

Partial Fuel Stratification to Control HCCI Heat Release Rates: Fuel Composition and Other Factors Affecting Pre-Ignition Reactions of Two-Stage Ignition Fuels

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ABSTRACT

Homogeneous charge compression ignition (HCCI) combustion with fully premixed charge is severely limited at high-load operation due to the rapid pressure-rise rates (PRR) which can lead to engine knock and potential engine damage. Recent studies have shown that two-stage ignition fuels possess a significant potential to reduce the combustion heat release rate, thus enabling higher load without knock.

This study focuses on three factors, engine speed, intake temperature, and fuel composition, that can affect the pre-ignition processes of two-stage fuels and consequently affect their performance with partial fuel stratification. A model fuel consisting of 73 vol.% isooctane and 27 vol.% of n-heptane (PRF73), which was previously compared against neat isooctane to demonstrate the superior performance of two-stage fuels over single-stage fuels with partial fuel stratification, was first used to study the effects of engine speed and intake temperature. The results for PRF73 show that increasing engine speed from 1200 to 1600 rpm causes almost no change in ϕ -sensitivity, which is defined by the advancement of combustion phasing for an increase in equivalence ratio. Consequently, the maximum combustion pressure rise rate (PRR_{max}) can be reduced substantially with partial fuel stratification at this higher speed as it was at 1200 rpm. In contrast, increasing intake temperature from 60°C to 174°C eliminates the low temperature heat release of PRF73. Despite the single-stage ignition at this temperature,

PRF73 still shows a weak but definitive ϕ -sensitivity, likely due to the relatively strong intermediate temperature heat release before hot ignition. As a result, PRR_{max} was reduced modestly with partial fuel stratification. This PRF73 result is distinctively different from that of isooctane at the same intake temperature. To study the importance of fuel composition, PRF73 is compared with a low-octane, gasoline-like distillate fuel, termed Hydrobate, which could be readily produced from petroleum feedstocks. With the similar HCCI reactivity to PRF73, Hydrobate shows little difference in ϕ -sensitivity and performs similarly with partial fuel stratification compared to PRF73. This result indicates that it is the overall fuel HCCI reactivity, rather than the exact fuel composition, that determines the ϕ -sensitivity and the consequent performance with partial fuel stratification.

INTRODUCTION

Despite being called homogeneous charge compression ignition, HCCI combustion is not a homogeneous process. The inhomogeneity comes primarily from the thermal stratification that naturally occurs in the charge as a result of heat transfer between the charge gas and the cylinder walls, and in some cases, from imperfect mixing of fresh charge and residual gases [1, 2, 3]. The naturally occurring thermal stratification is critical to reduce pressure rise rates (PRR) of HCCI combustion, which otherwise would be as steep as that predicted by single-zone kinetic modeling [4]. Enhancing thermal stratification is thus a promising way to extend HCCI to higher load operation by moderating the overly fast PRR.

However, manipulating the thermal field inside cylinder is inherently difficult [5].

Due to the difficulties associated with adjusting thermal stratification to control the HCCI PRR (or heat release rate, HRR), interest has turned to mixture stratification, which is more straightforward to produce and control. Stratifying the mixture field has been studied via intake port fuel injection (PFI) [6, 7, 8, 9, 10, 11] and direct injection (DI) [12, 13, 14, 15, 16, 17, 18, 19, 20]. The PFI studies showed that some mixture stratification could be preserved at the start of combustion [6, 11], which, however, had little effect on the combustion process, except for the cases where a high-cetane (high autoignition reactivity) fuel, dimethyl ether (DME), was used [9, 10]. Similar results were also found when the fuel was directly injected early in the intake stroke [13, 18]. Such lack of impact with PFI and early DI is likely because the mixture stratification, weakened during the compression stroke by in-cylinder turbulence, was too weak at the start of autoignition to affect the combustion of the fuels used in these studies which had significantly lower cetane number (lower autoignition reactivity) than DME [6, 7, 8, 11]. In fact, many of the fuels had high octane numbers (above those of typical gasoline), and they may not have been sensitive to mixture stratification, as discussed below. On the other hand, better results have been achieved using fuels with autoignition characteristics between diesel fuel and gasoline (i.e. more reactive than gasoline but less reactive than diesel fuels), together with direct fuel injection in the latter part of the compression stroke [14, 16, 18, 19]. With such fuel/injection combinations, appropriate mixture stratifications can be produced, allowing the chemical kinetics of these fuels to significantly impact the HCCI HRR.

Suitable mixture formation and appropriate fuel autoignition chemistry are thus two critical elements for mixture stratification to be effective in reducing HCCI HRR [14, 18, 21]. Sjöberg and Dec argued that in order for mixture stratification to slow down the combustion process, the zones with different equivalence ratio (ϕ) need to autoignite at different timings, i.e. high- ϕ zones autoignite sooner and low- ϕ zones autoignite later [14]. The relationship between the autoignition timing and equivalence ratio was termed “ ϕ -sensitivity”. With a carefully designed experiment, the authors have shown that the ϕ -sensitivity of two-stage ignition fuels is much stronger than that of single-stage fuels [18, 21], i.e. the autoignition timing of two-stage fuels advances significantly as ϕ increases, while the autoignition timing of single-stage fuels does not. In subsequent partial fuel stratification tests [14, 18], where most fuel was premixed and a fraction of fuel (up to 22%) was directly injected late in the compression stroke, two-stage fuels, in particular, PRF73 (isooctane:n-heptane=73:27 by volume),

exhibited an exceptional ability to reduce the HRR at a high-load operating point while maintaining clean, efficient, and stable HCCI combustion. However, a single-stage fuel, isooctane, showed no tendency to reduce HRR under the test conditions. These results are consistent with those reported by Dahl et al. [16] and Wada and Senda [19]. Dahl et al. showed that with a similar amount of mixture stratification created by late DI, the PRR of a two-stage fuel (RON~50) was reduced more effectively than a single-stage fuel, gasoline (RON=100), in a high residual engine operated with negative valve overlap. Wada and Senda found that a fuel showing strong low-temperature heat release (LTHR), PRF45, had a larger PRR reduction than a fuel showing weak LTHR, PRF80. However, NO_x emissions in these studies were very high, over an order of magnitude higher than the US 2010 limit (0.27 g/kWh) [16, 19].

The essence of ϕ -sensitivity is the pre-ignition reaction rate varying as a function of equivalence ratio. However, equivalence ratio is only one factor that affects pre-ignition reaction rate. Other factors, such as temperature, pressure, and time available for reaction, are all important for pre-ignition progress. For example, LTHR, the sign of two-stage ignition which is commonly present for ϕ -sensitive fuels¹, is inhibited by increased temperature and engine speed, whereas it is typically enhanced by increased pressure. For a fuel with strong ϕ -sensitivity that performs well with partial fuel stratification at a base condition, understanding how changes in these parameters affect engine performance is important for the practical use of this technique. This work, following recent work comparing two-stage fuel (PRF73) vs. single-stage fuel (isooctane) [18], studies the effects of increased engine speed and intake temperature on the partial fuel stratification of PRF73. Also, since PRF73 is not a realistic fuel, a distillate fuel having similar HCCI reactivity (definition given in the subsection “PRF73 vs. Hydrobate” in Results and Discussion) to PRF73, is tested in the last section. The results help to elucidate the role of fuel chemical composition in determining the performance of partial fuel stratification.

EXPERIMENTAL

Engine Facility

The HCCI research engine used for this study was derived from a Cummins B-series six-cylinder diesel engine, which is a typical medium-duty diesel engine with a displacement of 0.98 liters/cylinder. Figure 1 shows a schematic of the engine, which has been converted for single-cylinder operation by deactivating cylinders 1-5. The active HCCI cylinder is fitted with a compression-ratio (CR) = 14 custom piston, as shown in Fig. 1b, which provides an open combustion chamber with

¹Two-stage ignition (or LTHR) is not absolutely necessary for a fuel to be ϕ -sensitive. Results from this work and a concurrent work [22] suggest that strong intermediate temperature heat release (ITHR) can also enable ϕ -sensitivity.

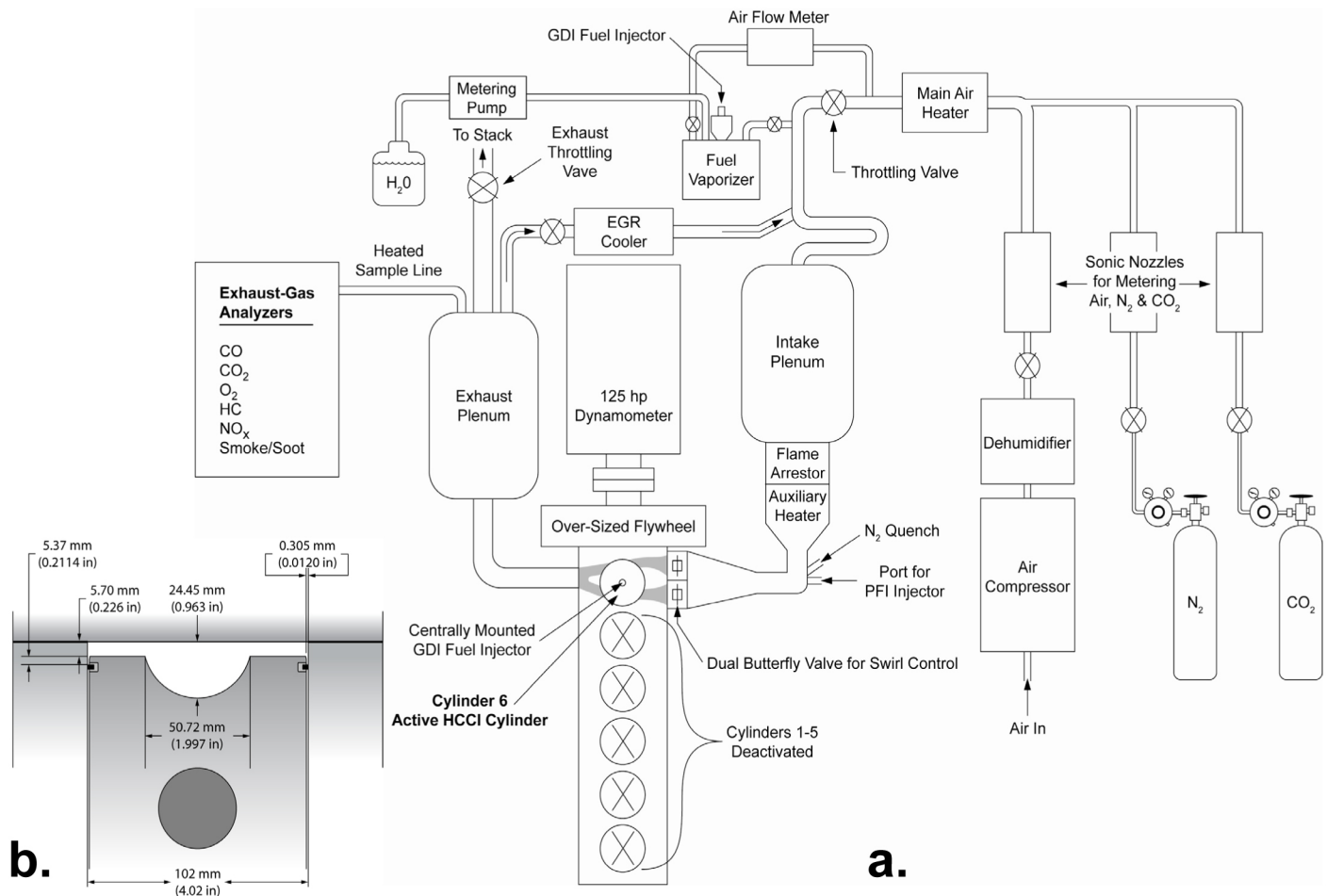


Fig. 1. Schematic of the HCCI engine facility (a) and combustion chamber geometry of the CR = 14 piston at TDC (b).

a large squish clearance and a quasi-hemispherical bowl. The engine specifications and operating conditions are listed in Table 1. The configuration of the engine and facility is identical to previous studies with PRF73 and isooctane [18].

To achieve partial fuel stratification, a combination of premixed and DI fueling was used. The premixed fueling system, shown at the top of the schematic in Fig. 1a, consists of a gasoline direct injector (GDI) mounted in an electrically heated fuel-vaporizing chamber and appropriate plumbing to ensure thorough premixing with the air and EGR upstream of the intake plenum. The DI fueling is achieved via a different GDI injector (Bosch, 8-hole) mounted centrally in the cylinder head. A positive displacement fuel flow meter was used to determine the total amount of fuel supplied.

Table 1. Engine Specifications

Displacement (single-cylinder)	0.981 liters
Bore	102 mm
Stroke	120 mm
Connecting Rod Length	192 mm
Geometric Compression Ratio	14:1
No. of Valves	4
IVO	0° CA ^a
IVC	202° CA ^a
EVO	482° CA ^a
EVC	8° CA ^a
Swirl Ratio	0.9
Fueling System	Fully Premixed / GDI
DI Injector	Bosch, 8-hole
Included Angle	70°
Hole Size	Stepped-hole, min. hole dia. = 0.125 mm
Injection Pressure	120 bar
Coolant/Oil Temperature	100°C

^a0° CA is taken to be TDC intake. The valve-event timings correspond to 0.1 mm lift.

The intake air was supplied by an air compressor and precisely metered by a sonic nozzle. Simulated EGR containing N_2 , CO_2 and H_2O in proportions that would result from complete combustion of the fuel (here called complete stoichiometric products or CSP) was used in this work. Nitrogen and carbon dioxide were supplied from gas bottles and metered with sonic nozzles. Water was supplied via a variable-speed rotary pump while the mass flow rate was determined by continuously monitoring the weight of the supply bottle on an electronic scale. The water was vaporized in the same chamber as the fuel. These EGR components were mixed with the air and fuel upstream the intake plenum to ensure sufficient mixing.

In this work, an equivalence ratio based on total charge mass, rather than air alone, is used, which is called charge-mass

equivalence ratio (ϕ_m) and is defined as
$$\phi_m = \frac{(F/C)}{(F/A)_{stoich}}$$
, where F/C is the mass ratio of fuel and total inducted charge gas (i.e. fresh air and EGR), and $(F/A)_{stoich}$ is the mass ratio of stoichiometric fuel/air mixture for complete combustion. This provides a convenient and consistent way to compare data with the same supplied energy content per unit charge mass (i.e., the same dilution level) for operating conditions with different fuels and different EGR levels. Note that ϕ_m is the same as conventional air-based ϕ when no EGR is used. It should also be noted that the air-based ϕ is < 1 for all conditions presented, so combustion is never oxygen limited.

The intake tank and plumbing were preheated to 50 - 60°C to avoid condensation of the fuel or water from the EGR gases. The intake temperature was precisely controlled by an auxiliary heater mounted close to the engine. The cooling water and lubricating oil were maintained at 100°C during the tests.

Data Acquisition

Cylinder pressure was measured with a transducer (AVL QC33C) mounted in the cylinder head approximately 42 mm off center. The pressure transducer signals were recorded at $1/4^\circ$ crank angle (CA) increments for 100 consecutive cycles. The cylinder-pressure transducer was pegged to the intake pressure near bottom dead center (BDC) where the cylinder pressure reading was virtually constant for several degrees. Intake temperatures were monitored using thermocouples mounted in the two intake runners close to the cylinder head. For all data presented, 0° CA is defined as TDC intake (so TDC compression is at 360°). This eliminates the need to use negative crank angles or combined bTDC, aTDC notation.

The crank angle of the 50% burn point (CA50) was used to monitor the combustion phasing on the fly during the experiment. CA50 was determined from the cumulative apparent heat-release rate (AHRR), computed from the

cylinder-pressure data (after applying a 2.5 kHz low-pass filter [23]). Computations were performed for each individual cycle, disregarding heat transfer and assuming a constant ratio of specific heats ($\gamma = c_p / c_v$) [24]. The average of 100 consecutive individual-cycle CA50 values was then used to monitor CA50 and for the CA50 values reported. The pressure-rise rates and ringing intensities (as defined in Ref. [25]) are computed from the same low-pass-filtered pressure data. For each cycle, the maximum pressure-rise rate was analyzed separately with a linear fit over a moving $\pm 0.5^\circ$ CA window. Similar to CA50, these individual-cycle values were then averaged over the 100-cycle data set.

A second method of computing the HRR was used for detailed HRR-curve analysis. Here, the heat release was computed in a more refined way from the ensemble-averaged pressure trace (with the 2.5 kHz low-pass filter applied), using the Woschni correlation for heat transfer [24] and a variable γ which updates as a function of burn duration. In using the Woschni correlation, the main coefficient, C , and a coefficient in the gas velocity term, C_2 , were adjusted for each combustion condition so that the heat release rate is zero before and after the combustion (constant coefficients were used for comparable operating conditions). Using the ensemble-averaged pressure trace has benefits from the standpoint of reduced noise on the heat-release traces. On the other hand, it can lead to overestimated burn durations if the cycle-to-cycle variations are large. However, for the condition where this was applied, the phasing was fairly stable with the standard deviation of CA50 over 100 fired cycles averaging $< 1.2^\circ$ CA. Moreover, the results of this detailed HRR analysis are mainly used for comparisons of the early part of the heat release, leading up to hot ignition. Since these early autoignition reactions persist for $15^\circ - 25^\circ$ CA, the relatively small cycle-to-cycle variation in CA50 will have little effect.

Exhaust emissions data were also acquired, with the sample being drawn just downstream of the exhaust plenum using a heated sample line (see Fig. 1a). CO , CO_2 , HC , NO_x , and O_2 levels were measured using standard exhaust-gas analysis equipment. Soot emissions were not measured here. However, negligible soot emissions had been detected in previous work under similar operating conditions [18].

Test Conditions

This study focuses on three parameters that could affect pre-ignition reaction rate and consequently, ϕ -sensitivity and HCCI performance with partial fuel stratification. The test conditions are listed in Table 2. In each case, ϕ -sensitivity is first tested, followed by partial fuel stratification tests.

Table 2. Test Conditions

Test	Engine speed	T_{in}	Fuel
1600 vs. 1200 rpm	—	60°C	PRF73
$T_{in} = 174$ vs. 60°C	1200 rpm	—	PRF73
PRF73 vs. Hydrobate	1200 rpm	60°C	—

The ϕ -sensitivity test is conducted in a carefully designed experiment to isolate fuel chemistry effect from thermal and residual-gas effects on ignition timing as ϕ is varied. The latter effects primarily result from wall heating and the varying temperature and composition of residual-gas at different ϕ . An alternative firing method is used, as in Ref. [18, 21], where 19 cycles fire at a baseline ϕ , followed by 1 cycle firing at the ϕ of interest, for which the data are acquired. The engine operating conditions, including intake temperature, intake pressure, CSP level, etc., are kept constant throughout the ϕ -sweep. The only change is the fueling rate of the 20th cycle.

To change the fueling rate from cycle to cycle, direct fuel injection is required. However, several issues need to be addressed. First, since DI fuel vaporization may significantly alter the in-cylinder thermal conditions and mixture homogeneity, most fuel is premixed with air in the fuel vaporizer and only a small portion is direct injected to make up the required ϕ . For example, for a baseline ϕ (or ϕ_m) of 0.42, 80% of the baseline fuel (corresponding to $\phi = 0.34$) is premixed. DI is then used to add $\phi = 0.08$ to reach the ϕ of 0.42. For a test $\phi > 0.42$, more DI ($\phi > 0.08$) is added to the same amount of premixed fueling ($\phi = 0.34$). Similarly, for $\phi < 0.42$, less DI ($\phi < 0.08$) is added. Note that the test ϕ can not be lower than 0.34 in this case. Also, the cooling from DI fuel vaporization changes slightly as ϕ is varied. Second, in order to generate as homogeneous of a mixture as possible, an early DI timing, 40°CA, is used. This timing was determined from a preliminary DI timing sweep at the baseline ϕ to ensure mixture homogeneity and no piston wetting by comparing the performance with the fully premixed case.

The partial fuel stratification tests, as mentioned earlier, required premixing most fuel with air in the intake system and directly injecting a small fraction of fuel in the *latter* part of the compression stroke. To evaluate the performance with partial fuel stratification, both DI timing and DI fraction sweeps were conducted, as in Ref. [18]. For the DI timing sweep, the DI fraction was held constant, and for the DI fraction sweep, the DI timing was held constant. For both sweeps, T_{in} and ϕ_m were held constant and CSP was adjusted

to maintain a constant CA50. All data were taken at an intake pressure of 100 kPa.

It should be pointed out that although the performance results are not reported in each case, care was taken to make sure that the data were collected under the conditions where the HCCI combustion was clean ($ISNO_x < 0.1$ g/kWh), complete (combustion efficiency $> 95\%$), stable ($COV_{IMEP} < 2\%$), and non-knocking (ringing intensity < 5 MW/m²), unless otherwise noted.

RESULTS AND DISCUSSION

PRF73: 1200 vs. 1600 rpm

Engine speed is an important parameter that can affect pre-ignition reactions as it changes the time available for the reactions. Increasing engine speed generally inhibits LTHR, as shown in Refs.[26, 27, 28, 29]. Thus, it could reduce ϕ -sensitivity and affect the performance with partial fuel stratification. To test this effect, engine speed was incrementally increased above the 1200 rpm baseline speed used in Ref. [18] for PRF73. During this process, the combustion phasing (CA50) was kept at 371°CA by reducing CSP and keeping T_{in} at 60°C. 1600 rpm was reached where almost no CSP was required to maintain the combustion phasing.

ϕ -Sensitivity of PRF73 at 1600 rpm

The ϕ -sensitivity of PRF73 at 1600 rpm is shown in Fig. 2, together with the result at 1200 rpm from Ref. [18]. Since ignition timing is more relevant than main combustion phasing², the ϕ -sensitivity is shown in terms of 10% burn point, CA10³, rather than CA50. A lower range of ϕ was used at 1600 rpm to obtain a similar range of combustion phasing as at 1200 rpm. This avoids excessive engine knock because the ringing intensity is proportional to dP/dt [25]. At 1600 rpm, the time (dt) for the pressure rise event becomes shorter, which requires dP to be lower, i.e. less fuel energy, for a given ringing intensity at the same CA50.

PRF73 shows a strong ϕ -sensitivity at 1600 rpm, with a similar $\Delta(CA10) / \Delta(\phi_m)$ slope to that at 1200 rpm. This indicates that the pre-ignition chemistry is still active at this speed. As shown in Fig. 3, LTHR is still present at 1600 rpm. Also the cumulative heat release during the first-stage ignition accounts for a similar percentage of the total cumulative heat release at both speeds, 3.8% at 1600 rpm and 4.2% at 1200 rpm. Moreover, the heat release from 353 to 363°CA, the so called intermediate temperature heat release

²Ignition timing is directly determined by autoignition chemistry which depends on ϕ for these fuels, while CA50 is determined by both ignition timing and burn duration, and the latter is mostly a function of thermal stratification rather than ϕ .

³The CA10 reported here is determined from the apparent heat release in a similar manner to that described in the Experimental section for CA50. For two-stage ignition, the CA10 refers to the 10% burn point of the main combustion where the calculation starts at the minimum point between the LTHR peak and main combustion peak on the HRR curve. Thus CA10 is representative of the main hot-ignition point.

(ITHR) which is defined as the heat release from the minimum point after LTHR to roughly 5°CA before CA10, is remarkably similar at the two speeds. The strong ϕ -sensitivity predicts that partial fuel stratification would still work well at 1600 rpm.

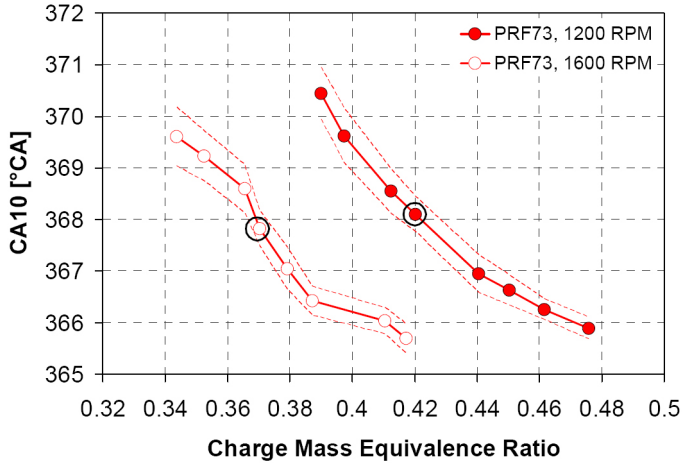


Fig. 2. ϕ -sensitivity of PRF73 at 1600 and 1200 rpm. Black circles indicate baseline points. Baseline at 1600 rpm: $\phi_m = 0.37$, intake $[O_2] = 20.7\%$, $CA_{50} = 371^\circ CA$. Baseline at 1200 rpm: $\phi_m = 0.42$, intake $[O_2] = 16.7\%$, $CA_{50} = 371^\circ CA$. Dashed lines correspond to one standard deviation earlier or later than the mean. $T_{in} = 60^\circ C$ at both speeds.

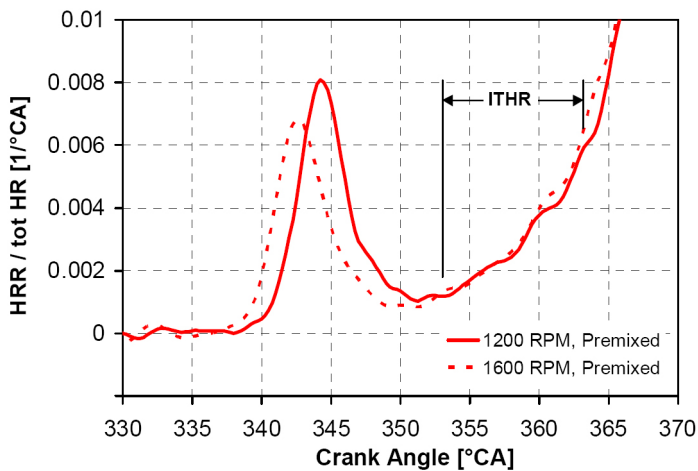


Fig. 3. Pre-ignition heat release (LTHR and ITHR) of PRF73 at 1600 and 1200 rpm. Fully premixed charge. At 1600 rpm, $\phi_m = 0.39$, $CA_{50} = 371^\circ CA$, $T_{in} = 60^\circ C$, intake oxygen concentration = 20.2%. At 1200 rpm, $\phi_m = 0.44$, $CA_{50} = 371^\circ CA$, $T_{in} = 60^\circ C$, intake oxygen concentration = 16.5%.

The similar ϕ -sensitivity at 1200 rpm and 1600 rpm, and the similar pre-ignition heat release seem to suggest that engine speed is not important for the pre-ignition chemistry. This is

inconsistent with the rules in chemical kinetics because from 1200 rpm to 1600 rpm the time available for reactions is reduced by 25%. However, at 1600 rpm, CSP diluents were mostly removed in order to maintain the similar combustion phasing, which resulted in a 22% increase in intake oxygen concentration. The increased oxygen concentration tends to accelerate pre-ignition reaction rate, thus offsetting the effects of the reduced reaction time.

The global reaction rate for pre-ignition reactions can be expressed as

$$d[Prod] = k[F]^m [O_2]^n dt$$

Eq. 1

where $d[Prod]$ is the amount of product being formed, k is the rate constant, $[F]$ and $[O_2]$ are the fuel and oxygen concentrations, m and n are the order of reaction with respect to fuel and oxygen, and dt is the time available for the reaction to occur. Assume that $d[Prod]$ is proportional to the cumulative pre-ignition heat release, $Q_{LTHR+ITHR}$, and $[F]^m$ is proportional to the total cumulative heat release from the combustion, Q_T . The latter is valid because Q_T equals the fuel energy for complete combustion, which is proportional to $[F]$ times heating value of fuel. Also m is ~ 1 , as reported for isooctane [30] around 700 - 900 K. Therefore, Eq. 1 becomes

$$\frac{Q_{LTHR+ITHR}}{Q_T} \propto \frac{d[Prod]}{[F]^m} = k[O_2]^n dt$$

Eq. 2

The similar $Q_{LTHR+ITHR}/Q_T$ in Fig. 3 for the two engine speeds suggests that the $k[O_2]^n dt$ term in Eq. 2 should also be similar at the two speeds. Given the 25% decrease in dt and 22% increase in $[O_2]$ from 1200 to 1600 rpm, Eq. 2 requires $n \approx 1$ in order to cancel the changes in dt and $[O_2]$, and to produce the similar $Q_{LTHR+ITHR}/Q_T$. Note that due to the dynamic reaction conditions in the engine cylinder, the value of n does not necessarily agree with those obtained from chemical kinetics experiments, e.g. [30], which showed $n \sim 1.8 - 2.8$ for isooctane at 700 - 900 K.

Besides the higher oxygen concentration, other factors may also contribute to cancelling the effect of reduced time available for reaction on the HCCI reaction. It is noted that the compressed-gas temperature at 335°CA (right before LTHR) is about 20 K higher at 1600 rpm, which is due to the higher γ resulting from lower ϕ and less CSP usage, as well as the reduced heat transfer losses (per charge mass) at higher engine speed. The higher compressed-gas temperature works together with the increased O_2 concentration to prevent the combustion phasing from retard at the higher speed. The timing for LTHR is in fact more advanced at 1600 rpm. However, due to the negative-temperature-coefficient (NTC) behavior of hydrocarbon oxidation, LTHR is inhibited by the