

Ethanol Autoignition Characteristics and HCCI Performance for Wide Ranges of Engine Speed, Load and Boost

2010-01-0338

Published
04/12/2010Magnus Sjöberg and John E. Dec
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ABSTRACT

The characteristics of ethanol autoignition and the associated HCCI performance are examined in this work. The experiments were conducted over wide ranges of engine speed, load and intake boost pressure (P_{in}) in a single-cylinder HCCI research engine (0.98 liters) with a CR = 14 piston.

The data show that pure ethanol is a true single-stage ignition fuel. It does not exhibit low-temperature heat release (LTHR), not even for boosted operation. This makes ethanol uniquely different from conventional distillate fuels and offers several benefits: a) The intake temperature (T_{in}) does not have to be adjusted much with changes of engine speed, load and intake boost pressure. b) High P_{in} can be tolerated without running out of control authority because of an excessively low T_{in} requirement.

However, by maintaining true single-stage ignition characteristics, ethanol also shows a relatively low temperature-rise rate just prior to its hot ignition point. Therefore, ethanol does not tolerate as much combustion-phasing retard as fuels that exhibit LTHR and/or pronounced intermediate-temperature heat release. Since combustion retard is important for avoiding excessive pressure-rise rates, the distinct single-stage ignition characteristic of ethanol can be considered a drawback when reaching for higher loads. Nonetheless, an IMEP_g of 11.3 bar was demonstrated for P_{in} = 247 kPa.

Finally, the latest ethanol chemical-kinetics mechanism from the National University of Ireland - Galway was evaluated against the experimental engine data using a multi-zone

model. Overall, the mechanism performs very well over wide ranges of operating conditions.

INTRODUCTION

The homogeneous charge compression ignition (HCCI) combustion process offers good fuel economy and very low nitrogen-oxide (NO_x) and particulate emissions. Therefore, HCCI combustion is one option for improving the efficiency of the spark-ignited gasoline engine. HCCI is also pursued in order to reduce the requirement for NO_x aftertreatment in the latest generation of compression-ignited diesel engines. However, several technical hurdles need to be overcome before HCCI can be broadly applied in production engines. For example, controlling the combustion phasing and increasing the power output while maintaining acceptable pressure-rise rate (PRR) are two important research areas.

The autoignition reactivity of the fuel is a very important parameter impacting the fuel's potential suitability for an HCCI combustion system. This is particularly important to consider for emerging alternative fuels, whose reactivities can vary greatly [1]. If the fuel has high resistance to autoignition (*i.e.* high octane number), high charge temperatures are required during the compression stroke in order to ensure autoignition. This can pose a problem for low-load operation since the available exhaust heat may be insufficient for raising the temperature of the fresh charge to the required level [2]. Also, a higher intake temperature (T_{in}) leads to lower charge density for a given intake pressure (P_{in}), which typically has a negative influence on the peak load that can be obtained [3,4]. In addition, the high temperature required for autoignition also leads to high peak-combustion temperatures, so excessive NO_x can become the load-limiting factor, even for well-mixed "classical" HCCI [3].

On the other hand, if the fuel is very prone to autoignite (*i.e.* has a low octane number), the lowest possible T_{in} in combination with large quantities of exhaust-gas recirculation (EGR) may be required to obtain an acceptable 50% burn point (CA50), typically at or slightly after TDC. Since EGR gases displace air, the intake mole fraction of oxygen, $[O_2]$, is reduced with increasing amount of EGR. Therefore, the load-limiting factor for very reactive fuels can be oxygen deprivation [3]. Also, if the fuel is very reactive, it may not be suitable for use in combustion systems that revert to SI operation for parts of the load/speed range. This is because high resistance to autoignition (*i.e.* high octane number) is required to avoid engine knock for SI operation, particularly for engines that employ intake-pressure boost [5].

Worldwide, the most widespread alternative fuel for light-duty engines is currently ethanol. The most common production methods are based on fermentation of corn or sugarcane. In addition, many predictions suggest that cellulosic ethanol has the potential to increase ethanol production substantially. Practically all gasoline SI engines tolerate some fraction of ethanol in the fuel ($\sim 10\%$), and most SI engines are readily adapted for operation on fuels that contain up to 85% ethanol (*i.e.* flex-fuel engines) [5]. Based on the importance of ethanol as an alternative fuel and the current trend towards more advanced and efficient engines, it is important to fully understand the characteristics of ethanol when used in advanced combustion systems for internal combustion engines. A literature search shows that a number of studies of ethanol HCCI combustion have been conducted [*e.g.* 6,7,8]. Jointly, these studies cover rather wide ranges of operating conditions. However, because of differences in engine geometry, how the engines were operated, and how the data are presented, it is very hard to form a comprehensive view of the autoignition characteristics of ethanol for HCCI operation. The current study tries to fill this apparent gap in the literature.

Furthermore, modeling of the combustion processes is often considered a key element when developing advanced engines. Because of this, it is important that well validated chemical-kinetics mechanisms be available. This is particularly true for emerging alternative fuels, which may have characteristics that differ substantially from traditional fuels like gasoline. Therefore, the current study evaluates the fidelity of a newly developed ethanol mechanism.

SCOPE AND OBJECTIVES

The primary objective of this study is to experimentally investigate the autoignition behavior of ethanol under HCCI conditions across relatively wide ranges of operating conditions. Integral to this assessment are comparisons of the autoignition and heat-release characteristics of ethanol to those of other (non-oxygenated) fuels. The second objective is to assess the fidelity of a newly developed chemical-

kinetics mechanism for ethanol. This is done by detailed comparisons of multi-zone model predictions with the acquired engine data.

First, the experimental setup, data acquisition and analysis are described. This is followed by a description of the chemical-kinetics mechanism and the model setup. The results are then divided into five main parts:

1. Combustion-phasing sweep by changing T_{in} at $\phi = 0.40$, 1200 rpm, and $P_{in} = 100$ kPa.
2. Engine-speed sweep at $\phi = 0.38$, $P_{in} = 100$ kPa, while holding CA50 = 372°CA by adjusting T_{in} .
3. Fuel/air-equivalence ratio (ϕ) sweep to detect CA10 changes at $T_{in} = 143^\circ\text{C}$, $P_{in} = 100$ kPa and 1200 rpm.
4. Intake-boost pressure sweep at $\phi = 0.40$, 1200 rpm, while holding the 10% burn point (CA10) = 369.0°CA by adjusting T_{in} .
5. Demonstration of high IMEP_g for boosted operation at 1200 rpm, using a lower $\phi = 0.36$ and $P_{in} = 247$ kPa.

The evaluation of the chemical-kinetics mechanism for ethanol is performed in conjunction with each of the parameter sweeps in parts 1 - 4 above.

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 the same as for recent studies (*e.g.* Ref. [3]).

<figure 1 here>

Furthermore, the schematic in Fig. 1 shows that the piston used for these experiments with ethanol, iso-octane and gasoline provides an open combustion chamber with a large squish clearance and a quasi-hemispherical bowl. The geometry renders a geometric compression ratio (CR) of 14:1. The bowl of this piston is deeper than the shallow scallop design used in several previous publications (*e.g.* Ref. [4]). In particular, all data with PRF80 fuel that are presented here were acquired with a CR = 14 piston that has a more shallow piston bowl. However, comparative measurements show that both the T_{in} requirements and the heat-release rate (HRR) are nearly identical, regardless of piston-bowl geometry. Thus, the results for PRF80 can be directly compared with those of the other three fuels in this study. Finally, note that the custom-design piston provides a small topland-ring crevice, amounting to only 2.1% of the top-

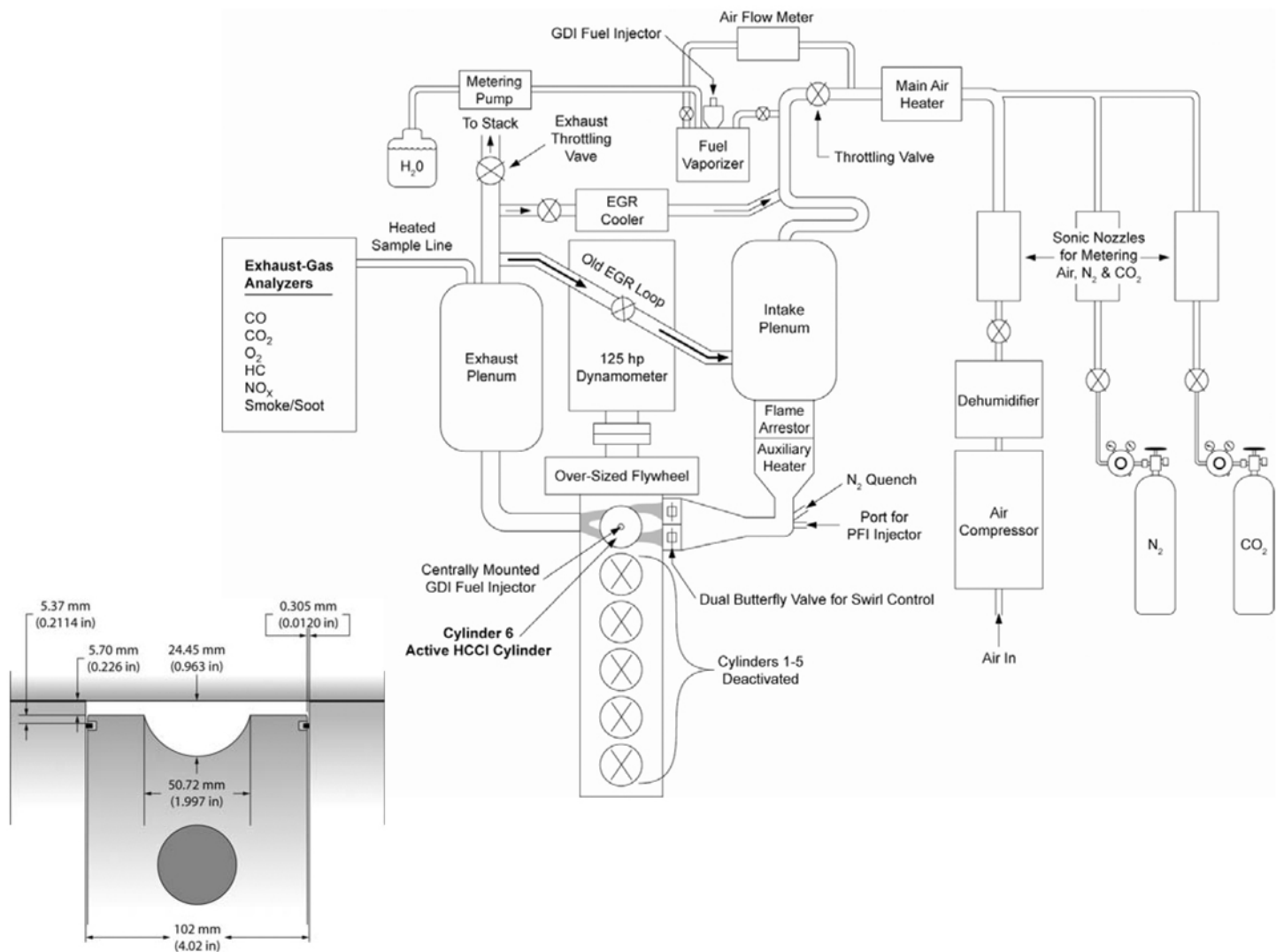


Figure 1. Schematic of the HCCI engine facility, and combustion-chamber dimensions at TDC with the CR = 14 piston.

dead-center (TDC) volume, including the volume above and behind the top piston ring.

For all operating conditions of this study, the engine was fueled using a fully premixed fueling system featuring an electrically heated fuel vaporizer (Fig. 1). The intake air was metered with a sonic nozzle. A main air heater and tank heaters (not shown) were used to preheat the mixture of air and fuel. An auxiliary air heater mounted close to the engine was used to precisely control the intake temperature of the inducted charge. For all operating conditions, the exhaust back pressure was kept at atmospheric level by maintaining a fully open exhaust throttling valve. Engine specifications are listed in Table 1. A detailed description of the engine modifications for HCCI operation can be found in Ref. [9].

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

*Valve closing and opening timings refer to 0.1 mm lift.

Intake temperatures were monitored using thermocouples mounted in the two intake ports close to the cylinder head. Firedeck temperatures were monitored with a thermocouple embedded in the cylinder head so that its junction was about

44 mm off the cylinder center and 2.5 mm beneath the surface. Surface temperatures were estimated by extrapolating the thermocouple reading to the surface, using the thickness of the firedeck and assuming that its back surface was at the 100°C cooling-water temperature.

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 1/4° crank angle (CA) increments for at least 100 consecutive cycles per data point. To compute the PRR, each individual cycle is first low-pass filtered (< 2.5 kHz, see Ref [9]) and then analyzed with a linear fit over a moving, $\pm 0.5^\circ\text{CA}$ window to extract the maximum PRR. The reported PRR_{max} values are computed by averaging the PRRs of at least 100 individual cycles. 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 fuels that show LTHR, the LTHR is excluded when the cumulative heat release is computed. Effectively, the reported CA50 for operating points with LTHR refers to 50% burn point for the main combustion event, starting at the crank angle of minimum heat-release rate between the low- and high-temperature combustion events. Referring to the main combustion event alone is considered more relevant for quantifying the main-combustion timing. Note that intermediate-temperature heat-release (ITHR) occurs just before the hot-ignition point, so the ITHR will be included as a part of the main combustion event both for fuels with and without LTHR.

A second method of computing the HRR was used for the presented HRR traces. Here, the heat-release rate 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 [10].

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 100 cycles), the known cylinder volume, and the trapped mass. The trapped mass equals the sum of the supplied air, fuel, and residuals, the latter being computed by applying the ideal gas law to the clearance volume at TDC-valve-overlap, using a pressure that was determined from cycle-simulation modeling (using Ricardo's WAVE program) and an estimated residual temperature based on exhaust blowdown to this pressure. The average molecular weight used for the calculation of the charge temperature during the compression stroke corresponds to that of the trapped gases - including fresh air, retained residuals, and fuel. During the combustion event, and in proportion to the mass fraction burned, the molecular weight in the calculations is gradually changed to that of the measured exhaust composition. This

exhaust molecular weight is then used for the remainder of the expansion stroke and for computing the trapped mass.

Exhaust emissions data were also acquired, with the sample being drawn from the exhaust plenum using a heated sample line (see Fig. 1). For all conditions, the levels of CO, CO₂, HC, NO_x, O₂ were measured using standard exhaust-gas analysis equipment as shown in Table 2. Since the fuel is oxygenated, a separate test was performed to check the response of the HFID to ethanol. It was found that the carbon-atom-detection efficiency was 65%. Accordingly, the HC emissions reported here have been multiplied by 1.53 to correct for this, with the assumption that the HFID response is dominated by ethanol molecules in the exhaust [11]. Initial measurements with the smoke meter showed that the smoke levels were virtually zero since the fuel was well mixed with the air. Therefore, smoke was not measured for all data points.

TABLE 2. Emissions Analysis Equipment

CO	Non-Dispersive Infrared Detector, Rosemount 880A
CO ₂	Non-Dispersive Infrared Detector, CAI 602 NDIR
HC .	Heated Flame Ionization Detector (HFID), CAI 600 HFID
NO _x	Chemiluminescence Analyzer, Rosemount 951A
O ₂	Paramagnetic Analyzer, Rosemount 755R
Smoke	Optical-Density of Filter Paper, AVL415S

Because HCCI combustion is very sensitive to temperature, the engine coolant and oil were both fully preheated to 100°C before starting the experiments. 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 fuels used for this study are neat (100%) ethanol, iso-octane, gasoline, and PRF80 (an 80/20 blend of the primary reference fuels, iso-octane and n-heptane). All of these fuels are fairly volatile, and this facilitates the charge preparation process. Table 3 shows the fuel compositions and other relevant parameters. It can be noted that the mass-based heating value of ethanol is substantially lower than the other fuels since ethanol is oxygenated. However, the stoichiometric air/fuel-ratio is also lower for ethanol. Consequently, for the same ϕ , the heating values of the fuel/air-mixtures are nearly identical for the four fuels. Since ethanol tends to absorb water from the ambient air, care was taken to minimize the exposure of the ethanol to the ambient air by keeping fuel containers sealed and to displace air with nitrogen gas above the fuel in the fuel tank.

TABLE 3. Fuel Properties

Fuel:	Ethanol	Iso-Octane	Gasoline	PRF80
Iso-Octane %vol.	0	100	Unknown	80
n-Heptane %vol.	0	0	Unknown	20
Saturates %vol.	100	100	73.1	100
Olefins %vol.	0	0	4.2	0
Aromatics %vol.	0	0	22.7	0
RON	107	100	90.8	80
MON	89	100	83.2	80
Antiknock Index (RON+MON)/2	98	100	87.0	80
C-atoms	2	8	6.78	7.78
H-atoms	6	18	13.6	17.56
O-atoms	1	0	0	0
Molecular weight	46.07	114.2	95.2	111.1
A/F Stoichiometric	9.00	15.13	14.8	15.14
Lower heating value for gas-phase fuel [MJ/kg]	27.75	44.65	43.17	44.71
Lower heating value for stoichiometric charge [MJ/kg]	2.775	2.769	2.734	2.770

CHEMICAL-KINETICS MODELING SETUP

The chemical-kinetic modeling approach used in this work is similar to one used previously by the authors [12]. The calculations were carried out using a special multi-zone version of the Senkin application of CHEMKIN III developed at Sandia [13,14]. The model treats each zone as a single lumped mass with uniform composition and thermodynamic properties. The chemistry is treated independently for each zone. The only coupling between zones is the pressure, which is assumed to equilibrate instantaneously as heat is released in any of the zones. The total volume of all zones is modeled according to the standard slider-crank relationship [10], using the geometry and specifications of the Sandia HCCI research engine shown in Table 1. As a result, the volume of each zone effectively depends on its mass and temperature relative to the other zones. The number of zones and the thermal distribution are described in the in Appendix A, which also includes a comparison with single-zone modeling.

A newly developed reaction mechanism for ethanol is used [15]. The ethanol mechanism has 58 species and 310 reactions. It is developed to be an integrated part of a gasoline surrogate mechanism [16]. This much larger surrogate mechanism is a joint effort between the National University of Ireland (NUI) - Galway (Curran, Serinyel, and Metcalfe) and Lawrence-Livermore National Lab (LLNL) (Pitz and Mehl).

For simplicity, heat transfer effects were not modeled. However, to ensure a charge-pressure history during the compression stroke that is very similar to that of the experiment, the model was set up with CR = 12.8. This is somewhat lower than the nominal CR = 14 used in the experiment.

The amount and composition of the reactants were computed based on careful analysis of the engine experiment, including emissions measurements. The air was modeled using the correct proportions of N₂, O₂ and CO₂, where atmospheric argon was lumped as atmospheric N₂. The residuals were modeled using CO₂, H₂O, N₂, CO, unburned fuel, and air. For this modeling work, no attempt was made to capture the effect of partially burned fuel that is encountered experimentally in residuals, and so the measured exhaust hydrocarbon mole fraction was converted to an ethanol mole fraction in the residuals. It should be noted that the amount of residuals is low as a result of the use of conventional valve timings. In this study, the residual mass fraction ranges from 2.1% to 5.8%, depending on the boost pressure, engine speed, and residual temperature.

RESULTS

As described in conjunction with Fig. 1, a CR = 14 piston was installed for all tests. However, the choice of compression ratio influences the T_{in} requirements, thus affecting the performance of a given fuel [3,17,18]. This should be considered when comparing the data presented here with data acquired in other engines using different compression ratios.

COMBUSTION-TIMING SWEEP / T_{IN}-SENSITIVITY

This section deals with the use of T_{in} adjustments to control the combustion phasing for a fixed engine speed of 1200 rpm and P_{in} = 100 kPa. Precise CA50 control is particularly important at high loads, since too-advanced CA50 can lead to excessive PRR and engine knock [19]. Below, the degree of response of the combustion phasing to a change of T_{in} will be referred to as T_{in} sensitivity.

Figure 2 shows how the T_{in} has to be adjusted to achieve a certain CA50 for ethanol, iso-octane and PRF80. Directly

relevant is Fig. 3, which shows that both ethanol and iso-octane exhibit single-stage ignition behavior without LTHR. As a result, their T_{in} requirements are comparable. Even so, Fig. 2a shows that iso-octane requires more than 33°C higher T_{in} than ethanol for this range of CA50. This shows that ethanol has a higher autoignition reactivity than iso-octane under these conditions (1200 rpm and $P_{in} = 100$ kPa). The term autoignition reactivity will be used extensively throughout the paper and refers to how easy it is to achieve autoignition for the fuel in question. For operation with a constant CR, low residual fraction, and no EGR - as in this study - the autoignition reactivity is quantified by the required T_{in} to achieve autoignition. A fuel with high reactivity requires low T_{in} whereas a fuel with low reactivity requires high T_{in} . In contrast to ethanol and iso-octane, PRF80 requires a much lower T_{in} , so it is plotted by itself in Fig. 2b. Under these operating conditions, PRF80 exhibits LTHR, as illustrated in Fig. 3, and this explains why its T_{in} has to be low.

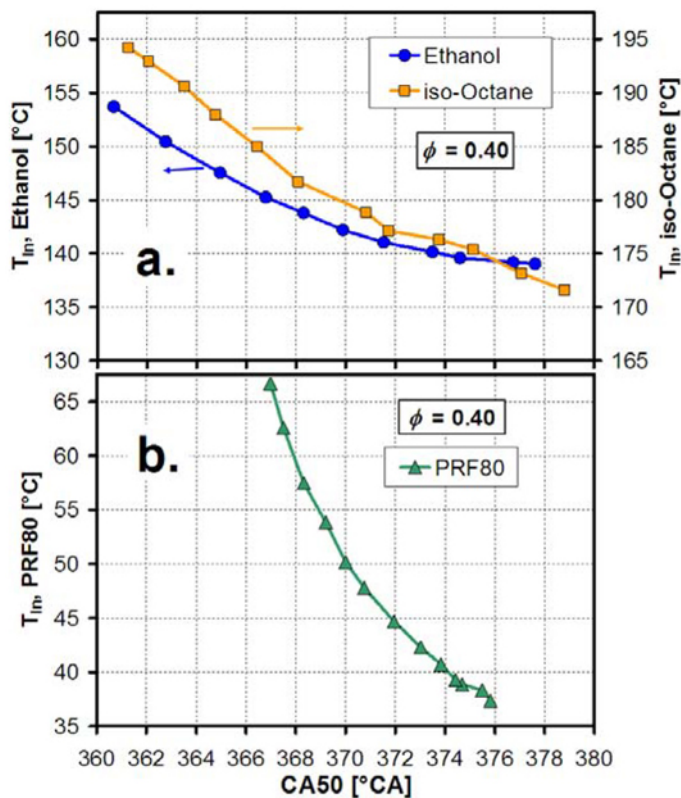


Figure 2. Required T_{in} as a function of desired CA50 for ethanol, iso-octane, and PRF80. $\phi = 0.40$, 1200 rpm, and $P_{in} = 100$ kPa.

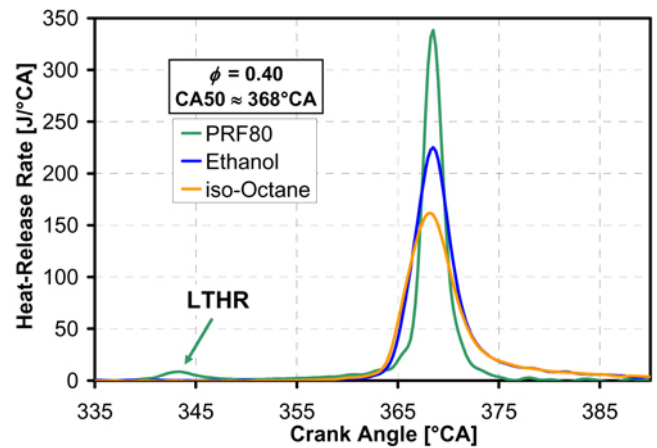


Figure 3. HRR traces for ethanol, iso-octane, and PRF80. CA50 $\approx 368^\circ\text{CA}$, $\phi = 0.40$, 1200 rpm, and $P_{in} = 100$ kPa.

Not only are the T_{in} requirements different between the fuels, the slope of the curves in Fig. 2 are different as well. PRF80 has the steepest slope, so among these fuels its combustion phasing has the lowest sensitivity to changes of T_{in} . Its low T_{in} sensitivity can be explained by its LTHR in combination with enhanced ITHR [4]. Figure 3 clearly shows the LTHR, and Fig. 4 zooms in on the ITHR that precedes the main combustion. The presence of LTHR reduces the sensitivity of the autoignition timing to changes of the charge temperature because the amount of LTHR increases with decreasing T_{in} , thus counteracting the direct influence of changes in T_{in} on the charge temperature at TDC. The enhanced ITHR in the 350 - 363°CA range (see Fig. 4) increases the temperature-rise rate (TRR) just before the hot-ignition point, as Fig. 5 shows. As explained in detail in [4], with a higher TRR, the timing of transition into hot ignition becomes less sensitive to changes of the charge temperature. Consequently, the higher TRR due to enhanced ITHR contributes to the low T_{in} sensitivity for PRF80, as Fig. 2b shows.

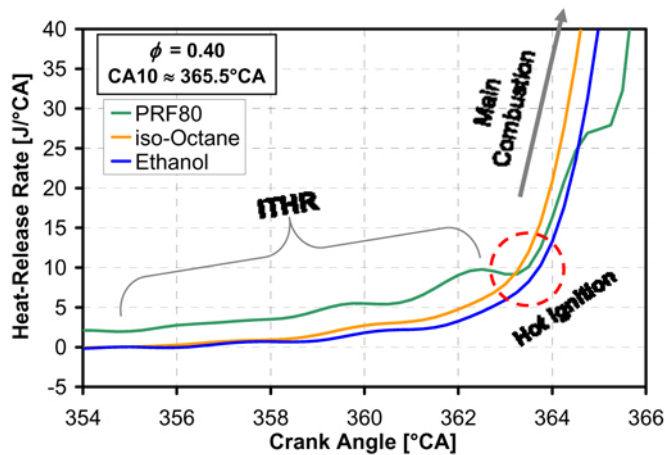


Figure 4. HRR during the early part of the autoignition event for ethanol, iso-octane, and PRF80. CA10 ≈ 365.5°CA, $\phi = 0.40$, 1200 rpm, and $P_{in} = 100$ kPa.

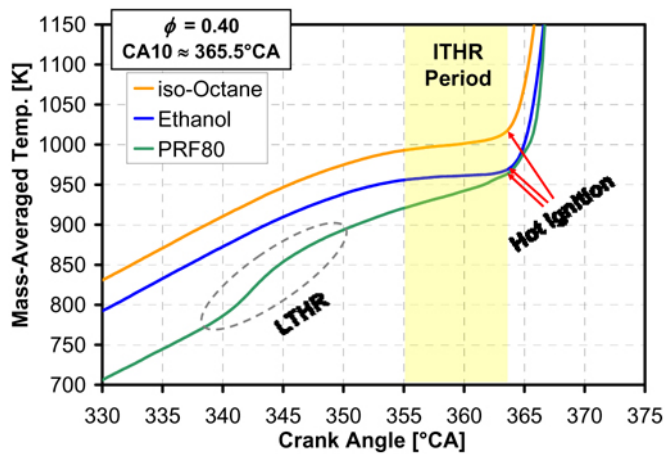


Figure 5. Temperature rise during the late compression stroke and early part of the autoignition event for ethanol, iso-octane, and PRF80. CA10 ≈ 365.5°CA, $\phi = 0.40$, 1200 rpm, and $P_{in} = 100$ kPa.

In contrast, Fig. 2 shows that the CA50 of both ethanol and iso-octane are much more sensitive to changes of T_{in} . Neither ethanol nor iso-octane exhibit LTHR and Fig. 4 shows much less ITHR for these fuels. Consequently, the TRR prior to hot ignition is also much lower, as can be seen in Fig. 5. When the hot-ignition temperature is approached with a shallow slope (*i.e.* low TRR), the crank angle of transition to hot ignition becomes very sensitive to changes of charge temperature (vertical displacement of the temperature trace). This explains the higher T_{in} sensitivity. Examination of Fig. 2a reveals that ethanol has a slightly higher T_{in} sensitivity than iso-octane. This is consistent with the somewhat lower ITHR and TRR prior to the hot ignition. In this sense, ethanol is a more pronounced single-stage-ignition fuel than iso-octane. This could make it harder to control the combustion

timing for operation with retarded combustion phasing using ethanol.

It is important to maintain stable combustion with low cycle-to-cycle variations. This can be an issue for operation with more retarded combustion phasing. Figure 6 shows the standard deviation of IMEP_g as a function of CA50 for ethanol, iso-octane and PRF80. All fuels exhibit larger variations with increasing CA50 retard. As explained in Ref. [4], this happens because the TRR becomes lower with CA50 retard as the piston-expansion cooling becomes more rapid for later crank angles. With a lower TRR, the onset of hot ignition becomes more sensitive to cycle-to-cycle variations of the charge temperature, as exemplified in Fig. 7, which is reproduced from Ref. [4]. Associated with larger variations of the hot-ignition timing are also larger variations of IMEP_g. In Fig. 6, the curves for ethanol and iso-octane are nearly overlapping. With a 2% limit of tolerable IMEP_g variations, this means that both these single-stage ignition fuels have an identical CA50 retard limit of 373°CA. Based on their similar TRR prior to hot ignition, it could have been expected that the CA50 retard limit be similar. However, since Fig. 5 shows that ethanol has slightly lower TRR, it would also be expected that ethanol would tolerate slightly less CA50 retard. This slight inconsistency is believed to be related to the somewhat higher IMEP_g that ethanol produces, as will be shown below. It should be remembered that Fig. 6 compares IMEP_g variations, not variations of the autoignition timing.

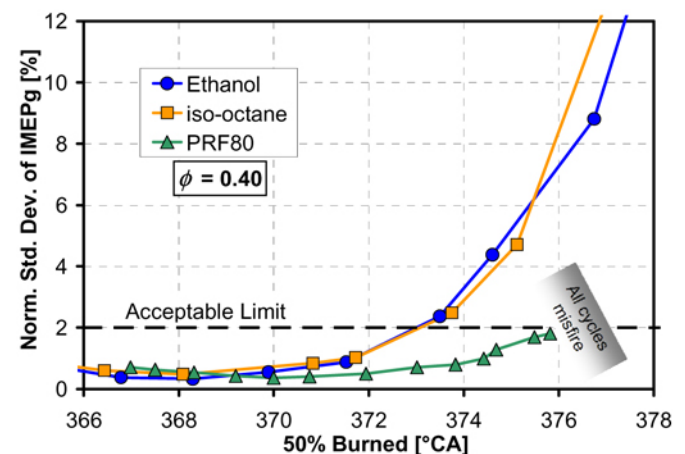


Figure 6. Standard deviation of IMEP_g normalized by $(IMEPg - IMEP_{g,motored})$ as a function of CA50 for ethanol, iso-octane, and PRF80. $\phi = 0.40$, 1200 rpm, and $P_{in} = 100$ kPa.