

Influence of Fuel Autoignition Reactivity on the High-Load Limits of HCCI Engines

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ABSTRACT

This work explores the high-load limits of HCCI for naturally aspirated operation. This is done for three fuels with various autoignition reactivity: *iso*-octane, PRF80, and PRF60. The experiments were conducted in a single-cylinder HCCI research engine (0.98 liter displacement), mostly with a CR = 14 piston installed, but with some tests at CR = 18. Five load-limiting factors were identified: 1) NO_x-induced combustion-phasing run-away, 2) wall-heating-induced run-away, 3) EGR-induced oxygen deprivation, 4) wandering unsteady combustion, and 5) excessive exhaust NO_x.

These experiments at 1200 rpm show that the actual load-limiting factor is dependent on the autoignition reactivity of the fuel, the selected CA50, and in some cases, the tolerable level of NO_x emissions. For *iso*-octane, which has the highest resistance to autoignition of the fuels tested, the NO_x emissions become unacceptable at IMEP_g = 473 kPa. This happens before wandering and unsteady combustion becomes an issue for IMEP_g > 486 kPa. The NO_x is caused by high peak-combustion temperatures resulting from the high intake temperature required for this low-reactivity fuel. *iso*-octane operation with a CR = 18 piston reduces the intake-temperature requirement. Consequently, the exhaust NO_x issue vanishes while the IMEP_g can be increased to 520 kPa before wall-heating-induced run-away become an issue. For a very reactive fuel like PRF60, large amounts of EGR are required to control the combustion phasing. Therefore, the maximum IMEP_g becomes limited at 643 kPa by the available oxygen as the EGR gases displace air. A fuel of intermediate reactivity, PRF80, exhibits the highest IMEP_g for the conditions of this study – 651 kPa. For this fuel, the maximum IMEP_g becomes limited by NO_x-induced run-away. This happens because even small amounts of NO_x recycled via residuals enhance the autoignition sufficiently to advance the ignition point. This leads to higher peak-combustion temperatures and more NO_x formation, thus making a very rapid run-away situation inevitable.

INTRODUCTION

The homogeneous charge compression ignition (HCCI) combustion process offers good fuel economy and very low nitrogen-oxide (NO_x) and particulate emissions. Therefore, engine manufacturers are considering HCCI combustion as one option to improve the efficiency of the spark-ignited gasoline engine, and also to reduce NO_x aftertreatment requirement for the latest generations of compression-ignited diesel engines. However, several technical difficulties need to be resolved before HCCI can be widely implemented in production engines. Among these, controlling the combustion phasing and increasing the power output while maintaining acceptable pressure-rise rates (PRR) continue to be major issues.

The autoignition quality of the fuel is an important parameter impacting the design of HCCI engines and the methods used to control the combustion phasing and the heat-release rate (HRR). HCCI operation has been demonstrated for a variety of fuels that have autoignition qualities spanning a wide range [1,2,3,4].

The autoignition quality can also influence the observed power output. For example, Ref. [5] demonstrates that PRF80 (a 80/20 volume mix of the primary reference fuels, *iso*-octane and *n*-heptane) can provide substantially higher indicated mean effective pressure (IMEP_g) than *iso*-octane when operated with a fuel/air-equivalence ratio (ϕ) of 0.40. This happens because PRF80 is more reactive and can be operated with a lower intake temperature (T_{in}) compared to *iso*-octane. A lower T_{in} leads to higher charge density and thus more inducted fuel when ϕ is kept constant. In addition, the data in Ref. [5] show that the cycle-to-cycle variations increase with combustion-phasing retard for both fuels, but also that the two-stage autoignition PRF80 has less cycle-to-cycle variation for a given amount of combustion-phasing retard. This is an important aspect that potentially can help to reach higher loads since extensive combustion-phasing retard is required in order

to keep the PRR below acceptable limits as the fueling is increased.

For a given displacement, the power output is proportional to both the brake mean effective pressure (BMEP) and the engine speed. However, to limit the parameter space, this study compares the performance of the different fuels at a fixed engine speed of 1200 rpm and naturally aspirated operation. Both the engine speed and the intake-boost pressure influence the observed autoignition reactivity and the amount of low-temperature heat release (LTHR) [6]. Because of this, the differences between the fuels may grow or diminish for operation with boost and at other engine speeds. Also, the choice of compression ratio (CR) influences the performance of the engine/fuel combination [7,8,9]. These aspects should be considered when comparing the data presented here with data acquired at other operating conditions in other engines.

SCOPE AND OBJECTIVES

The main objective of this study is to experimentally investigate how the choice of fuel influences the maximum obtainable IMEP_g while maintaining steady operation with acceptable PRR and NO_x emissions. Furthermore, and equally important, the load-limiting factor(s) will be identified for each operation condition. The fuels considered are iso-octane, PRF80 and PRF60. The engine speed was 1200 rpm and the engine was operated with $P_{in} = 100$ kPa, simulating naturally aspirated conditions. CR = 14 was used for all three fuels. In addition, iso-octane was also evaluated at a higher CR of 18 for which high-load data have been previously published by the authors [10].

Following the description of the experimental setup, data acquisition and analysis, this paper covers six areas:

1. The three fuels are compared at the same degree of charge dilution to highlight combustion-process differences that arise from variations in the autoignition reactivity.
2. The importance of adjusting the combustion phasing (CA50) with load is demonstrated for PRF80.
3. The fundamentals responsible for the beneficial heat-release-smoothing effects of combustion-phasing retard are reviewed using multi-zone modeling.
4. With adjustments of CA50 to maintain a moderate PRR of 5 bar/°CA¹, the IMEP_g is pushed to the limit for each fuel.
5. A detailed examination is made of each fuel separately, whereby the load-limiting factors are identified and the load limits are explored for operation also at PRR = 3 and 7 bar/°CA.

¹ At the conditions studied, the engine knock/ringing is not considered unacceptable until PRR > 8 bar/°CA.

6. Based on the potential importance of NO_x feedback via residuals, the sensitivity of CA50 to NO_x addition is measured for each fuel. These results are presented in the Appendix.

EXPERIMENTAL SETUP

The engine used for this study is based on a Cummins B-series diesel engine, which is a typical medium-duty diesel engine with a displacement of 0.98 liters/cylinder. A schematic of the setup is shown in Fig. 1. The configuration of the engine and facility is nearly the same as for previous studies [e.g. 5,6,10-12], except for one substantial change: a new CR = 14 piston is used. As the schematic in Fig. 1 shows, this piston features a hemispherical bowl in the center. Compared to the shallower scallop of the piston used previously, this results in slightly higher surface-to-volume ratio at TDC. In addition, some squish flow can be expected. Because of this, slightly higher heat-transfer rates were anticipated. However, both motored and fired operation indicated a minimal effect. For example, the reduction of the thermal efficiency was measured to less than 0.2% (i.e. less than 0.5% increase of the fuel consumption). The reason for the change in piston geometry was to facilitate the concurrent testing of a variable-valve timing (VVT) system (not reported here). In case of an accidental valve impact onto the piston, the new piston design reduces the risk of bending of the valve stem as the valve is being pushed up against the hydraulic pressure. However, for all tests presented here, the traditional camshaft - push rod - rocker arm arrangement was used. The custom-design piston provides a small top-land-ring crevice, amounting to only 2.1% of the top-dead-center (TDC) volume, including the volume behind the top piston ring.

For all operating conditions, except for the NO_x sensitivity measurements presented in the Appendix, the engine was fueled using a fully premixed fueling system featuring an electrically heated fuel vaporizer. The intake gases were metered with separate sonic nozzles for air, CO₂, and N₂. To supply H₂O to the intake charge, a metering pump was used to draw water from a bottle placed on a digital scale and feed it into the fuel vaporizer. An auxiliary air heater mounted close to the engine was used to precisely control the intake temperature (Fig. 1). Engine specifications are listed in Table 1. A detailed description of the engine modifications for HCCI operation can be found in Ref. [12].

Cylinder pressure measurements were made with a transducer (AVL QC33C) mounted in the cylinder head approximately 42 mm off center. The pressure transducer signals were digitized and recorded at ¼° crank angle (CA) increments for at least 100 consecutive cycles. (Except for the NO_x sensitivity data, for which 40 alternate-fire cycles were recorded.) The reported PRRs are computed based on the maximum pressure-rise rate averaged over at least 100 cycles (each cycle is analyzed separately with a linear fit over a moving

TABLE 1. Engine Specifications

Displacement (single-cylinder).....	0.981 liters
Bore.....	102 mm
Stroke.....	120 mm
Connecting Rod Length.....	192 mm
Nominal Geometric Compression Ratio.....	14:1
No. of Valves.....	4
IVO.....	0°CA*
IVC.....	202°CA*
EVO.....	482°CA*
EVC.....	8°CA*
Intake Air Swirl Ratio, Both Ports Combined.....	0.9

* 0°CA is taken to be TDC intake, so TDC combustion is 360°CA. The same camshaft is used as in previous studies, but the presented numbers for valve closing and opening are slightly adjusted to better represent the timing for 0.1 mm lift.

$\pm 0.5^\circ\text{CA}$ window after low-pass filtering ($< 2.5\text{ kHz}$)). Similarly, the 50% burn point (CA50) was first computed from the low-pass filtered pressure trace for each individual cycle (without heat-transfer correction), and then averaged. However, it should be noted that for operation with the presence of LTHR, the LTHR is excluded when the cumulative heat release is computed. Effectively, the reported combustion phasings refer to

CA50 for the main combustion event, starting at the crank angle of minimum heat-release rate between the low- and high- temperature combustion events. Presenting the data referring to the main combustion event alone is considered more relevant from the standpoint of quantifying the timing of the main combustion event.

Charge temperatures during the closed part of the cycle (*i.e.* compression/expansion) are computed using the ideal-gas law in combination with the measured pressure (ensemble-averaged over at least 100 cycles, except for Fig. 24b), the known cylinder volume, and the trapped mass. The average molecular weight used for the calculation during the compression stroke corresponds to that of the trapped gases - including fresh gases, EGR and retained residuals, and the fuel. During the combustion event, and in proportion to the mass fraction burned, the molecular weight gradually changes to that of the measured exhaust composition. This exhaust molecular weight is then used for the remainder of the expansion stroke.

The fuels used were blends of the primary reference fuels (PRF), iso-octane and n-heptane. The PRF blends allow selection of autoignition reactivity by varying the blending proportions. They are also fairly volatile, and this facilitates the charge preparation. Table 2 shows the fuel compositions and other relevant parameters.

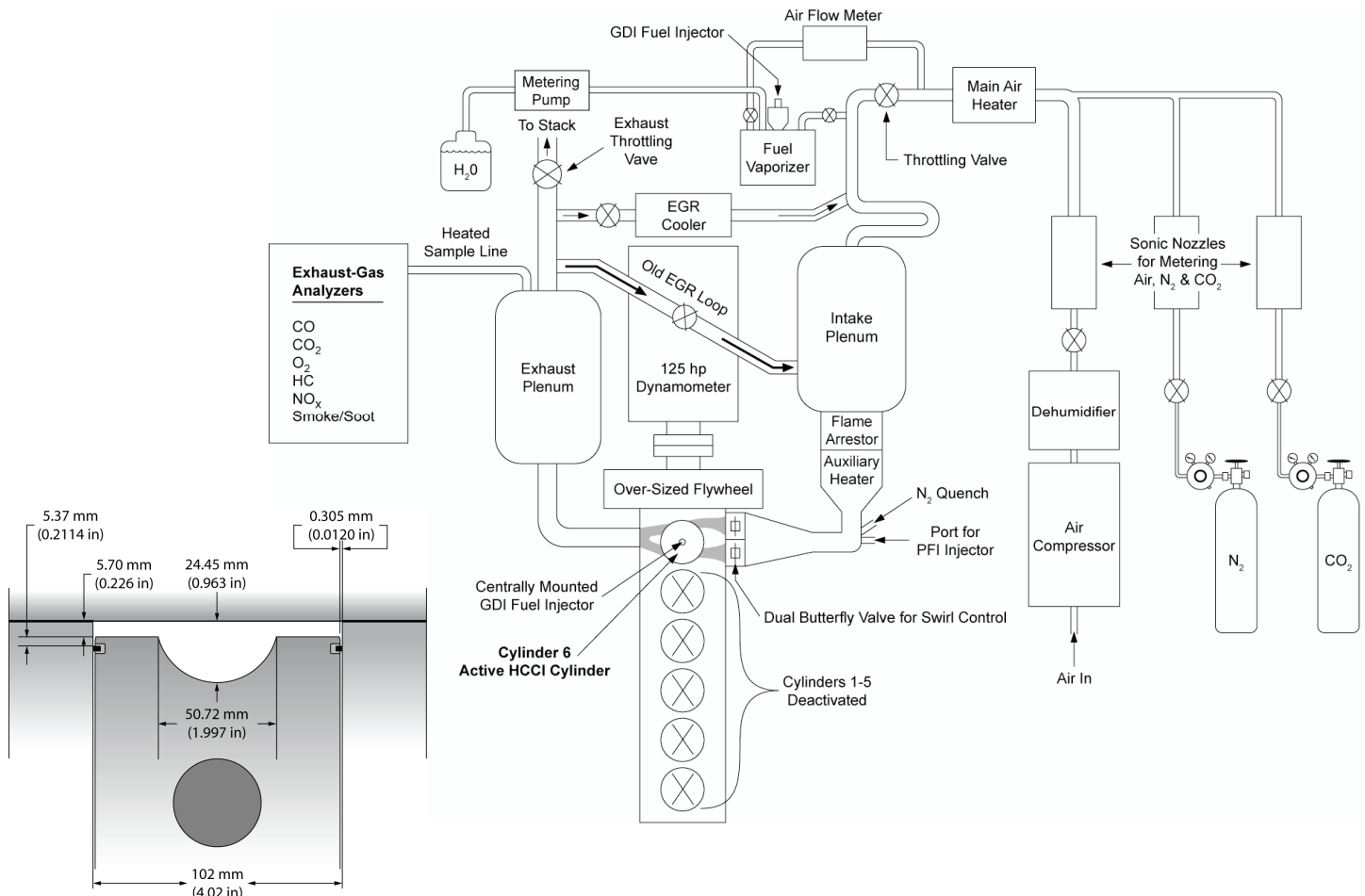


Figure 1. Schematic of the HCCI engine facility, and combustion-chamber dimensions at TDC with the CR = 14 piston.

TABLE 2. Fuel Properties

Fuel	Iso-Octane	PRF80	PRF60
Iso-Octane %vol.	100	80	60
n-Heptane %vol.	0	20	40
C-atoms	8	7.78	7.57
H-atoms	18	17.56	17.14
Molecular weight	114.23	111.15	108.21
A/F Stoichiometric	15.13	15.14	15.15
Lower heating value for gas-phase fuel [MJ/kg fuel]	44.65	44.71	44.76
Lower heating value for stoichiometric charge [MJ/kg air-fuel mixture]	2.769	2.770	2.772
Boiling point / range at 1 atm [°C]	99.2	98.4* - 99.2	98.4* - 99.2

* The boiling point for pure n-heptane is 98.4°C.

Because HCCI combustion is very sensitive to temperature, the engine coolant and oil were both fully preheated to 100°C before starting the experiments. In addition, the intake tanks and plumbing were preheated to at least 50°C to avoid any condensation of the water supplied with the simulated EGR. 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.

BASIC EGR CONSIDERATIONS

In an engine operating lean with complete combustion, EGR consists of air and complete stoichiometric products (CSP). Typically there are combustion inefficiencies, and this generates trace species like carbon monoxide (CO), hydrocarbons (HC) and partially-oxidized hydrocarbons. In addition, NO_x can be formed if the combustion temperatures are sufficiently high. All these species can potentially influence the autoignition. To avoid the influence of these combustion by-products, and to simplify the interpretation of the data, this study uses simulated EGR (except for Figs. 5 and 6, which use real EGR via the “old EGR loop” shown in Fig. 1). The simulated EGR consists of a mixture of air with the three components of complete stoichiometric products (CSP),

TABLE 3. Composition of simulated EGR (CSP) for all three fuels (% mole fraction). Average molecular weight (M) is also given.

Fuel:	Iso-Octane	PRF80	PRF60
CO ₂	12.47	12.45	12.44
H ₂ O	14.03	14.05	14.08
N ₂	73.50	73.49	73.48
M	28.71	28.71	28.70

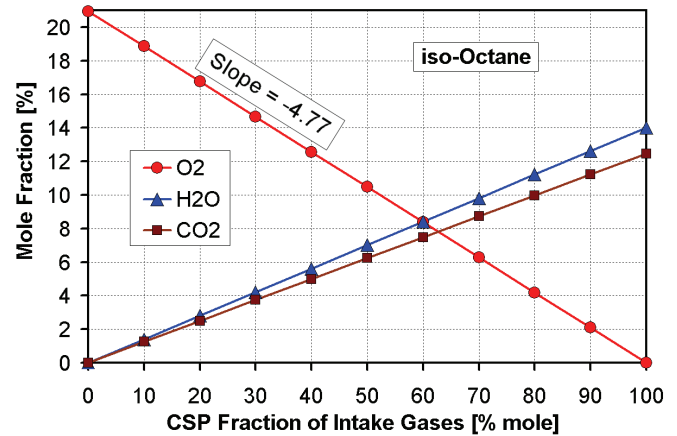
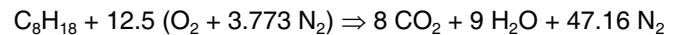


Figure 2. Intake mole fraction of O₂, CO₂, and H₂O as a function of CSP mole fraction. Excluding fuel.

namely CO₂, H₂O and N₂. The relative proportions of these components vary slightly with fuel-type and can be computed based on the average number of C and H atoms listed in Table 2. For iso-octane, complete stoichiometric combustion can be written as:



where atmospheric argon and CO₂ have been lumped into the atmospheric N₂, following Ref. [13]. For complete combustion with $\phi = 1$, the gas composition (excluding fuel) changes from: 20.95% O₂ and 79.05% N₂ for intake air, to products with 12.47% CO₂, 14.03% H₂O and 73.50% N₂ for wet exhaust. This exhaust composition will be referred to as CSP. As Table 3 shows, the CSP composition varies only marginally with changes in PRF number.

To simulate various amounts of EGR, air and CSP were metered into the intake system to form a homogeneous mixture. Figure 2 demonstrates how the intake gas composition changes with CSP mole fraction. The mole fractions of CO₂ and H₂O ([CO₂] and [H₂O]) both increase linearly with increasing fraction of CSP, while [O₂] decreases linearly. When evaluating data with simulated EGR, it can be beneficial to consider the intake [O₂]. For such cases, Fig. 2 can be used to convert the given %CSP to [O₂].

RESULTS

INTAKE TEMPERATURE CONSIDERATIONS

This study compares the load capabilities of three fuels with different autoignition reactivities. As discussed in the introduction, the intake-temperature requirement can influence on the observed IMEP_g. Therefore, the intake temperatures that were used in this study are discussed first.

Plotted in Fig. 3b is the T_{in} that was used for each fuel type at a fueling rate corresponding to a charge²/fuel mass ratio (C/F) of 34.4 and a PRR of 5 bar/°CA. Iso-

² The charge mass is the sum of the supplied air and CSP constituents, excluding the fuel.

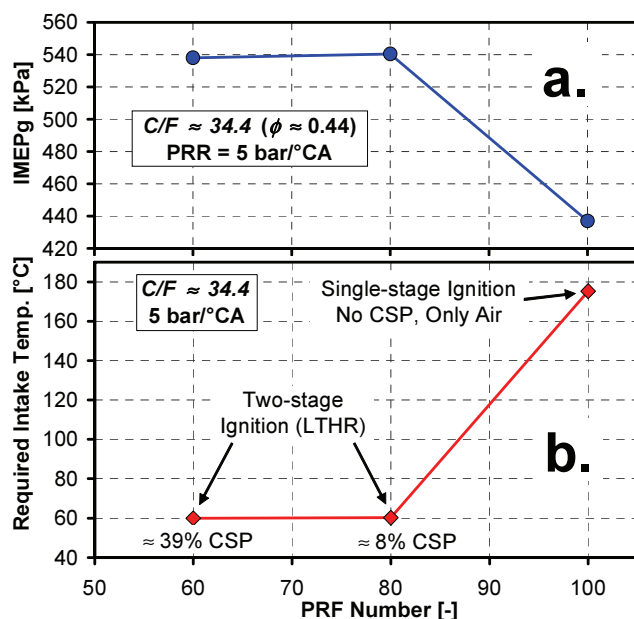


Figure 3. IMEP_g and T_{in} as a function of PRF number for operation with air dilution only for iso-octane, and with CSP addition for PRF80 and PRF60. 1200 rpm. $C/F \approx 34.4$, corresponding to $\phi = 0.44$, had there been no CSP addition.

octane was operated with air dilution only (no CSP or real EGR), so the required T_{in} was determined by the CA50 that gives a PRR of 5 bar/°CA. As can be seen, iso-octane (PRF100) required a relatively high T_{in} of 175°C. This happens because iso-octane exhibits single-stage ignition at these operating conditions³. On the other hand, PRF80 and PRF60 exhibit two-stage ignition with LTHR for these operating conditions, as evident in Fig. 4c. This LTHR accelerates the temperature rise towards the end of the compression stroke and around TDC, shown in Fig. 4b. Therefore, T_{in} has to be reduced in order to achieve an appropriate combustion phasing after TDC. However, both PRF80 and particularly PRF60 are so reactive that without EGR it would have been necessary to drop T_{in} well below ambient for the higher fueling rates investigated. Clearly, this is not practical. Instead, T_{in} was set to 60°C to avoid condensation of water in the intake system and CA50 was then controlled by adjusting the amount of CSP.

As shown by the annotation in Fig. 3b, PRF80 required 8% CSP to achieve $PRR = 5 \text{ bar/}^\circ\text{CA}$, while PRF60 required 39%. Figures 4a and 4b show that this CSP addition makes both the temperature and pressure rise associated with LTHR comparable for the two PRF blends. Furthermore, Fig. 3a shows how the IMEP_g varies between these fuels. PRF80 and PRF60 exhibit the highest power output and iso-octane the lowest. This happens because P_{in} was maintained at 100 kPa while

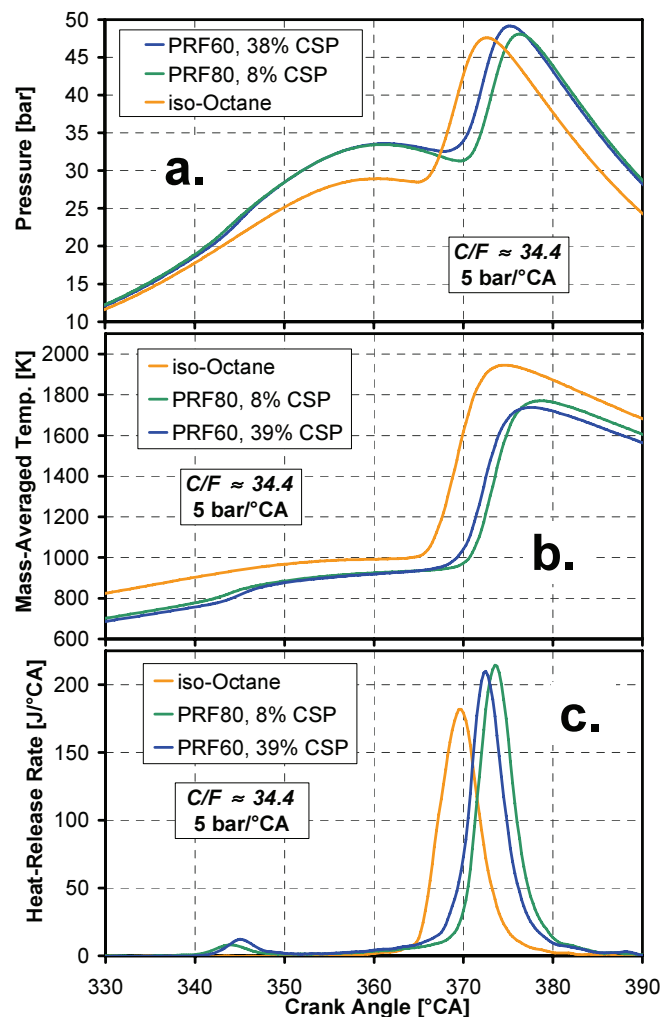


Figure 4. Pressure, temperature and HRR traces for operation with $PRR = 5 \text{ bar/}^\circ\text{CA}$ and $C/F \approx 34.4$.

$C/F \approx 34.4$. Since a higher T_{in} lowers the charge density, less charge mass is inducted for each intake stroke for the iso-octane case. For this example with $C/F \approx 34.4$ for all fuels, this also means that less fuel mass is inducted for the iso-octane case. This explains why iso-octane has 19% lower IMEP_g in this example. As will be discussed below, higher IMEP_g can be achieved with iso-octane by increasing the fueling rate. Nonetheless, it will be clear that the higher required T_{in} for iso-octane is detrimental for its high-load limits. On the other hand, the T_{in} requirement can be reduced by using a higher CR, and this will also be examined.

ADJUSTMENTS OF CA50 FOR CONSTANT PRR

For HCCI to be practical for automotive use, fairly wide load ranges must be covered. Within the load range, the combustion phasing must be easy to control in a robust and repeatable manner. As will be clear from the results presented below, the combustion phasing generally becomes more sensitive to small disturbances in charge temperature and composition as the load is increased towards the upper load limit. This work does not consider operation with closed-loop CA50 control which

³ As shown in Ref. [2], iso-octane can exhibit two-stage ignition with LTHR under conditions of elevated intake pressure. Also, low engine speed can allow the development of LTHR even for naturally aspirated conditions [14].

can allow continuous operation at combinations of CA50 and fueling rate that spontaneously lead to misfire or uncontrollable combustion-phasing advancement (*i.e.* run-away) [7]. Instead, the upper load limit in this study is determined by the combination of fueling and CA50 which can be operated continuously and steadily by only applying slow ($\sim$ minute timescale) adjustments of T_{in} (for iso-octane) and CSP/EGR rate (for PRF80 & PRF60) to correct for minor disturbances. As will be shown, above this IMEP_g limit it becomes impossible to obtain steady operation. However, the factor that makes steady operation impossible often changes with both fuel type and CA50, as will be shown.

In the process of determining these steady-state high-load limits, the fueling rate was increased stepwise from moderate fueling rates to high fueling rates while data were recorded for each steady operating point. To allow efficient data acquisition and subsequent comparison between fuels, as many parameters as possible should be held constant as the fueling rate is increased. In previous studies by the authors, data were often compared at a fixed CA50 [*e.g.* 6,11,12]. However, when spanning very wide ranges of fueling rates up to the load limit, it becomes impossible to work with a predetermined CA50 while maintaining acceptable engine performance.

This point is illustrated by the two cases shown in Figs. 5 and 6. First consider the case where CA50 is held fixed, as shown by the red diamonds in Fig. 5. Figure 5a shows how the PRR changes with fueling rate (IMEP_g) when CA50 is held fixed at 372°C/A by adjusting the EGR rate for each operating point. The corresponding pressure traces are shown in Fig. 6a. As can be seen, the PRR increases rapidly with increasing fueling rate. This happens because the total pressure rise is higher (Fig. 6a) while the combustion duration decreases (Fig. 5c). For IMEP_g > 560 kPa, the PRR exceeds the acceptable level of 8 bar/°CA, which corresponds to a ringing intensity of 5 MW/m² [10,11,14,15]. Conversely, if the fueling rate is reduced significantly below the plotted range, the combustion becomes so slow that combustion inefficiencies arise, along with increasing risk for complete misfire.

These problems can be avoided if CA50 is adjusted with fueling rate such that a reasonable PRR is maintained across the IMEP_g range of interest. This is demonstrated by the curves with blue squares in Fig. 5. The corresponding pressure traces are shown in Fig. 6b. Figure 5b shows how CA50 has to be adjusted with fueling rate to maintain a constant PRR of 7 bar/°CA (Fig. 5a). As can be seen, a more retarded CA50 is required when the fueling is increased. In addition to avoiding excessive ringing, Fig. 6b shows that the more retarded CA50 for higher fueling rates leads to a slight reduction of the peak combustion pressures, despite the higher IMEP_g. In contrast, the constant-CA50 data show a substantial increase of the peak pressure for increased fueling rates (Fig. 6a). Finally, with a constant PRR, the combustion duration is also constant, as shown in

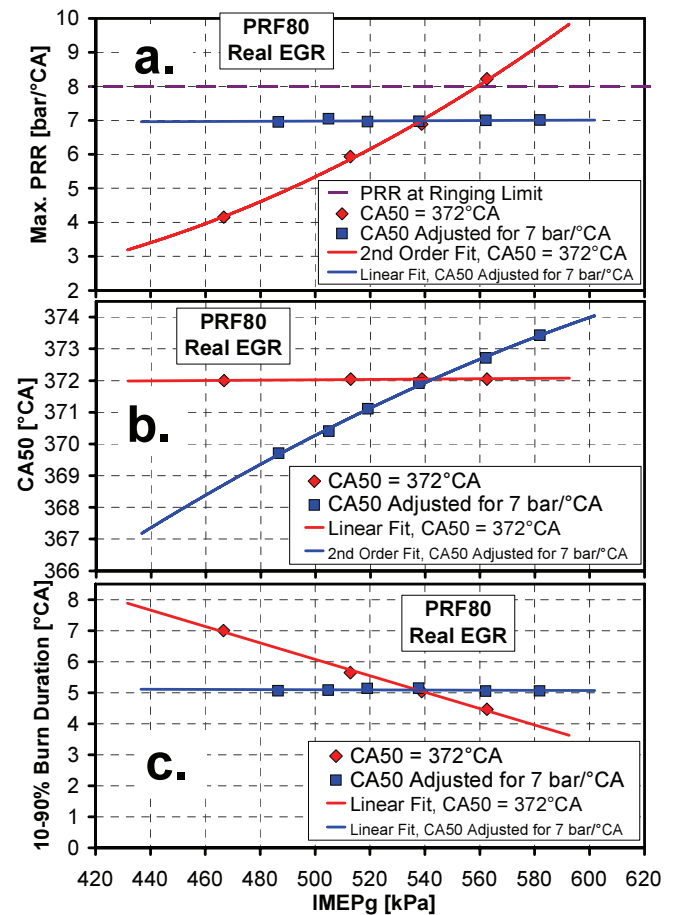


Figure 5. a) PRR as a function of IMEP_g both for operation with CA50 = 372°C/A and with CA50 variable, b) corresponding CA50, c) corresponding 10-90% burn duration.

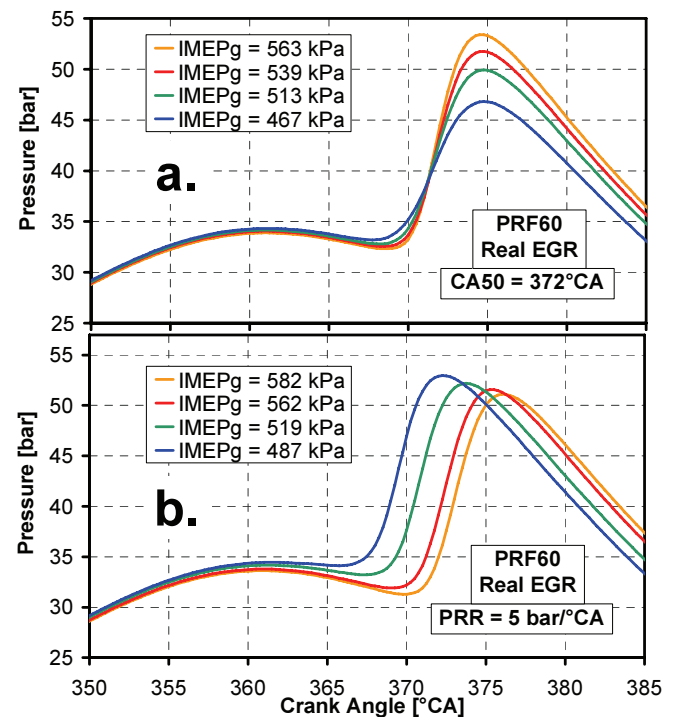


Figure 6. Pressure traces corresponding to Fig. 6. a) CA50 = 372°C/A, b) CA50 variable, constant PRR = 5 bar/°CA