to give the correct compression ratio.

<figure 6 here>

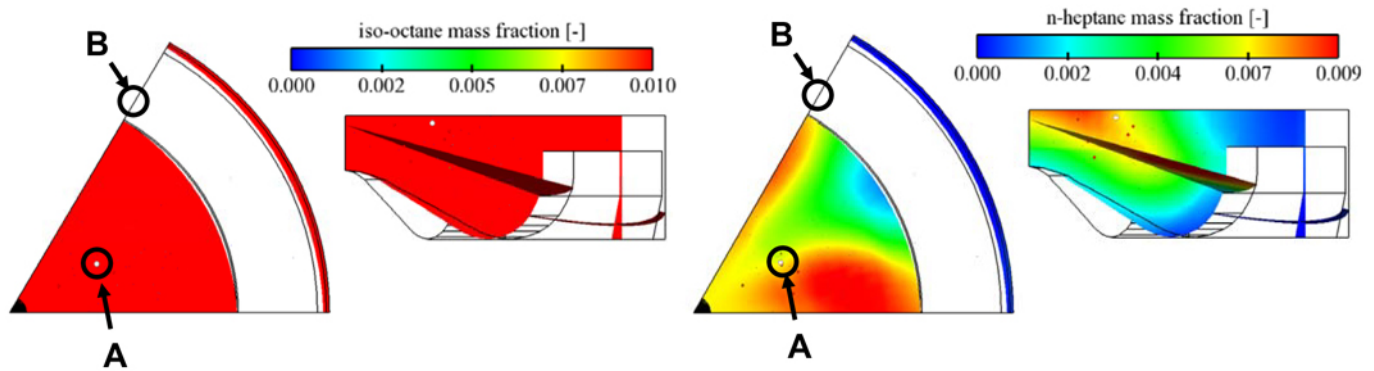


Figure 7. CFD predicted fuel distribution just prior to combustion, note that a large portion of the more reactive fuel component resides in the bowl. The A and B regions are the points of experimental optical access of Locations A (bowl) and B (squish) respectively

RESULTS AND DISCUSSION

OPERATING CONDITION

For all experiments and computations the engine was operated at the steady-state condition seen in Table 6. Using the injection strategy described in Table 6, a reactivity gradient is achieved within the fuel distribution. The CFD predicted distribution of iso-octane and n-heptane at -20 deg ATDC prior to combustion can be seen in Figure 7. The figure demonstrates that there is a uniform distribution of iso-octane and a inhomogeneous distribution of n-heptane, with the most reactive fuel mixture locally in the bowl.

Table 6. Experimental and computational engine conditions

Nominal IMEP (bar)	4.5
Engine speed (rev/min)	1300
IVC timing ($^{\circ}$ ATDC)	-143
EGR rate (%)	0
Equivalence ratio (-)	0.24
Intake temperature ($^{\circ}$ C)	32
Intake pressure (bar)	1.37
Total fuel (mg/cycle)	60.1
Percent gasoline of total fuel by mass	68 %
Mass of diesel fuel (mg/cycle)	19.2
Mass of gasoline (mg/cycle)	40.9
Diesel injection pressure (bar)	800
Diesel SOI1 ($^{\circ}$ ATDC)	-58
Diesel SOI2 ($^{\circ}$ ATDC)	-37
Fraction of diesel fuel in pulse 1	0.62
Diesel injection duration 1 ($^{\circ}$ CA)	5.07
Diesel injection duration 2 ($^{\circ}$ CA)	2.34

The sampled experimental engine-out emissions can be seen in Table 7. The emissions and performance for the 4.5 bar IMEP condition offer further evidence of the low emissions and high thermal efficiency potential of dual-fuel operation that was demonstrated at the same engine speed with mid load operation in References [14 and 15]. Thermal efficiency at the present conditions was diminished because of the non-optimized combustion phasing; however, changes to the fuel reactivity blend could be used to increase thermal efficiency through later combustion phasing.

Table 7. Engine out emissions and performance

NO _x	0.016 g/kW-hr
PM	0.002 g/kW-hr
HC	4.691 g/kW-hr
CO	15.047 g/kW-hr
CO ₂ (exhaust)	464.761 g/kW-hr
Brake power	8.12 kW
Brake Torque	59.66 N-m
COV of IMEP	2.14 %
ISFC	185.88 g/kW-hr
PRR	4.13 bar/deg
Indicated net thermal efficiency	45 %

Experimental and computational cylinder pressure and heat release were compared to confirm that the model adequately predicts the measured combustion process. As seen in Figure 8, the cylinder pressure and heat release rate of both the experiment and simulation agree well.

<figure 7 here>