

Smoothing HCCI Heat Release with Vaporization-Cooling-Induced Thermal Stratification using Ethanol

Magnus Sjöberg and John E. Dec
Sandia National Laboratories

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ABSTRACT

Ethanol and ethanol/gasoline blends are being widely considered as alternative fuels for light-duty automotive applications. At the same time, HCCI combustion has the potential to provide high efficiency and ultra-low exhaust emissions. However, the application of HCCI is typically limited to low and moderate loads because of unacceptably high heat-release rates (HRR) at higher fueling rates.

This work investigates the potential of lowering the HCCI HRR at high loads by using partial fuel stratification to increase the in-cylinder thermal stratification. This strategy is based on ethanol's high heat of vaporization combined with its true single-stage ignition characteristics. Using partial fuel stratification, the strong fuel-vaporization cooling produces thermal stratification due to variations in the amount of fuel vaporization in different parts of the combustion chamber. The low sensitivity of the autoignition reactions to variations of the local fuel concentration allows the temperature variations to govern the combustion event. This results in a sequential autoignition event from leaner and hotter zones to richer and colder zones, lowering the overall combustion rate compared to operation with a uniform fuel/air mixture.

The amount of partial fuel stratification was varied by adjusting the fraction of fuel injected late to produce stratification, and also by changing the timing of the late injection. The experiments show that a combination of 60 – 70% premixed charge and injection of 30 – 40 % of the fuel at 80°CA before TDC is effective for smoothing the HRR. With CA50 held fixed, this increases the burn duration by 55% and reduces the maximum pressure-rise rate by 40%. Combustion stability remains high but engine-out NO_x has to be monitored carefully. For operation with strong reduction of the peak HRR, ISNO_x rises to around 0.20 g/kWh for an IMEP_g of 440 kPa. The single-cylinder HCCI research engine was operated naturally aspirated without EGR at 1200 rpm, and had low residual level using a CR = 14 piston.

INTRODUCTION

The homogeneous charge compression ignition (HCCI) combustion process offers high thermal efficiency and very low nitrogen-oxide (NO_x) and particulate emissions. Therefore, HCCI combustion is one available option for improving the efficiency of the spark-ignited gasoline engine. HCCI-type combustion is also being implemented in the latest generation of compression-ignited diesel engines in order to reduce the requirement for NO_x aftertreatment. However, several technical hurdles need to be overcome before HCCI combustion will see broad application. Maintaining an acceptable pressure-rise rate (PRR) to avoid knocking at high loads is one important research area. One effective way to reduce the PRR is to retard the combustion phasing [1,2]. However, the degree of combustion-phasing retard that can be applied while maintaining high combustion stability varies with fuel type [3]. Specifically, combinations of fuel type and operation strategy that render strong early heat release just prior to the main combustion allow more combustion-phasing retard [4].

Since petroleum is a limited resource, at present there is great interest in developing alternative fuels. Worldwide, the most widespread alternative fuel for light-duty engines is currently ethanol. Practically all gasoline SI engines tolerate some fraction of ethanol in the fuel (~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. Consequently, a recent comprehensive HCCI study was conducted by the current authors to map out the autoignition characteristics of ethanol [6]. One of the fundamental findings was that neat ethanol is a true single-stage ignition fuel with very little early heat release prior to the onset of main combustion, regardless of engine speed and intake pressure boost.

Because ethanol is a true single-stage ignition fuel with very little early heat release, the amount of combustion-phasing retard that can be applied while maintaining stable combustion is less than for other fuels. Therefore, ethanol offers less potential for applying combustion-phasing retard to increase power output in HCCI engines than does gasoline [4,6]. This fact has to be considered in the light of expected higher availability of ethanol as a motor fuel [7], both as E85 and intermediate blends (e.g. E15 – E30). However, with a change of fuel composition, several other important factors change simultaneously. For example, both the stoichiometric air/fuel-ratio (AFR_{st}) and latent heat of vaporization differ considerably between gasoline and ethanol. As a result, for a given engine load, the vaporization-cooling potential is more than four times greater for ethanol. For a combustion system like HCCI, compensation must be provided for this additional cooling to ensure robust autoignition and combustion. On the other hand, this strong vaporization cooling can potentially be exploited to change the in-cylinder thermal field. This may be a very important consideration, since for classical HCCI at moderate to high loads, the combustion rate is controlled by the sequential autoignition from hotter to colder in-cylinder zones [8].

SCOPE AND OBJECTIVES

Fuel stratification has the potential to create thermal stratification due to uneven vaporization cooling. If the naturally occurring thermal stratification due to heat transfer can be enhanced, this should lead to longer burn duration. Compared to conventional fuels, ethanol has a high latent heat of vaporization and strong cooling potential. Based on this, the primary objective of this study is to experimentally examine the use of direct injection of ethanol to create fuel stratification and achieve a longer HCCI combustion event with reduced peak HRR. For better understanding of the in-cylinder processes, some of ethanol's autoignition and thermodynamic characteristics are examined in detail. To put the results in context, comparisons are made with previously published data for other fuels at similar operating conditions. In addition, using previous data for iso-octane, some of the test engine's characteristics regarding both fuel stratification and the naturally occurring thermal stratification due to heat transfer are discussed.

While the study is mainly experimental, chemical-kinetics modeling is used to provide fundamental insights of ethanol's thermodynamic and autoignition characteristics. In addition, some CFD modeling results are included to quantify the in-cylinder thermal field caused by normal heat transfer.

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. Review of ethanol's distinct single-stage autoignition characteristics and the sensitivity of the autoignition timing to changes of the charge temperature in comparison with data for other fuels.
2. Fundamental investigation of the sensitivity of the autoignition timing to changes of the fuel/air-equivalence ratio (ϕ -sensitivity) for gas phase only.
3. Quantification of experimentally attainable vaporization cooling using direct injection of liquid ethanol (in comparison with iso-octane), and the influence of vaporization cooling on the ϕ -sensitivity of ethanol.
4. Discussion of ways to achieve vaporization-cooling-induced thermal stratification and its relationship to the naturally occurring thermal stratification caused by normal wall heat transfer.
5. Demonstration of the use of partial fuel stratification with ethanol to achieve an enhanced thermal stratification with lower peak combustion rates.

Finally, a summarizing comparison is made between this application of partial fuel stratification using ethanol and previously published applications of partial fuel stratification using other types of fuels.

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. Refs. [4,6]).

Furthermore, the schematic in Fig. 1 shows that the piston used for the current experiments with ethanol 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. [3]). However, tests show that the engine performance is nearly identical. Nonetheless, it can be noted that the data for fuels other than ethanol that are presented here (but previously published) were acquired with pistons that have more shallow piston bowls. In the case of optical data, flat-top pistons were used.

To achieve partial fuel stratification, a combination of premixed and direct injection (DI) fueling was used. The premixed fueling system, shown at the top of the schematic in Fig. 1, consists of a GDI injector mounted in an electrically heated fuel-vaporization chamber and appropriate plumbing to ensure thorough premixing with the air upstream of the intake plenum. The DI fueling is accomplished using a second GDI injector mounted centrally in the cylinder head. For the current tests with ethanol, an 8-hole

Bosch injector was used at a fuel pressure of 120 bar. The included angle was 70°. A positive-displacement fuel-flow meter was used to determine the amount of fuel supplied. 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. Intake temperatures were monitored using thermocouples mounted in the two intake ports close to the cylinder head. Intake pressure (P_{in}) was measured with a pressure transducer mounted on the intake runner. The reported absolute P_{in} values are crank-angle averaged over 200 cycles. Engine specifications are listed in Table 1. A detailed description of the engine modifications for HCCI operation can be found in Ref. [9].

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 $\frac{1}{4}^\circ$ crank angle (CA) increments for typically 200

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.

consecutive cycles per operating point. To compute the maximum pressure-rise rate (PRR_{max}) for an operating point, each individual cycle is first low-pass filtered (< 2.5 kHz) and then analyzed with a linear fit over a moving 0.5°CA window to extract the PRR_{max} of that cycle. The reported PRR_{max} associated with an operating point is then computed by averaging all PRR_{max} values of the 200 individual cycles. Similarly,

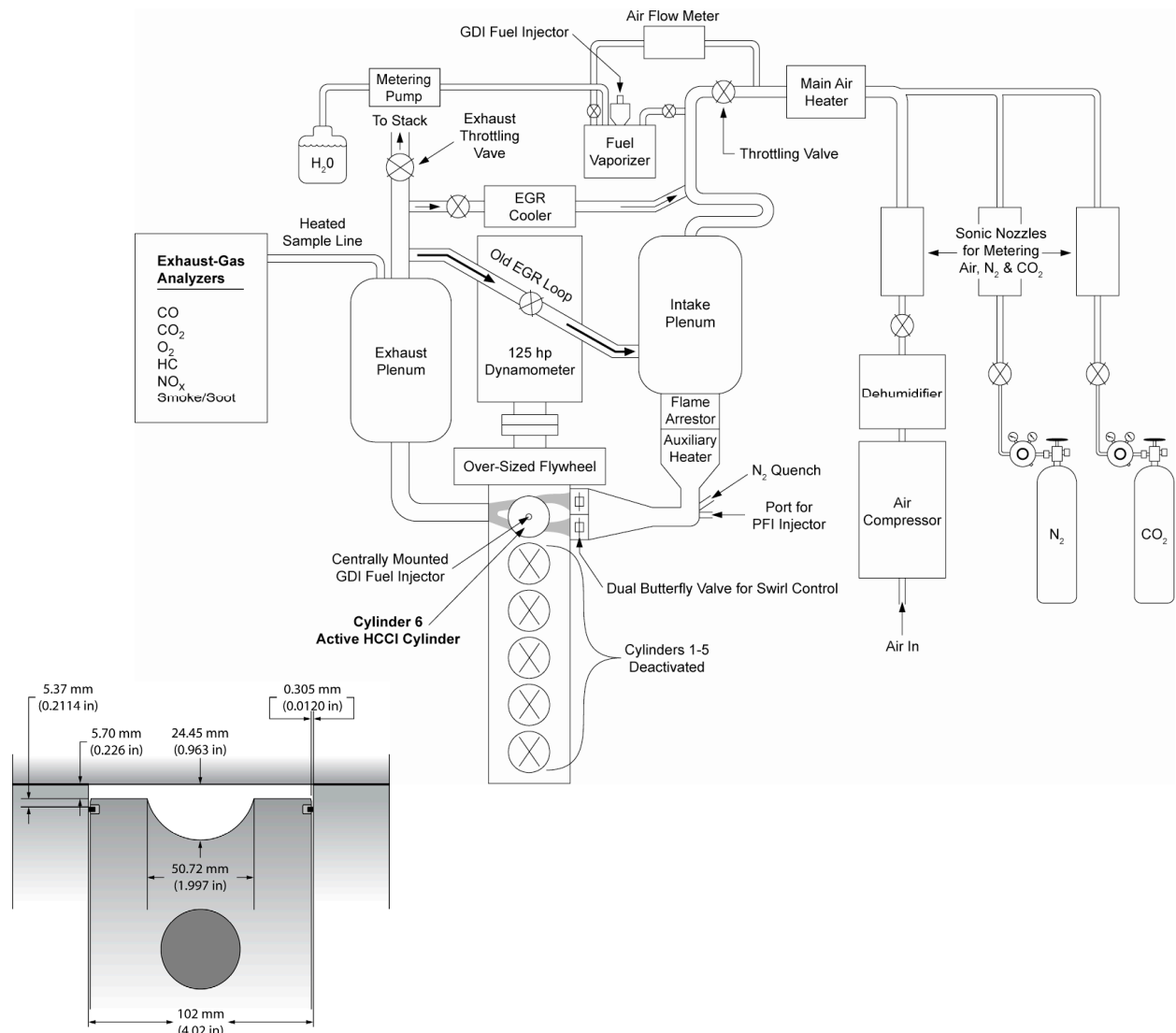


Figure 1. Schematic of the HCCI engine facility, and combustion-chamber dimensions at TDC with the CR = 14 piston.

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.

A second method of computing the heat-release rate was used for the presented HRR traces. Here, the heat-release rate was computed in a more refined way from the 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 and expansion) are computed using the ideal-gas law in combination with the measured pressure (ensemble-averaged over 200 cycles), the known cylinder volume, and the trapped mass. The trapped mass equals the sum of the supplied air, fuel, and residuals. The residual mass is 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 iteratively estimated residual temperature based on exhaust-blowdown cooling to this pressure. The average molecular weight used to calculate 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 average 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 residual mass.

Exhaust emissions data were also acquired, with the sample being drawn from just downstream of the exhaust plenum using a heated sample line. 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 ethanol 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 readout during engine operation is dominated by unburned fuel (*i.e.* ethanol molecules) in the exhaust [11]. Smoke measurements were also made with an automated smoke meter, but no soot emissions were detected.

Because HCCI combustion is very sensitive to temperature, the engine coolant and oil were both preheated to 100°C before starting the experiments.

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, CAI 600 HFID
NO _x	Chemiluminescence Analyzer, Rosemount 951A
O ₂	Paramagnetic Analyzer, Rosemount 755R
Smoke	Optical-Density of Filter Paper, AVL415S

TABLE 3. Fuel Properties

Fuel:	100% Ethanol	100% Iso-Octane
RON	107	100
MON	89	100
Antiknock Index (RON+MON)/2	98	100
C-atoms	2	8
H-atoms	6	18
O-atoms	1	0
Molecular Weight [g/mole]	46.07	114.2
A/F-Stoichiometric [kg air/ kg fuel]	9.00	15.13
Specific Heat Capacity - C _p [J/g·K] @ 700K	2.58	3.26
Heat of Vaporization [MJ/kg] @ 298 K	0.84	0.31
Lower Heating Value for Gas-phase Fuel [MJ/kg fuel]	27.75	44.65
Lower Heating Value for Stoichiometric Charge [MJ/kg]	2.775	2.769

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 main fuel used for this study is neat (100%) ethanol, and this fuel was used for all operation with partial fuel stratification. In addition, 190-proof ethanol (95% ethanol, 5% water by volume), and neat iso-octane were used for the separate vaporization-cooling measurements. All of these fuels are fairly volatile, and this facilitates the charge preparation process. Table 3 shows selected fuel data for ethanol and iso-octane. In the first results section, the autoignition characteristics of ethanol are compared with iso-octane, gasoline, and two PRF blends. The properties of the three latter fuels can be found in previous work [6,12].

CHEMICAL-KINETICS MODELING SETUP

The chemical-kinetic modeling approach used in this work is identical to one used recently by the authors [6,12]. 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. In the current study, 11 zones were used and the thermal distribution across the zones is described in Appendix A. The use of a multi-zone model was favored over a single-zone model since the former more accurately reproduces the pressure rise and combustion rate of the experiment.

A newly developed reaction mechanism for ethanol was used [15]. The ethanol mechanism has 58 species and 310 reactions, and it has been validated against experimental flow-reactor and shock-tube data. 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). Additionally, as a part of a collaboration between Sandia and the University of New South Wales (UNSW) in Australia, two other mechanisms that are available in the open literature, Refs. [17,18], were examined [19]. However, neither of these ethanol mechanisms had sufficient reactivity so they required unrealistically high charge temperature to reproduce the experimental combustion phasing, therefore they were not used in this work.

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 experimental CR = 14. The air was modeled using the correct proportions of N₂, O₂ and CO₂, where atmospheric argon was lumped with atmospheric N₂. The residuals were modeled using CO₂, H₂O, N₂, CO, unburned fuel, and air. It should be noted that the amount of residuals was low as a result of the use of conventional valve timings. For operation using ethanol, the residual mass fraction was around 4.2%.

RESULTS

The engine speed was kept at 1200 rpm throughout this study. Unless noted, the intake pressure (P_{in}) was set to = 100 kPa, simulating naturally aspirated operation.

EARLY AUTOIGNITION HEAT RELEASE

The successful use of vaporization cooling to enhance the in-cylinder thermal stratification and in this way achieve an extended burn duration requires selection of a suitable fuel. As mentioned in the Introduction, the fact that ethanol has a much smaller amount of heat release prior to the main combustion is a characteristic feature that distinguishes ethanol from other common fuels. As will be shown, this characteristic feature of ethanol is very important for the use of vaporization cooling to smooth HCCI heat

release. Thus, this section compares the early heat release of ethanol with that of several other fuels.

Figure 2 plots the heat release just prior to onset of the main combustion for ethanol and four other fuels. From here forward, the heat release just prior to the main combustion will be called intermediate-temperature heat release (ITHR) in accordance with the terminology used in previous work [20]. The low-octane PRF blends stand out with high ITHR. This stems partly from the low-temperature combustion (which occurs in the 338-350°C range, outside the plot area) of these PRF blends, which creates a large number of reactive fuel fragments [20]. Conversely, the CHEMKIN model predicts that the ethanol molecule is stable up to a temperature of approximately 960K. Consequently, Fig. 2a shows that ethanol does not start to break down until roughly 10°C prior to hot ignition. The timing of the hot ignition is indicated by the rapid rise in HRR around 364°C. As a result, ethanol exhibits a very low ITHR prior to hot ignition. Iso-octane and gasoline also show low ITHR for these operation conditions, albeit not quite as low as ethanol. As a side note, Fig. 2a shows that significant amounts of both acetaldehyde and formaldehyde are formed during the autoignition process of ethanol. Aldehydes are known to influence the autoignition timing [3,21,22], but these intermediate species are probably not very important for combustion-phasing control of this low-residual engine as long as the combustion efficiency remains high. However, they may be of greater importance for high-residual engines, in particular if significant amounts remain unburned and participate in the next cycle.

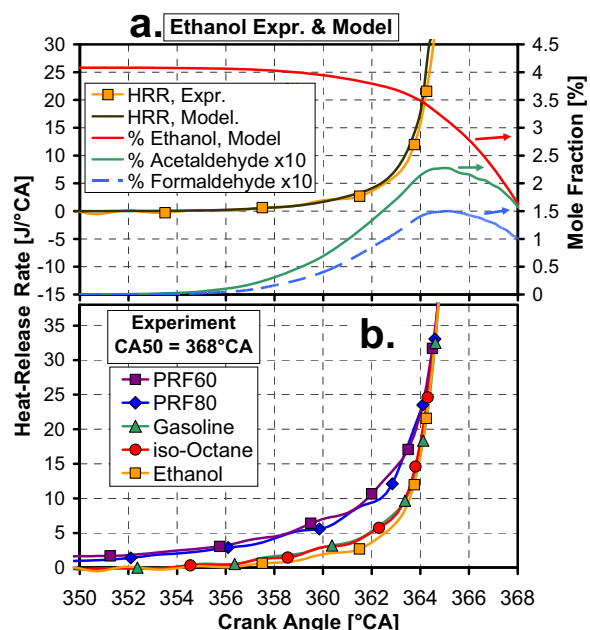


Figure 2. $\phi = 0.40$. a) Ethanol experimental and model ITHR, and model prediction of ethanol breakdown, acetaldehyde and formaldehyde formation. b) Comparison of the ITHR for five fuels. For ease of interpretation, non-ethanol curves are shifted slightly (0.2 – 1.2°C) to the left to make the curves cross at 364.8°C. Modified from Ref. [12].

It can be noted that the predicted ITHR in Fig. 2a is very similar to the experimental curve for ethanol, providing confidence in the multi-zone modeling approach. Also, the bottom-dead-center temperature (T_{bdc}) required to match the 10% burn point (CA10) of the model to the experimental CA10 is less than 1°C different from the experimental value of 154°C.

THERMAL SENSITIVITY OF ETHANOL AUTOIGNITION TIMING

Figure 3 shows how T_{in} has to be adjusted to achieve a certain CA10 for ethanol, iso-octane and PRF80. Both ethanol and iso-octane exhibit single-stage ignition behavior without low-temperature heat release (LTHR). As a result, their T_{in} requirements are comparable. Even so, Fig. 3a shows that iso-octane requires between 34 and 41°C higher T_{in} than ethanol for this range of CA10. This shows that ethanol has a higher autoignition reactivity than iso-octane under these conditions (1200 rpm and $P_{in} = 100$ kPa). This higher reactivity is in agreement with the lower MON of ethanol, as Table 3 shows. (MON numbers are acquired at 900 rpm with high T_{in} , so they are more relevant than RON for this comparison. RON numbers are acquired at 600 rpm and low T_{in} [6].) In contrast to ethanol and iso-octane, PRF80 requires a much lower T_{in} , so it is plotted separately in Fig. 3b. Under these operating conditions, PRF80 exhibits LTHR, and this explains why its T_{in} has to be low.

Not only are the T_{in} requirements different between the fuels, the slope of the curves in Fig. 3 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 [3]. 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°C range (see Fig. 2b) increases the

temperature-rise rate (TRR) just before the hot-ignition point. As explained in detail in [3], 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 (Fig. 3b).

In contrast, Fig. 3a shows that the CA10 of both ethanol and iso-octane are much more sensitive to changes of T_{in} . Neither ethanol nor iso-octane exhibit LTHR, and Fig. 2b shows much less ITHR for these fuels. Consequently, the TRR prior to hot ignition is also much lower, and this explains the higher T_{in} sensitivity. Examination of Fig. 3a 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.

ϕ -SENSITIVITY OF ETHANOL AUTOIGNITION TIMING

With this understanding of ethanol's high thermal sensitivity, the influence of changes to the fuel concentration on ethanol's autoignition is investigated. Gas-phase effects are examined first, followed by vaporization-cooling effects. However, with the existing experimental hardware, the required gas-phase-only data cannot be conveniently generated using fully premixed fueling. This is the case because as the amount of fuel is adjusted to change ϕ in a continuously firing engine, the charge temperature at BDC (T_{bdc}) also changes despite T_{in} being held constant. These changes of T_{bdc} occur because the varying amounts of fuel burned affect both in-cylinder wall temperatures (T_{wall}) and residual gas temperatures ($T_{residuals}$) [6]. It would be difficult and time consuming to try to compensate for this by adjusting both T_{in} and the coolant temperature to achieve constant T_{bdc} and T_{wall} . Additionally, $T_{residuals}$ would still change with ϕ . Instead of trying to use experiments to generate the desired gas-phase data, the model was set up to simulate fully premixed operation with constant T_{bdc} . Please note that the model was extensively compared with engine results in Ref. [6], and generally good agreement was found. In particular, the model response to changes of ϕ agreed fairly well with the experiment. Figure 4 shows the model response to changes of the supplied ϕ when T_{bdc} is held constant. The results are insightful. With increasing ϕ , the autoignition timing is retarded.

To understand why the autoignition of ethanol is retarded with increasing ϕ , Fig. 5 plots the temperature traces for $\phi = 0.30$ and 0.60 . As can be seen, the compressed-gas temperature 5°CA before TDC is 47 K lower for the higher- ϕ case. This is a thermodynamic effect caused by a higher heat-capacity of the charge, leading to a lower ratio of specific heat capacities (lower γ). This is a well-known cooling effect that is used regularly to suppress engine knock at high loads in SI gasoline engines by operating the engine rich of stoichiometric [23].

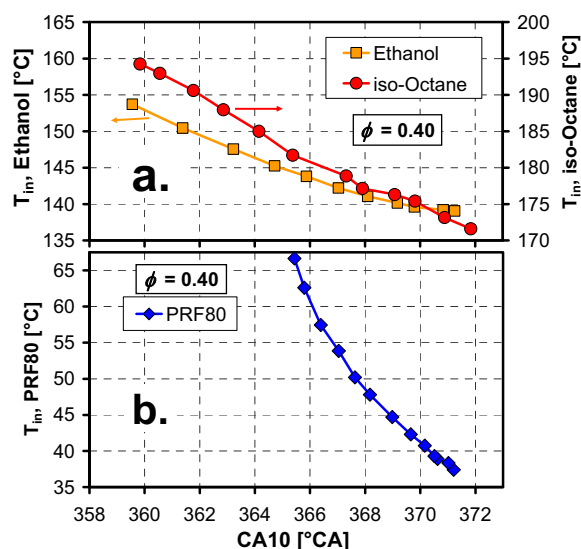


Figure 3. Required T_{in} as a function of CA10 for ethanol, iso-octane, and PRF80. $\phi = 0.40$.

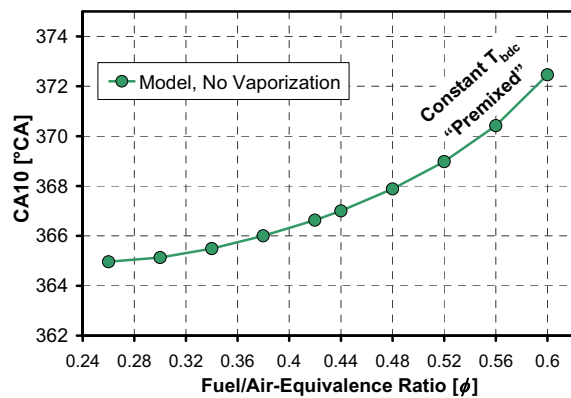


Figure 4. Model prediction of premixed engine operation. CA10 is plotted against ϕ for constant $T_{bdc,max} = 152^\circ\text{C}$ (see Appendix A for definition of $T_{bdc,max}$). Only gas-phase ethanol. Reproduced from Ref. [6].

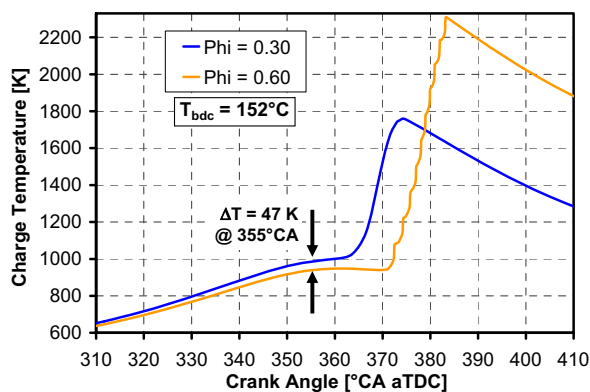


Figure 5. Model prediction of temperature traces for operation with $T_{bdc,max} = \text{const} = 152^\circ\text{C}$ with $\phi = 0.30$ and 0.60 . Ethanol, 1200 rpm, and $P_{in} = 100$ kPa. Reproduced from Ref. [6].

However, the autoignition-suppression effect resulting from gas-phase thermodynamic cooling is greater for ethanol than for traditional non-oxygenated fuels like gasoline. (In the following example, iso-octane serves as a gasoline surrogate since its thermodynamic properties are more accurately known.) First, the stoichiometric air/fuel ratio is 40.5% lower for ethanol; 9.0 vs. 15.1 for iso-octane. As Fig. 6 shows, this requires 68% more fuel mass to be supplied to achieve the same ϕ . With the same ϕ , the delivered chemical energy is practically the same since also the lower heating value of ethanol is 40.5% lower than that of iso-octane. Ethanol has substantially lower mass-specific heat capacity than iso-octane [6,24]. Nonetheless, because the required amount of fuel is 68% greater, the total heat capacity of the fuel in gas phase becomes 33% higher than for iso-octane. (The heat capacities of the two fuels were computed for a temperature of 700 K, which is roughly half-way between T_{bdc} and the ignition temperature.) This fact, combined with the high temperature sensitivity of ethanol autoignition (see Fig. 3a), explains why Fig. 4 shows such a strong retarding effect of increasing ϕ .

To better understand the fuel-chemistry contribution to the gas-phase ϕ -sensitivity plotted in Fig. 4, additional

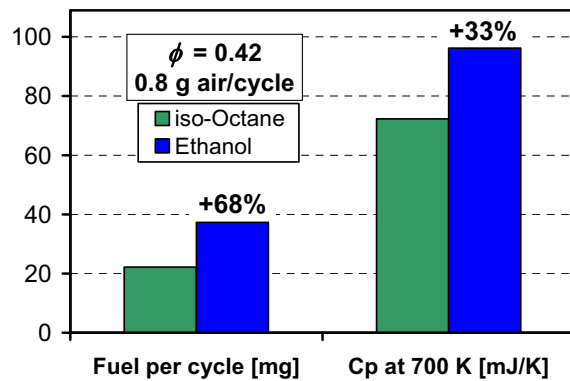


Figure 6. Illustration of differences in fueling rate and heat capacity of the fuel between iso-octane and ethanol. Reproduced from Ref. [6].

computations were performed. First, the model was exercised with all the reactions disabled. This allowed the determination of the T_{bdc} adjustment required to compensate for the increase of heat capacity with ϕ and achieve the same temperature at 355°CA . Figure 7a shows how $T_{bdc,max}$ had to be adjusted to achieve a constant compressed-gas temperature at 355°CA , which is when significant breakdown of ethanol starts according to Fig. 2a. (See Appendix A for definition of $T_{bdc,max}$.) With the cooling effect of more gas-phase ethanol removed, the CA10 trend reverses, as plotted in Fig. 7b and illustrated by the curved arrow. With thermodynamic effects removed, cases with higher ϕ ignite earlier, indicating that there is a small direct effect of the fuel concentration on the rate of the autoignition reactions.

Figure 8 illustrates the fuel-chemistry effects by plotting the temperature and heat-release traces for two different ϕ , using the $T_{bdc,max}$ from Fig. 7. For each ϕ , the compressed-gas temperatures are identical until 353°CA regardless of the reactions being

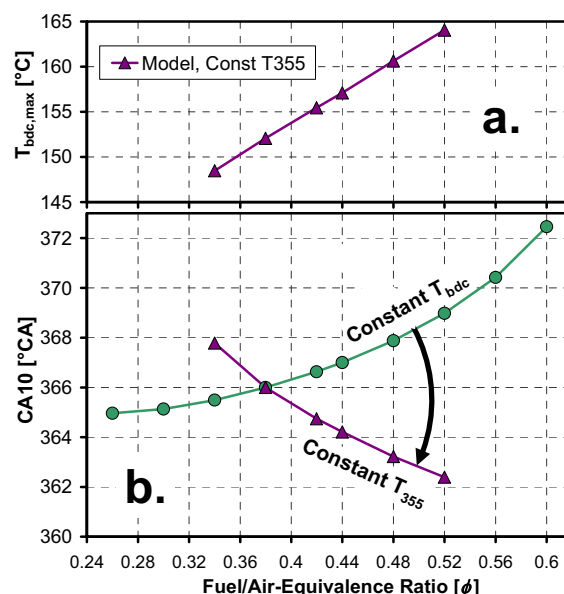


Figure 7. Effect of removal of γ -effect on ϕ -sensitivity. Gas-phase only. Ethanol, 1200 rpm and $P_{in} = 100$ kPa.