

High Efficiency, Low Emissions RCCI Combustion by Use of a Fuel Additive

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ABSTRACT

Heavy-duty engine experiments were conducted to explore reactivity controlled compression ignition (RCCI) combustion through addition of the cetane improver di-tert-butyl peroxide (DTBP) to pump gasoline. Unlike previous diesel/gasoline dual-fuel operation of RCCI combustion, the present study investigates the feasibility of using a single fuel stock (gasoline) as the basis for both high reactivity and low reactivity fuels. The strategy consisted of port fuel injection of gasoline and direct injection of the same gasoline doped with a small volume percent addition of DTBP. With 1.75% DTBP by volume added to only the direct-injected fuel (which accounts for approximately 0.2% of the total fueling) it was found that the additized gasoline behaved similarly to diesel fuel, allowing for efficient RCCI combustion. The single fuel results with DTBP were compared to previous high-thermal efficiency, low-emissions results with port injection of gasoline and direct injections of diesel. The comparison between fueling strategies found that the higher volatility of gasoline enabled a reduction in the direct injection pressure from 800 (bar) with diesel to 400 (bar) with gasoline. At the tested conditions, the peak gross indicated based thermal efficiency was over 57%. The emissions trends and magnitudes of the single fuel strategy were also comparable to those of the diesel/gasoline dual-fuel strategy, and both engine-out NO_x and PM met EPA HD 2010 emissions mandates without aftertreatment. Also, the decreased low temperature heat release with the single fuel strategy was found to lower compression work and increased thermal efficiency by approximately 1% over the diesel/gasoline case. The results demonstrate that a very small percentage of an appropriate additive can be used to establish a sufficiently large reactivity gradient to match the performance of a dual fuel strategy when operated in the RCCI combustion regime.

INTRODUCTION

Rising fuel costs and a focus on the reduction of greenhouse gases has necessitated increased thermal 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 thermal efficiency and low emissions.

Many strategies have been investigated to meet the future requirements of clean, efficient internal combustion engines. Most of the current strategies utilize low temperature premixed combustion. Premixed strategies such as homogeneous charge compression ignition (HCCI), and its derivatives, premixed charge compression ignition (PCCI) and partially premixed combustion (PPC), have historically been very sensitive to fuel chemistry. For instance, recent experiments performed by Bessonette et al. [1] 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. [2] investigated dual-fuel PCCI operation as means for reducing the EGR requirements of PCCI strategies. Using premixed iso-octane and direct injection diesel fuel, they were able to operate in PCCI mode up to 12 bar IMEP. Furthermore, they showed that stratification of fuel reactivity

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(rather than only equivalence ratio) resulted in reduced rates of heat release and reasonable combustion noise.

Based on the work of Bessonette et al. [1] and Inagaki et al. [2], 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.

To explore the benefits of an optimized fuel for premixed combustion, Kokjohn et al. [3] and Hanson et al. [4] initially demonstrated a premixed dual fuel strategy in a heavy-duty engine. The optimized strategy is described in Reitz et al. [5] where the processes utilizes in-cylinder blending and control of fuel reactivity distributions. Splitter et al. [6] experimentally demonstrated that the resulting combustion process is staged, wherein combustion progresses from areas of locally high fuel reactivity to areas of locally low fuel reactivity. The staged combustion process results in significant extension of the duration of the premixed combustion event. The extension of the process has been experimentally demonstrated to enable high thermal efficiency, low emissions and low pressure rise rate operation for loads as high as 16 bar IMEP in Splitter et al. [7]. Although the charge preparation strategy used in these studies exhibits both reactivity and equivalence ratio stratification, modeling results by Kokjohn et al. [8] has suggested that the combustion process is dominated by the large reactivity gradient and not by local equivalence ratio effects.

Although these studies demonstrated operation of the reactivity controlled compression ignition (RCCI) strategy, they used dual fueling. It is of interest to explore whether the RCCI combustion process can be realized with use of a single fuel and an ignition improving additive. To explore this possibility the present study investigates a method to operate RCCI combustion though the use of a single fuel plus an additive to increase the cetane number of gasoline for the high reactivity stream. The fuel selected for this study is low reactivity commercially available pump gasoline, which is delivered to the engine by both port and direct injection systems. However, since a single fuel is unable to generate a reactivity gradient, the gradient is generated by blending a small volume percent addition of a reactivity enhancing additive to only the direct injected gasoline. The effect of the present single fuel reactivity enhanced strategy is compared to previous dual fuel operation results by Hanson et al. [4].

EXPIEREMENTAL SETUP

ENGINE

A heavy-duty 2.44 L Caterpillar 3401 Single-Cylinder, Oil-Test Engine (SCOTE) was used for all the engine tests, and

operated in its stock configuration. The specific engine lab setup is given in Figure 1, with the stock engine geometry and configuration given in Table 1.

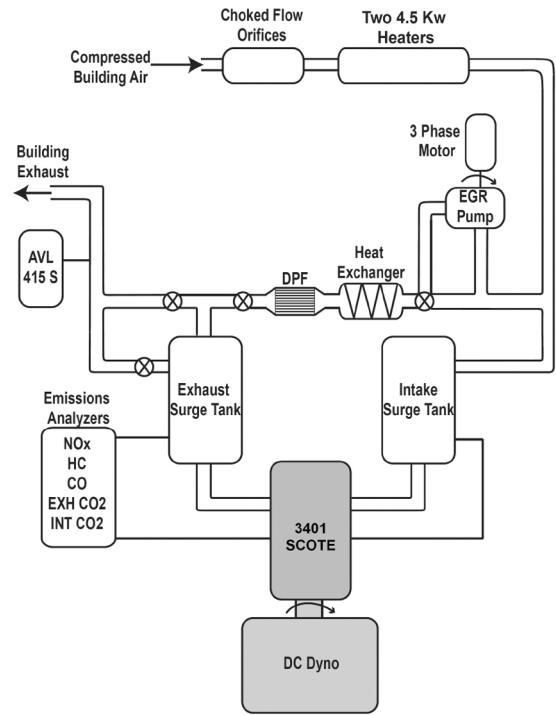


Figure 1. Diagram of the engine lab

Table 1. Test engine geometry

Base engine type	Caterpillar SCOTE
Bore x stroke (cm)	13.72 x 16.51
Connecting Rod Length (cm)	21.16
Squish height (cm)	0.157
Displacement (L)	2.44
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 (CA° ATDC Firing)	-335
Intake valve closing (CA° ATDC Firing)	-143
Exhaust valve opening (CA° ATDC Firing)	130
Exhaust valve closing (CA° ATDC Firing)	-355

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, and low pass filtered at the engines resonance mode as described by Eng [9]. 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 (mg/m^3) 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 was used for all tests. Table 4 shows the fuel properties obtained from an independent lab analysis.

REACTIVITY ENHANCEMENT ADDITIVE

To increase the reactivity of the direct injected fuel, a reactivity enhancing chemical was added to the 91 PON gasoline. Reactivity enhancing chemicals such as 2-ethylhexyl nitrate (2-EHN) and di-tert butyl peroxide (DTBP) have historically been used to increase fuel reactivity with diesel fuels [10, 11]. These select chemicals have been found to be advantageous at increasing reactivity (decreasing ignition delay) due to the presence of at least one low strength bond, which provides a low activation energy radical initiation initial step [12]. Optical combusting spray measurements by Higgins et al. [13], have demonstrated that when doped with fuels, cetane improvers transport with the base fuel in sprays; furthermore, their research demonstrated that although cetane improvers accelerate ignition, they have little effect on the energies of the combustion process of the base fuel.

Table 2. Gasoline fuel properties

Distillation Curve	ASTM D86
Initial Boiling Point ($^\circ\text{C}$)	38.9
Temperature 10% evaporated ($^\circ\text{C}$)	69.4
Temperature 50% evaporated ($^\circ\text{C}$)	105.0
Temperature 90% evaporated ($^\circ\text{C}$)	160.6
Final Boiling Point ($^\circ\text{C}$)	215.6
Lower Heating Value (MJ/kg)	43.2
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) (ppm)	4.6

For gasoline like fuels, research by Tanaka et al. [14] is particularly interesting. In that research, rapid compression machine experiments demonstrated that for gasoline-like fuels, 2% DTBP addition may have greater effect at decreasing ignition delay than 2% addition of 2-EHN. Similar research with high octane fuels by Alam et al. [15] demonstrated that DTBP can effectively be used to increase the cetane number of LPG to that comparable to diesel. These DTBP studies demonstrate that small additions of peroxide compounds can be used to enhance the reactivity of low reactivity fuels with improved effectiveness over 2-EHN, which have been shown by [10, and 11] to have better effectiveness in diesel fuels. Furthermore, low temperature combustion (LTC) research by Bunting et al. [16] and Ikes [17] have demonstrated that using 2-EHN can lead to increased NO_x emissions through the introduction of fuel borne NO_x . Since the present study considered gasoline, operated in an LTC regime, DTBP was used as the direct injection additive.

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

Previous research by Eng et al. [18] clearly demonstrated the effect of small additions of DTBP to gasoline-like fuels in low load HCCI operation. In that study DTBP addition was found to offer significant ignition delay and fuel consumption reductions.

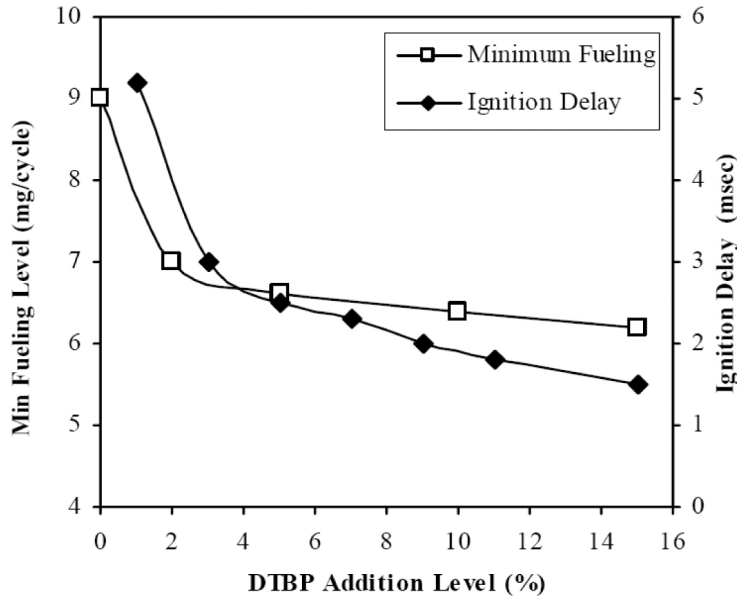


Figure 2. HCCI ignition delay and fueling requirement as a function of % DTBP addition to iso-octane [18].

The trend of Figure 2 shows a two mode piece-wise behavior of the ignition delay as a function of percent DTBP addition. As can be seen, the results of Eng et al. [18] show significant promise for the use of small percentage additions of DTBP (less than 3%) as a means to increase fuel reactivity.

INJECTION SYSTEM

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

Table 3. Port fuel injector specifications

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

Table 4. Common rail injector specifications

Number of holes	6
Hole Diameter (μm)	250
Included spray angle (°)	145
Injection pressure (bar)	400

REACTIVITY ENHANCEMENT STRATEGY

Based on the results of Eng et al. [18] in Figure 2, RCCI engine experiments using port injection of un-additized gasoline and direct injection of DTBP additized gasoline were conducted. DTBP was added to only the direct injected fuel in volume addition percentages of 3.5%, 1.75%, 0.75% and 0%. The direct injected portion of the fuel is approximately 10% of the total fueling, thus the percentages DTBP with respect to the total fueling are 0.35%, 0.175% and 0.075%. A diagram of the fueling strategy is seen in Figure 3.

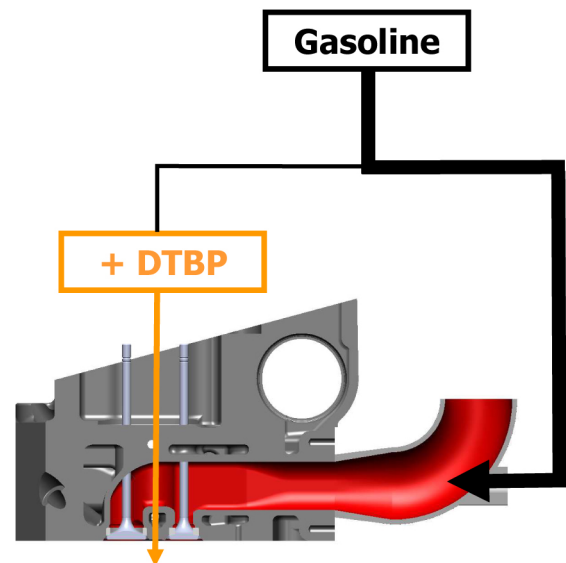


Figure 3. Section view diagram describing fuel delivery method of port and direct injection gasoline streams.

Note that DTBP is only added to the direct injected gasoline, but both the direct injected and port injected gasoline is from the same fuel stock.

RESULTS AND DISCUSSION

DIRECT INJECTION FUEL PRESSURE EFFECTS

Unlike previous dual fuel RCCI experiments by Hanson et al. [4] and Splitter et al. [6] the direct injection fuel pressure in the present study was reduced from 800 bar to 400 bar. The reduction of the direct injected fuel pressure was a result of using gasoline as compared to diesel fuel. Shi [19] has computationally demonstrated that the distillation characteristics of gasoline and diesel fuels result in significant differences in the spray structure for identical injection pressure. Specifically his results suggest that the high volatility of gasoline results in vapor formation faster, reducing spray penetration. In the present study his predictions were confirmed where initial testing at 800 bar direct injection pressure of gasoline resulted in higher NO_x emissions as compared to identical injection timing and pressure gasoline/diesel dual fuel results by Hanson et al. [4]. The results suggest that the 800 bar direct injected gasoline produces rich pockets that are required for PCCI but not RCCI. As the injection pressure was reduced to 400 bar low NO_x operation was realized due to improved charge preparation of the direct injected spray, and was used for all tests in the present study.

6 BAR IMEP OPERATION

Initially the effect of DTBP addition and single fuel operation was studied at the light load condition of 6 (bar) IMEP. The experimental operating conditions for this study are seen in [Table 5](#).

Table 5. 6 (bar) IMEP operating conditions

Total fueling (kg/hr)	2.72
Engine Speed (rev/min)	1300
EGR (%)	0
Intake Temperature ($^{\circ}\text{C}$)	40
Intake Pressure (kPa)	174.4
Exhaust Pressure (kPa)	184.1
Port fueling percentage (%)	90
Port injection pressure (bar)	4.14
Port Injection Timing (CA° ATDC)	-320
Direct injection pressure (bar)	400
SOI1 (first direct injection) Start of Injection Timing (CA° ATDC Firing)	-55
SOI2 (second direct injection) Start of Injection Timing (CA° ATDC Firing)	-36
SOI1 fuel percentage (%) (percent of direct injected fuel only)	60

The light load condition was selected for simplicity as the starting point because EGR was not required for low PRR operation. Operation without EGR enables investigation of

only the fuel reactivity effects without potentially confounding effects between EGR and DTBP, or EGR diluent effects that could result in unknown engine performance. DTBP percentages of 3.5%, 1.75%, 0.75%, and 0% addition by volume were tested. At the 6 (bar) condition, operation with PRR below approximately 10 bar/deg was achievable with the 3.5%, 1.75% and 0.75% DTBP addition fuels without the need for EGR. However, operation with 0% DTBP addition was unrealizable, and thus no cylinder pressure or emissions data were collected. The inability to operate without addition of DTBP demonstrates that a reactivity gradient is required for RCCI combustion and at the tested conditions a single low reactivity fuel is incapable of operating in a RCCI combustion mode.

As seen in [Figure 4](#), as the percentage of DTBP is decreased combustion is phased later in the cycle. This is most clear at the 0.75% DTBP addition level, where both later phasing of the high and low temperature heat releases is observed. As the percentage of DTBP is decreased the reactivity gradient of the in-cylinder blended fuel is decreased. This results in a globally and locally higher octane mixture, which resists combustion more than reactive mixtures. Also of note is the slight difference in the high temperature heat release of the 1.75% DTBP case. Although the fueling of all cases nominally constant, the 1.75% case inadvertently had approximately 2% lower fueling than the other tested cases, resulting in slightly lower heat release magnitude. [Table 6](#) displays the total fueling for each presented case to demonstrate the slight differences in fueling.

Table 6. 6 (bar) IMEP DTBP percentages fueling

DTBP (%)	0.75	1.75	3.5
Total Fueling (kg/hr)	2.70	2.66	2.72
Percent Port Fuel (%)	90	90	90

The combustion timings and trends of the DTBP sweep in [Figure 4](#) are consistent with those of Eng et al. [18], who used a single blended fuel. [Figure 2](#) shows that when the DTBP percentage is decreased beyond approximately 2%, significant combustion behavior differences occur. [Figure 5](#) provides further insight to the pressure and heat release rate trends of [Figure 4](#).