The influence of intake pressure and ethanol addition to gasoline on single- and dual-stage auto-ignition in an HCCI engine

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Abstract:

Autoignition in HCCI engines is known to be controlled by the combustion kinetics of the in-cylinder fuel/air mixture which is highly influenced by the amount of low-temperature and intermediate-temperature heat release (LTHR & ITHR) that occurs. At lower intake pressures (typically < 1.4 bar absolute), it has been observed that gasoline behaves as a single-stage heat release fuel, while at higher intake pressures (typically > 1.8 bar absolute) gasoline behaves as a two-stage heat release fuel. Furthermore, ethanol blending strongly affects heat release characteristics, and this warrants further investigation.

This paper experimentally investigates the conditions under which gasoline transitions from a single-stage heat release fuel to a two-stage heat release fuel as intake pressure is increased. Experiments were performed in single-cylinder HCCI engine fueled with two research-grade gasolines, FACE A and FACE C. These gasolines were tested neat, with 10% and 20% (by volume) ethanol addition. In addition, these results were compared to results previously obtained for PRF 85, and new results for PRF 84 with 10% and 20% ethanol addition. Moreover, the engine experiments were supported by rapid compression machine (RCM) ignition delay data for the same fuels.

The engine experiments revealed that there were minimal differences between the heat release profiles of the two gasolines, FACE A and FACE C, which was confirmed by the RCM experiments that showed similar ignition delay data for the two FACE fuels and PRF 84. On the other hand, with ethanol addition to these gasolines and PRF 84, the occurrence of LTHR shifted to higher intake pressures compared to ethanol-free cases, precisely from 1.4 bar intake pressure for neat fuel to 2.2 bar with 20% ethanol. Consequently, the intake temperatures required to
achieve constant combustion phasing for all mixtures were drastically altered. Simulations using a detailed chemical kinetic model were utilized to understand the effects of ethanol blending on the ignition characteristics of PRF 84. Addition of ethanol was found to act as a radical sink where it inhibits the radical pool formation during the low- (< 850 K) and intermediate- (850 – 1050 K) temperature chemistry regimes resulting in lower reactivity. These results help explain ethanol’s significant anti-knock qualities under boosted conditions in spark-ignition engines.

I. Introduction:

Homogeneous Charge Compression Ignition (HCCI) engines fundamentally rely on the autoignition of a fuel-oxidizer mixture for operation [1]. Therefore, it is critical to understand the auto-ignition behavior of any fuel used in an HCCI engine, so that the conditions for auto-ignition of the fuel-oxidizer mixture can be achieved in the engine at the appropriate part of the cycle. Further, other advanced engine concepts, such as Gasoline Compression Ignition (GCI) [2, 3] and Partially Premixed Compression Ignition (PPCI) [4, 5], also feature an auto-ignition process that influences the combustion behavior by controlling the degree of fuel-oxidizer mixing prior to combustion (followed by a mixing-controlled combustion regime). Understanding the auto-ignition of fuels in these engines is critical to their operation; however, due to the highly inhomogeneous mixture found in these other advanced engine concepts, the HCCI engine is perhaps a more suitable engine system for studying fuel auto-ignition [6].

In an HCCI engine, two types of auto-ignition are typically encountered: single-stage ignition and two-stage ignition [7, 8]. In general, fuels with low reactivity, such as methane, will ignite in a single stage; where the fuel autoignites upon reaching a certain temperature and pressure, and releases all its chemical energy [9, 10]. In contrast, highly reactive fuels, such as n-heptane, will typically display a two-stage autoignition process. In the first stage, heat is released
at low temperatures (typically < 850 K and on the order of 1% to 5% of the fuel’s chemical energy) [10], which is termed Low-Temperature Heat Release (LTHR). The second stage is the main auto-ignition event, which releases the majority of the fuel’s chemical energy. Single-stage or two-stage auto-ignition in an HCCI engine can be separated by whether a fuel does or does not produce LTHR under a set of operating conditions.

LTHR has been shown to depend on both fuel type and engine operating conditions. In [8], it is shown that a Primary Reference Fuel (PRF), PRF 80, can display either no LTHR behavior at low intake pressures and high engine speeds, or display LTHR at high intake pressures and low engine speeds. This behavior was further explored in [10]. The LTHR behavior was found to be sensitive to fuel composition (ratio of iso-octane to n-heptane), intake pressure, engine speed (residence time), and exhaust-gas recirculation (charge composition). In [10], it is shown that as the intake pressure of the engine is increased such that a fuel transitions from displaying no LTHR to some LTHR, the fuel’s resistance to auto-ignition diminishes greatly, and the engine operating conditions needed to maintain constant combustion phasing change significantly.

In [11], the LTHR behavior of PRF combustion was investigated in an HCCI engine using chemical kinetic modeling. A particular focus of that study was the intake pressure sensitivity of the fuel autoignition. This pressure sensitivity was shown to be dependent on O$_2$ addition reactions in the fuel’s low-temperature chemistry pathways, specifically addition of molecular oxygen to alkyl and hydroperoxy alkyl radicals (R+O$_2$ = RO$_2$ and QOOH + O$_2$ = O$_2$QOOH).

Previous investigations into LTHR in high-octane fuels have focused on PRF’s or traditional gasolines. However, interactions between alcohols and various gasoline components, such as alkanes, alkenes, and aromatic species, or blends of components, have not been as
thoroughly explored as the behavior of individual hydrocarbons and mixtures of hydrocarbons, although some previous work can provide guidance. In [12], Anderson et. al. demonstrated the strong effect of ethanol addition on the Research Octane Numbers (RON) of gasoline-ethanol blends. In [12], although ethanol increased gasoline’s RON rating significantly, the influence on the Motor Octane Number rating was minor, contributing to increased Octane Sensitivity, which is inversely correlates with the tendency towards low-temperature oxidation reactions. In [13], Stein et. al. demonstrated the strong knock resistance of ethanol and ethanol-gasoline blends in a boosted spark-ignition engine, attributing approximately half of ethanol’s knock resistance benefit to charge cooling from the high heat of vaporization of ethanol, and the rest of the benefit to improved chemical knock resistance. Foong et. al. reinforced the nonlinear blending influence of ethanol on the RON of gasoline in [13], supporting the findings of [12], and using both Primary Reference Fuels (PRF’s) as well as gasoline as base fuels. The experimental trends in [13] were later modeled in [15], and while the model was found to qualitatively reproduce the trends of the experiment, accurate prediction of autoignition was not observed. Kalaskar et. al. [16] provided more fundamental engine investigations on ethanol-PRF blending, using homogeneous motoring-engine experiments to investigate the changes in reactivity derived from ethanol blending over a wide range of temperature-pressure conditions. Of particular note was the reduction in low-temperature reactivity associated with the blending of ethanol and PRF’s. This study investigates the differences in autoignition behavior between two gasoline blends and one primary reference fuel at different intake pressures in an HCCI engine. In addition, the effects of adding ethanol to these gasolines and to the gasoline surrogate (PRF 84) are studied by adding 10% and 20% ethanol by volume to the three base fuels. The investigations were carried out using both experiments and modeling. Experimentally, the investigations were performed by conducting an intake pressure
sweep of each fuel to measure at which intake pressure the fuel begins to display LTHR while running in HCCI operation. The HCCI engine experiments are supported by rapid compression machine (RCM) experiments in which ignition delay times were measured for the fuels, under conditions similar to those encountered in the engine in the low-temperature regime. Then, RCM measurements were used to test an updated detailed chemical kinetic mechanism for PRF mixtures, which in turn was used to simulate the HCCI engine experiments, probing the effects of fuel composition and intake pressure on the auto-ignition process and LTHR occurrence.

II. Methodology:

a) Engine

All engine experiments were performed using a single cylinder of a 4-cylinder VW TDI engine, modified extensively for HCCI operation. These modifications include the addition of separate intake and exhaust tracts for the cylinder-of-interest, pressure transducers and thermocouples in the intake and exhaust tracts, and automotive-type oxygen sensors in the exhaust system. In-cylinder pressure sensing, port-fuel injection, and custom shallow-bowl pistons were also added. A more detailed description of the modifications can be found in [12]. A schematic of the experimental setup can be found in Figure 1, while engine specifications may be found in Table 1. In this engine experiment, fuel was introduced in the intake port immediately following the closure of the intake valve, allowing the fuel 490.5 crank-angle degrees (CAD) to evaporate before being introduced into the combustion chamber. It is assumed that the majority of the heat of vaporization is derived from surfaces, namely the walls of the intake port and the intake valve. Therefore, effects of fuel heat of vaporization and differences among fuels in this respect are expected to be small.
Figure 1: A representative schematic of the experimental engine.

Table 1: Key engine parameters and operating conditions.

<table>
<thead>
<tr>
<th>Experimental Engine Specifications and Operating Conditions</th>
<th>Fuel Injection System</th>
<th>Port Fuel Injection</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compression Ratio</td>
<td>17:1</td>
<td></td>
</tr>
<tr>
<td>Displacement</td>
<td>0.474 L</td>
<td></td>
</tr>
<tr>
<td>Bore</td>
<td>79.4 mm</td>
<td></td>
</tr>
<tr>
<td>Stroke</td>
<td>95.5 mm</td>
<td></td>
</tr>
<tr>
<td>Connecting Rod Length</td>
<td>144 mm</td>
<td></td>
</tr>
<tr>
<td>Coolant Temperature</td>
<td>95 °C</td>
<td></td>
</tr>
<tr>
<td>Oil Temperature</td>
<td>100 °C</td>
<td></td>
</tr>
<tr>
<td>Engine Speed</td>
<td>1400 RPM</td>
<td></td>
</tr>
<tr>
<td>Intake Pressure</td>
<td>1.0 - 2.3 Bar$_{\text{abs}}$</td>
<td></td>
</tr>
<tr>
<td>CA50</td>
<td>4, 6, 8, 10 CAD aTDC</td>
<td></td>
</tr>
<tr>
<td>Fuel Injection System</td>
<td>Port Fuel Injection</td>
<td></td>
</tr>
<tr>
<td>Fuel Pressure</td>
<td>45 PSI</td>
<td></td>
</tr>
<tr>
<td>Number of Valves per Cylinder</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Intake Valve Opening</td>
<td>2 °bTDC</td>
<td></td>
</tr>
<tr>
<td>Intake Valve Closure</td>
<td>47.5 °aBDC</td>
<td></td>
</tr>
<tr>
<td>Exhaust Valve Opening</td>
<td>47.5 °bBDC</td>
<td></td>
</tr>
<tr>
<td>Exhaust Valve Closure</td>
<td>8 °aTDC</td>
<td></td>
</tr>
<tr>
<td>Equivalence Ratio</td>
<td>0.4</td>
<td></td>
</tr>
<tr>
<td>Intake Temperature</td>
<td>23 - 171 °C</td>
<td></td>
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</tbody>
</table>
and the intake temperature was adjusted to attain the correct CA50, all at a fixed engine speed of 1400 RPM and fuel-air equivalence ratio of 0.4. Thus, for less reactive conditions, a higher intake temperature was required to achieve a fixed CA50, and for more reactive conditions a lower intake temperature was required.

At each engine operating condition, the in-cylinder pressure was measured for 300 consecutive cycles. In addition, each operating point was measured twice back-to-back to ensure repeatability. During post-processing, the 300 consecutive pressure traces were first filtered, using a Savitzky-Golay filter of 19 points, and then averaged. The calculation of the rate of heat release (ROHR) was made in a manner described in [18] using the average filtered pressure trace for each engine operating point. The method used accounts for wall heat losses via a Woschni model [19], mass loss due to blow-by, and changing specific heat ratios of the gas due to both temperature change as well as gas composition change from reactants to products (calculated from NASA thermodynamic tables). All constants in the model were tuned using motoring pressure traces and a cycle simulation model in AVL BOOST, as described in [20]. In addition to the ROHR, the in-cylinder mass-averaged temperature was calculated using the ideal gas model. A more detailed description of the calculation methods can be found in [21].

In this study, nine fuels were compared. Three base fuels were used, FACE A, FACE C, and PRF 84. Specifications of these fuels can be found in Table 2, as well as in [22]. FACE A and C were chosen for use in this study due to their general similarity as low-Octane Sensitivity gasolines with nearly identical RON and MON ratings, but with varying distributions of iso- and normal alkane fractions. FACE A and C also have octane ratings which are below common U.S. regular-grade 87 Anti-Knock Index gasoline, making them good candidates for ethanol blending, as is now typical in the U.S. The goal in studying such similar fuels was to determine
experimentally, in the HCCI system which is very sensitive to autoignition properties, whether meaningful differences in these fuels’ autoignition behavior could be observed, before moving on to the study of fuels with greater variations in composition and properties (as will be described in future manuscripts). PRF 84 was also incorporated into the experimental matrix as it is a useful kinetic surrogate for both FACE A and C, while also representing a fuel with varying physical properties in a system which should be relatively insensitive to them. Six additional fuels were created by blending each of the three base fuels with two levels of ethanol—10% and 20% ethanol by volume, in order to observe the effects of ethanol blending on low- and intermediate temperature oxidation, at blend levels which are relevant to U.S. gasoline. New experimental data was collected with two base fuels, FACE A and C; in addition to the six blends with ethanol. However, problems related to the experimental device hindered measurements for neat PRF 84. Accordingly, the new data was compared against previously obtained data for PRF 85 [10]. It is worth mentioning that the new data was acquired for constant combustion phasing (CA50) of 6 CAD aTDC, while for PRF 85 was 8 CAD aTDC; the same experimental apparatus was used in both cases, although with minor modifications between data sets. Despite these differences, the PRF 85 data can be still used for comparing trends, although quantitative comparisons are not made.

Table 2: FACE A and C fuel specifications in comparison with their primary reference fuel (PRF) surrogate, PRF 84 [22].

<table>
<thead>
<tr>
<th></th>
<th>FACE A</th>
<th>FACE C</th>
<th>PRF 84</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td>83.9</td>
<td>84.3</td>
<td>84.0</td>
</tr>
<tr>
<td>MON</td>
<td>83.5</td>
<td>83.0</td>
<td>84.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------------------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>Octane Sensitivity [-]</td>
<td>0.4</td>
<td>1.3</td>
<td>0.0</td>
</tr>
<tr>
<td>H/C Ratio [-]</td>
<td>2.29</td>
<td>2.27</td>
<td>2.26</td>
</tr>
<tr>
<td>Average Molecular Weight [g/mol]</td>
<td>97.8</td>
<td>97.2</td>
<td>112.0</td>
</tr>
<tr>
<td>n-alkanes [volume %]</td>
<td>11.7</td>
<td>24.4</td>
<td>16.0</td>
</tr>
<tr>
<td>iso-alkanes [volume %]</td>
<td>86.0</td>
<td>69.7</td>
<td>84.0</td>
</tr>
<tr>
<td>Aromatics [volume %]</td>
<td>0.6</td>
<td>3.9</td>
<td>0.0</td>
</tr>
<tr>
<td>Alkenes [volume %]</td>
<td>0.1</td>
<td>1.3</td>
<td>0.0</td>
</tr>
<tr>
<td>Cycloalkanes [volume %]</td>
<td>1.6</td>
<td>0.7</td>
<td>0.0</td>
</tr>
</tbody>
</table>

b) RCM

The RCM data in this study was generated at the University of Connecticut. The RCM facility has been previously described in detail in [23]. The University of Connecticut RCM employs a pneumatically driven creviced piston that is hydraulically arrested and locked, with a compression time of roughly 30 ms. The pressure measurement is taken with a Kistler 6125C pressure transducer, and the signal is amplified using a Kistler 5010B charge amplifier. The compressed temperature and pressure are altered via uncompressed pressure and compression ratio (which is varied via changes to the stroke and the clearance volume), while uncompressed temperature was held constant at 333 K. All mixtures of fuel and undiluted air at an equivalence ratio of 0.4 were prepared in a stainless-steel chamber separate from the RCM and allowed sufficient mixing time to ensure homogeneity.
The ignition delay times of six fuels were measured during the course of this study, for temperatures ranging from 632 to 745 K, at 20 and 40 bar pressures. The operating conditions were chosen to interrogate ignition delay times in the low-temperature regime, as well as the transition to Negative Temperature Coefficient (NTC) behavior. Further, as the effect of pressure was a focus of the engine investigations, the effect of doubling compressed pressure was also included in the RCM experiments as well. Additional considerations were the need to test conditions which resulted in ignition delays which were sufficiently long to be unaffected by the RCM compression stroke ($\tau_{\text{ign}} > 5$ ms) and short enough to be unaffected by heat transfer ($\tau_{\text{ign}} > 100$ ms). These goals and constraints led to the range of tested conditions.

The six fuels used in RCM experiments were FACE A, FACE C, PRF 84, and the E10 (base fuel + 10% ethanol by volume) blends of these three fuels. Both first stage and total ignition delays were determined from the measured pressure traces, using the time from the end of the compression stroke to the local maximum pressure derivative for each stage of the pressure rise (first stage, where applicable, and main pressure rise). To ensure repeatability, a minimum of five samples were taken at each condition to create a single reported data point; this reported data point was the measured value closest to the mean of the experiments. The uncertainty in all the reported RCM ignition delays measurements is less than 10% of the mean value.

c) 0-D Chemical Kinetic Modeling of Engine Experiments

The HCCI engine experiments were simulated using a 0D multi-zone model (coupled homogeneous batch reactors) created in CHEMKIN PRO [24]. The Chemkin model was used rather than a 3D CFD model to facilitate the use of detailed chemical kinetic mechanisms which
are required for better understanding of autoignition chemistry in HCCI engines [25]. Simulation results are only presented for PRF 84 and its mixtures with ethanol. Previous work has shown that PRF 84 is a suitable surrogate for FACE A and C gasolines under a range of HCCI-relevant pressure and temperature conditions [23, 26]; however, multicomponent surrogates may be required to accurately simulate FACE A and C at high pressures (> 20 bar) and low temperatures (< 750 K) [23]. Simulations using detailed chemical kinetic models with multicomponent surrogates (e.g., [27, 28]) were not pursued in this work.

The multi-zone HCCI model was created in the following manner: First, RANS CFD simulations of the experimental engine were carried out using CONVERGE™ [29] for non-reacting (no-fuel air-only motoring) cases to determine the temperature distribution at TDC for a given intake pressure and temperature. At TDC, the charge was divided into 20 zones, such that the maximum temperature in each zone varied by 10 K (except in the highest and lowest temperature zones, which had small mass fractions < 5%). These results were used to create a Chemkin multi-zone model. The model was created such that the average temperature and pressure of the model replicated the average temperature and pressure of the CFD results during the compression and expansion strokes, as can be seen in Figure 2 (a) and (b). The 20 zones in the Chemkin model use the same mass fractions as the 20 groupings from the CFD work, and all zones are initialized with uniform temperature, pressure, and composition. Differences in zone temperature in the model under non-reacting conditions are entirely due to varying heat transfer rates, and the relative heat transfer rates of each zone are shown in Figure 2 (c). The relative heat transfer rates of the zones have been scaled to give the same temperature distribution at TDC as in the CFD results. The temperature distributions of motoring conditions at TDC for two intake pressures and temperatures are shown in Figure 2 (d). The model acceptably reproduced the in-
cylinder temperature distribution predicted by the CFD simulation for both high and low intake pressures (1.0 bar to 2.2 bar), with high and low intake temperatures (~ 175 °C to ~ 30 °C), respectively. In use, the starting temperature of the model was varied to match the experimental CA50 with the CA50 of the multi-zone model.

The RCM ignition delay data for PRF 84 and PRF 84+10% ethanol were also simulated using CHEMKIN PRO. Those simulations were conducted using the batch reactor module while utilizing the experimental volume profiles to account for the facility heat loss effects.

The 0-D simulations in CHEMKIN PRO were conducted using three different mechanisms: Cai et. al. [30], Lawrence Livermore National Laboratory (LLNL) [25], and a newly updated PRF model. Cai et al. [30] developed an optimized model for PRF/toluene/ethanol mixtures (iso-octane, n-heptane and toluene) with 1027 species and 4236 reactions. The model was validated against ignition delay times, burning velocities, and jet stirred reactor and flow reactor data of pure fuels and binary, ternary and quaternary mixtures of n-heptane, iso-octane, toluene, and ethanol. The LLNL model includes the detailed combustion chemistry of PRF mixtures, 1-hexene and toluene, which are used as gasoline surrogates. The model demonstrates good agreement with shock tube and RCM experiments at pressures and temperatures relevant to advanced compression ignition engines. However, several engine studies [10, 23, 31] reported the inability of the current LLNL model to reproduce the LTHR behavior of gasoline-like fuels in HCCI engines, which motivated the update of the LLNL model.

The updated PRF model is based on updating the LLNL model with the recently developed n-heptane sub-model by Zhang et al. [32] and the iso-octane sub-model by Atef et al. [33]. In both sub-models, the thermochemistry and rate rules were updated using new group values [34]. In addition, 9 classes of reactions related to the low-temperature chemistry were updated using newly
computed rate rules from literature, which resulted in improved low-temperature reactivity for n-heptane and iso-octane as demonstrated by Zhang et al. [26] and Atef et al. [27]; respectively. The 9 classes are:

1- H-abstraction by OH, which was updated using experimentally driven rate rules from Sivaramakrishnan et al. [35] and Badra et al. [36]

2- The first and second addition to molecular oxygen (R+O_2=RO_2 and QOOH+O_2=O_2QOOH) which were updated based on the rate rules calculated by Villano et al. [37].

3- Isomerization of peroxy radicals to hydroperoxy alkyl radicals (RO_2=QOOH), which was updated using with rate parameters from Villano et al. [38]

4- The concerted elimination from peroxy radicals (RO_2=olefin+HO_2). This class is responsible for inhibiting reactivity at negative temperature coefficient region (NTC). In the n-heptane sub-model, the rate rules from Villano et al. [37] were implemented, while the rates by Auzmendi-Murua et al. [39] and Snitsiriwat et al. [40] were incorporated in the iso-octane sub-mechanism.

5- The formation of olefins and β-scission of hydroperoxy alkyl radicals were updated using the rate rules by Villano et al. [38] and Bugler et al. [41]; respectively.

6- The formation of cyclic ethers from hydroperoxy alkyl radicals; which is another inhibiting reaction. Rate parameters from Villano et al. [38] and Miyoshi [42] were implemented in the n-heptane and iso-octane sub-mechanisms; respectively.

7- The formation of ketohydroperoxides, which is the main chain branching pathway at low and intermediate temperatures. This class was updated using rate rules calculated by Sharma et al. [43].
Both sub-models have the same base chemistry [44], so the thermochemistry of n-heptane species and reaction classes from n-heptane sub-mechanism [32] was moved to the iso-octane published model [33, 45]. As will be shown later, the updated PRF model utilized here better predicts the RCM and HCCI engine data obtained in this study.

III. Results and Discussion:

Figure 2: Comparisons of pressure (a) and average temperature (b) profiles for RANS and 0-D models at 2.2 bar intake pressure under a non-reacting condition, as well as heat transfer multipliers and zone mass fractions (c) and example temperature and mass distributions at 1.0 bar and 2.0 bar intake pressure (and varying intake temperature) (d).
a) *Engine*

An HCCI engine was used to evaluate the autoignition properties of nine gasoline-type fuels. These fuels were composed of three neat gasolines, namely FACE A, FACE C, and PRF 85, and six gasoline-ethanol blends, FACE A, FACE C and PRF 84 with ethanol at 10% and 20% by volume. Figure 3 plots the intake temperatures required to maintain constant combustion phasing for each fuel at a given intake pressure. By holding combustion phasing constant at a fixed engine speed, the effective ignition delay time (time between the start of the compression stroke and autoignition) of the fuel-oxidizer charge is held constant. Thus, the required intake temperature is a function of a fuel’s overall reactivity at a given set of conditions and indicative of the type of heat release exhibited by the fuel at ignition.
Figure 3: Required intake temperature to maintain constant combustion phasing (6 CAD aTDC; 8 CAD aTDC for PRF 85) over a range of intake pressures for nine different fuels at 1400 RPM and an equivalence ratio of 0.4.

Figure 3 presents the intake temperature required to maintain constant combustion phasing at 6 CAD aTDC at a range of intake pressures for the 8 newly tested fuels. In addition, intake temperature data for PRF 85 from [10] is presented for comparison, due to the lack of available PRF 84 data. The PRF 85 data was taken under similar conditions in a prior experimental campaign, although the combustion phasing (CA50) was fixed at 8 CAD aTDC. Figure 3 demonstrates that at low intake pressures, all newly tested fuels required approximately the same
intake temperature (154 – 167 °C) to autoignite at a fixed combustion phasing, which indicates a similar level of reactivity among the fuels. In all cases increased intake pressures caused the intake temperature required to maintain constant combustion phasing to decrease, indicating an increase in fuel reactivity. In general, the tested fuels behaved similarly to one another at constant ethanol blending levels, perhaps unsurprising considering their similar chemical compositions.

The response of the fuels to intake pressure was observed to generally follow a trend of relatively linearly decreasing intake temperatures, followed by an inflection point, followed by a second approximately linear decrease in intake temperature, albeit with a heightened response to intake pressure. This behavior is best represented by the 10% ethanol blend data, in which the inflection point occurs at approximately 1.4 bar intake pressure and 110 °C intake temperature, which exists sufficiently far from the bounds of the range of experimental operating conditions that this trend may be clearly observed. In the case of the neat fuels, the inflection point occurs at approximately 1.2 bar intake pressure, reducing the availability of data on either side of the inflection point. Below 1.2 bar intake pressure with the neat fuels, the change in intake temperature required for constant combustion phasing as intake pressure changes is approximately -180 °C/Bar, while above this intake pressure it shifts to approximately 350 °C/Bar, or an approximate doubling in the sensitivity to intake pressure. At the highest intake pressure tested with FACE A and C, 1.5 bar, it is possible that the sensitivity to intake pressure is beginning to decrease, as is predicted by the modeling work presented later in this study, although insufficient data exists to make a firm determination. Finally, in the case of the 20% ethanol blends, the linear behavior exists over the majority of the tested intake pressure range, with a possible inflection point at approximately 2.1 bar intake pressure. Here, the FACE A + 20% ethanol blend exhibits the sharpest decrease in intake temperature of the three 20% ethanol blends. The FACE C + 20% ethanol and PRF 84 + 20%
ethanol blends exhibit a slight increase in sensitivity to intake pressure over the following two test points at 2.2 bar and 2.3 bar intake pressure.

Figure 4 (a) – (d) plots calculated heat release traces for the eight tested fuels at four different intake pressures. In general, the fuels exhibited similar behavior at a fixed level of ethanol blending, i.e. neat, 10%, or 20%. This is not to say that no differences were observed among the fuels at a given blend level of ethanol, only that these differences were small relative to the differences caused by ethanol addition. These results are consistent with the HCCI engine experiments by Shankar et al. [26].

Figure 4 (a) shows that at low intake pressures, all tested fuels, regardless of their ethanol content, exhibited single-stage heat release behavior. Figure 4 (b) shows the ROHR of 8 fuels at 1.4 bar intake pressure. This figure demonstrates that the FACE A and FACE C fuels exhibit LTHR at this intake pressure, which consequently increased their overall reactivity and rapidly decreased their intake temperature as previously shown in Figure 3. At the 1.8 bar intake pressure condition presented in Fig. 5 (c), fuels with 10% ethanol display obvious LTHR, which again coincided with the heightened intake temperature sensitivity to changes in intake temperature shown in Figure 3. Finally, considering Fig. 5 (d), which plots ROHR traces from the 2.2 bar operating condition, it may be seen that the fuels with 20% ethanol exhibit LTHR at this condition, although it is muted compared to what is observed in Figure 4 (b) & (c).
Figure 4: Heat release profiles in the LTHR and ITHR regions (labeled) for the 8 fuels tested (where possible) at different intake pressures: 1.0 bar (a), 1.4 bar (b), 1.8 bar (c), and 2.2 bar (d), at 1400 RPM and an equivalence ratio of 0.4.

The information presented in Figures 3 and 4, which plot intake temperatures required for constant combustion phasing and ensemble average rate of heat release profiles respectively, indicate a correlation between the observed heat release behavior leading up to the bulk autoignition and the required intake temperature. These figures show that under engine operating conditions which cause observable LTHR, lower intake temperatures are required to achieve constant combustion phasing, and heightened sensitivity to intake pressure exists. This indicates
that under these conditions, the required intake air temperature for autoignition is an indicator of
the fuel’s heat release behavior leading up to autoignition.

Conclusively from the data presented in Figures 3 and 4, it is obvious that fuel reactivity
increases with increasing intake pressure. However, this reactivity increases more in cases at which
the fuel demonstrates two auto-ignition stages. This indicates a strong correlation between LTHR
and reactivity, wherein LTHR increases the autoignition propensity of the fuel significantly.
Figures 3 and 4 show that the onset of LTHR as intake pressure is increased changes the slope of
the intake-pressure/intake-temperature relation, such that the slope becomes more negative
(greater absolute value) after the occurrence of LTHR. In addition, the heat release profiles show
that LTHR is more favored at higher intake pressures, likely due to the higher rates for low
temperature radical chain branching chemistry, as will be discussed later in the kinetic simulations
section. The experimental findings presented here agree well with previous work on low-
temperature oxidation in HCCI engines performed with PRF’s [8, 10] and PRF blends with ethanol
[16], in that increased intake pressure supports low-temperature oxidation of PRF’s [10], and
ethanol addition suppresses this behavior [16].

The aforementioned observations regarding the occurrence of LTHR and the change in
slope between required intake temperature and intake pressure has significant practical
implications. In transient operation of the engine, under conditions in which the intake pressure is
changing, it is expected that the intake temperature required for constant combustion phasing will
approximately follow the trends seen in Figure 3. Therefore, in the low intake pressure regime in
which LTHR does not occur, small changes in intake temperature would be required. However,
once LTHR onset occurs, the rate of change of intake temperature would increase significantly.
This could prove to be challenging for a control strategy, as the onset of LTHR has been shown to
be sensitive to the composition of the fuel. Since the reactivity of dissimilar fuels with varying LTHR onset pressures, such as the PRF 84 with 10% vs. 20% ethanol addition, can be similar at low intake pressures, operation at idle and low load may not be sufficient for an engine controller to estimate the high-load behavior of a fuel, especially with regards to the intake pressure at which LTHR onset begins. As intake pressure increases, the fuel will transition from single-stage ignition behavior to dual-stage behavior and the engine controller will be required to account for a significant change in reactivity; this challenge is compounded by the strong effect of ethanol on the onset of LTHR in intake pressure space, which may cause uncertainty as to the intake pressure level which will trigger LTHR. In the combustion strategy used in these experiments, the transition to LTHR would require a rapid drop in intake heating or other IVC temperature control method to achieve constant combustion phasing; however, such a strategy is not realistic for a light duty vehicle, and would need to be substituted for an alternative strategy, such as the application of exhaust gas recirculation.

Heretofore, all presented experimental results have been obtained with a combustion phasing of 6 CAD aTDC. In addition to this phasing, measurements were performed at 4 CAD aTDC, 8 CAD aTDC, and 10 CAD aTDC. These sweeps revealed that when using intake temperature to control combustion phasing, the amount of LTHR can be affected due to the changes in the temperature history during the compression stroke. Figure 5 shows the conditions under which LTHR begins to occur with significant magnitude by plotting the bulk-averaged temperature and in-cylinder pressure at the peak low-temperature heat release rate. Due to engine operability limits, primarily the experimental setup’s inability to produce sub-ambient intake temperatures, the full space of LTHR cannot be explored, however the outline of LTHR’s limits on the high-temperature and low-pressure boundary can be seen. For the residence time
encountered when running at 1800 RPM, pressure must exceed approximately 30 bar while the charge temperature is below approximately 850 K for LTHR to occur in appreciable amounts for the neat fuels. When 10% ethanol is added, a pressure of approximately 45 bar must be exceeded prior to the temperature surpassing 875 K. Finally, in the case of 20% ethanol addition, the pressure must exceed 65 bar while the temperature is below 900 K.

![Graph showing temperature and pressure of peak LTHR for all fuels and conditions tested.](image)

**Figure 5:** Temperature and pressure of peak LTHR for all fuels and conditions tested.

b) *RCM Experiments*

Ignition delay experiments were performed in a rapid compression machine (RCM) at both low (20 bar) and high (40 bar) pressure, with FACE C, FACE C, PRF 84, and +10% ethanol mixtures of these fuels. The fuel-oxidizer mixtures tested in the RCM matched those tested in the engine (except for the small fraction of internal exhaust residuals in the engine experiments): fuel
was mixed with undiluted air at an equivalence ratio of 0.4. The RCM experiments support the HCCI engine experiments, provide more fundamental data on the fuels and fuel mixtures, and help determine the suitability of a PRF surrogate for the two tested FACE fuels. The RCM experiments measured both the first stage (LTHR) ignition delay whenever applicable, as well as the total ignition delay for each fuel.

Figure 6 presents the measured total ignition delay time versus the inverse of compressed temperature ($T_c$). Generally, the ethanol addition decreases the fuel reactivity and increases the ignition delay time at both pressures; 20 and 40 bars. At the 20 bar condition, all six fuels exhibited significant NTC behavior in the measured temperature range. As seen in Figure 6 (a), total ignition delays among the three base fuels were quite similar at 20 bar compressed pressure. However, the ethanol addition to the three fuels caused measurable differences between PRF 84 and FACE A and FACE C, with PRF 84 exhibiting longer ignition delays in the Negative Temperature Coefficient (NTC) region than FACE A or FACE C. The first stage ignition delays at 20 bar, as seen in Figure 6 (c), showed the opposite trend to the total ignition delays; all fuels behaved similarly with 10% ethanol, while with neat fuels there was some variance.
Figure 6: Total Ignition Delays (top panels) and First Stage Ignition Delays (bottom panels) for mixtures of 6 different fuels with undiluted air at an equivalence ratio of 0.4 as measured in a Rapid Compression Machine at two different pressures; 20 bar for (a) and (b) and 40 bar for (c) and (d).

By increasing the pressure of the system to 40 bar, significant changes in ignition delay behavior are seen in Figure 6. First considering the overall ignition delays at this condition, which are seen in Figure 6 (b), the fuels no longer exhibit NTC behavior in the measured temperature range. This is due to shifting of the NTC region to a higher temperature range, as oxygen addition reactions in the low-temperature pathway are supported by the increased partial pressure of oxygen at the 40 bar conditions. Considering the differences in ignition delay behavior among the fuels,
Figure 6 (b) shows nearly identical ignition delays for the three E10 fuels at 40 bar. The three E0 fuels exhibit similar ignition delay times, but PRF 84 is slightly more reactive than the two FACE gasolines. Considering the first stage ignition delays shown in Figure 6 (d), neat PRF 84 has a slightly shorter first stage ignition delay than FACE A and C. Again, once ethanol is added, the first stage ignition delays for all three E10 fuels are indistinguishable.

Figure 6 (a) & (b) show that the three neat fuels show similar ignition delay times at the studied conditions which suggests that PRF 84 is a suitable chemical surrogate for FACE A and C as previously concluded in literature [23, 26]. However, some divergence is noticed during ethanol addition at low pressures (20 bar), and in the timing of the first stage heat release. This is similar to the behavior observed in the engine, in which the PRF 84 + 10% ethanol and + 20% ethanol exhibited nearly identical behavior to FACE A and FACE C with the same volume fractions of ethanol.

c) Kinetic Simulations

Chemical kinetic simulations were performed to elucidate the underlying causes of PRF84’s sensitivity to ethanol addition and boosted intake pressures. The three mechanisms, Cai [30], LLNL Gasoline Surrogate [25], and updated LLNL PRF, were evaluated against both the RCM data and HCCI engine data included in this paper. The three models incorporate different rate parameters for the low temperature chemistry reactions. Figure 7 compares the total rate for production of ketohydroperoxides (KHP) in the three models, both for iso-octane and n-heptane. The formation of KHP is the main branching pathway at low and intermediate temperatures. The figure shows that the rate of KHP formation in both n-heptane and iso-octane is highest in the updated model, which explains the higher reactivity of the updated model compared to the others.
Figure 7: Reaction rate constants for KHP formation in the three models, for iso-octane (a) and n-heptane (b).

Figure 8 (a) – (d) shows the simulation results using the three mechanisms against RCM ignition delay measurements for PRF 84 neat and +10% ethanol at 20 and 40 bar pressures. The lowest level of agreement is shown by the Cai et al. mechanism with a maximum deviation of 160% for PRF at 20 bar, 714 K and 0.4 equivalence ratio. The LLNL and updated models are in reasonable agreement with the experimental measurement, with better results shown by the LLNL mechanism especially for PRF+10% ethanol mixtures.
Figure 8. Ignition Delay Times for PRF84/air mixture at 20 bar (a) and 40 bar (b), and PRF 84 + 10% Ethanol at 20 bar (c) and 40 bar (d) with an equivalence ratio = 0.4. Insets represent 1st stage IDT using the updated model.

Figure 9 (a) – (c) shows the intake temperature – intake pressure trends predicted by the chemical kinetic mechanisms, as well as the experimental data. In the same manner as Figure 3, Figure 9 demonstrates the increase in fuel reactivity with increasing intake pressure as the low-temperature chain branching pathway is activated. The figures show generally poor agreement between the experimental data and the LLNL mechanism with regards to the inflection point which
indicates the onset of LTHR, with only Figure 9 (a) showing this regime (slope) change in the case of the original LLNL mechanism. While the original LLNL gasoline surrogate mechanism did not accurately predict the activation of the low-temperature pathway in intake pressure space, the Cai mechanism and the updated LLNL mechanism showed significantly better ability to simulate the experimental data; however, the agreement was still not sufficient to predictively model this LTHR indicating inflection point an engine. It is worth noting that the ignition event in the engine occurs above 800 K while the RCM experiments were conducted at lower temperatures and longer timescales, illustrating the behavior of the LLNL and Cai et al. mechanisms against different sets of data. Regardless, the experimental trend observed in the engine of a change of slope between $T_{in}$ required for constant combustion phasing and $P_{in}$ as LTHR onset occurs were reproduced, albeit at elevated pressures, and so the updated LLNL gasoline surrogate mechanism was used to gain insight into the activation of the low-temperature pathway, as well as to gain insight into the in-cylinder process under conditions which result in gasoline LTHR.
Figure 9. Experimental and simulated intake temperatures and pressures required for PRF 84/85 (a), PRF 84 + 10% Ethanol (b), and PRF 84 + 20% Ethanol (c) at 0.4 equivalence ratio and constant combustion phasing (CA50 = 6 CAD aTDC).

The effects of ethanol addition to PRF84 on auto-ignition in an HCCI engine were investigated by comparing HCCI engine simulation results for both PRF 84 and PRF 84 +10% ethanol (PRF 84 E10) at an intake pressure of 1.55 bar. The intake temperatures required to keep CA50 at 6 CAD aTDC in the simulations were 390 K and 426 K for PRF 84 and PRF 84 E10,
respectively. The PRF84 results show prominent LTHR, shown in Figure 10 (b), which increases the mixture temperature such that the temperature after the end of the LTHR matches that of PRF 84 E10, as shown in Figure 10 (a). Figure 10 (a) also show that the onset of hot ignition occurred at approximately the same temperature for both PRF 84 and PRF 84 E10, indicating a primarily thermal effect of LTHR.

![Graph showing HRR and temperature profiles for PRF 84 and PRF84+10% ethanol](image)

**Figure 10.** HRR (straight lines) (a) & (b) and temperature (dashed lines) -- (a) only -- profiles for PRF 84 (black) and PRF84+10% ethanol (red) mixtures,

The transition to the LTHR regime for PRF84 at elevated pressures is attributed to the low temperature chemistry of *iso*-octane (IC8) and *n*-heptane (NC7), which produces a radical pool that advances autoignition and decreases the required intake temperature to achieve the desired CA50. However, the addition of ethanol to the mixture replaces the relatively active fuel components (IC8 and NC7) with a less reactive one (C2H5OH). The chemistry of ethanol oxidation is shown in the flux analysis in Figure 11. Ethanol acts as a radical sink in the LTHR regime because it consumes OH and HO2 radicals and leads to HO2 and small molecules (CH3CO) which are stable at low temperature, as shown in Figure 11 and discussed by Kalaskar et al. [16] and Marinove et al. [46]. It is well-known that ethanol doesn’t exhibit low-temperature chemistry [46].
and shows a single-stage heat release in engines experiments as demonstrated by Sjoberg and Dec [47]. Figures 12 and 13 show the flux analysis for n-heptane and iso-octane at 1.55 intake pressure in both cases E0 and E10 mixtures. The analysis is conducted at 20% fuel consumption which corresponds to 872 K and 972 K for the E0 and E10 cases; respectively. The figures show that similar flux in both cases is going towards the formation of alkyl radicals through H-abstraction. However, less flux follows the 1st addition to molecular oxygen in E10 mixture and some of the alkyl radicals formed undergo beta-scission. This is more evident in the iso-octane flux, where 23% and 28% of the primary (AC8H17) and tertiary (CC8H17) alkyl radicals undergo beta-scission in E10 mixture. Moreover, 33% of DC8H17 isomerizes to AC8H17 in E10 mixture, which is one of the main classes characterizing the high temperature chemistry of alkanes. This explains the absence of LTHR in the E10 mixture. The main product of the hydroperoxy alkyl radicals (QOOH) formed by iso-octane is cyclic ethers, while the hydroperoxy heptyl radicals undergo a second addition to molecular oxygen followed by the formation of keto hydroperoxides or alternative isomerization. This different behavior results in lower reactivity of iso-octane compared to n-heptane.

Figure 14 plots the concentrations of HO$_2$ and H$_2$O$_2$ radicals in crank-angle space. HO$_2$ concentrations remain lower in E10 blends because *iso*-octane and *n*-heptane in E0 also produce HO$_2$ radicals via peroxy radical concerted elimination reactions. The build-up of HO$_2$ radicals decreases reactivity; however, the HO$_2$ radicals are converted to H$_2$O$_2$ via recombination reactions as the cylinder temperature increases. Prior to hot ignition, H$_2$O$_2$ concentrations are higher in PRF 84 E10 than PRF 84 (Figure 14), and at hot ignition, H$_2$O$_2$ decomposes to 2 OH resulting in a higher fraction of OH for the ethanol mixture, as seen in Figure 15. Similar behavior was observed by Haas et al. [48].
Figure 11. Flux analysis of ethanol at 10% fuel consumption from all zones.
Figure 12: Flux analysis for iso-octane at 20% fuel consumption and 1.55 intake pressure for E0 (black) and E10 (red) mixtures.
Figure 13: Flux analysis for n-heptane at 20% fuel consumption and 1.55 intake pressure for E0 (black) and E10 (red) mixtures.
Figure 14. $\text{HO}_2$ (straight lines) and $\text{H}_2\text{O}_2$ (dashed lines) profiles for PRF84 (black) and PRF84+10% ethanol (red). The dot-dash line represents hot ignition timing.

Figure 15. OH profile for PRF 84 (black) and PRF84+10% ethanol (red). The inset represents the OH-profile through the LTHR period.

Figure 16: Simulated rate of production of OH for PRF 84 and PRF 84 + 10% ethanol at 1.55 bar intake pressure and 20% fuel consumption.
Figure 16 shows the different reactions contributing to consumption/production of OH for the two mixtures; E0 and E10; at 1.55 bar intake pressure and 20% of fuel consumption which corresponds to -11.9 CAD and -1.1 CAD for E0 and E10, respectively. It is worth mentioning that, -11.9 CAD lies within the LTHR region in the E0 mixture. Overall, OH is being produced in the E0 mixture with a rate of 4.46E-4 mole/cm3.s and consumed with a rate of 4.25E-4 mole/cm3.s in the E10 mixture. The main reactions consuming OH in the E10 mixture are the H-abstraction from iso-octane to produce iso-octyl radicals, while the reaction of formaldehyde with OH (CH2O+OH<=>HCO+H2O) is responsible for OH consumption in E0 mixture. The main path for producing OH is the dissociation of hydrogen peroxide (H2O2(+M)<=>OH+OH(+M)) in the E10 mixture, where the main source of H2O2 is HO2 that is one of the main products in the ethanol chemistry. On the other hand, the O-O scission in CH3O2H is the main production path for OH in the E0 mixture.

In the case of PRF 84, the radical pool produced in the LTHR regime accelerates fuel consumption when compared to PRF 84 E10, as shown in Figure 17, even though the CA50 is fixed at 6 CAD in both cases. Approximately 40% of PRF 84 is consumed in the LTHR regime, while a negligible amount of PRF 84 E10 is consumed at the same CAD. In case of E10, the addition of ethanol suppresses the LTHR and the rate of conversion is the same throughout the cycle. This is illustrated by the conversion profiles of NC7 and IC8 in Figure 17.
Finally, the Chemkin multi-zone model was used to understand the effect of LTHR throughout the cylinder of an HCCI engine. Figure 5 shows that LTHR was observed experimentally at temperatures below ~850 Kelvin and at elevated pressures, that changed with the level of ethanol addition to the fuel, but that ranged from 30 bar (neat PRF 84) to 60 bar (PRF 84 E10). This knowledge, coupled with the knowledge of temperature distributions in HCCI engines, such as in [46], suggest that different regions of the combustion chamber may experience higher or lower LTHR intensity based on their temperature – pressure trajectory. This hypothesis is borne out in Figure 18, which plots the heat release rate for different zones in the multi-zone model against temperature, for -15.5 to -4.7 CAD aTDC, the range of peak LTHR. Figure 18 shows that over the same crank-angle range, zones that are at different temperatures exhibit varying levels of LTHR; here, the hottest zones are the least active, while the coolest zones release the most heat, with the heat release rate varying between the hottest and coolest zones by a factor of six. This has implications for both the experiment and the simulations. In the experimental system, the varying

Figure 17. Conversion profiles of NC7 (left) and IC8 (right) for E0 (black) and E10 (red).

Dotted line represents end of LTHR for PRF 84.
levels of LTHR will reduce the differences in temperature across the combustion chamber, likely influencing the onset of autoignition, combustion duration, Ringing Intensity, and emissions. In the simulation, the varying levels of LTHR will result in different levels of fuel conversion prior to hot ignition in the different zones, as well as concentrations of key radicals. While in the physical system there is mixing between different regions of the combustion chamber, in Chemkin multi-zone model mass transfer between zones is not modeled; this may in turn affect the accuracy of the simulation.

![Figure 18. Temperature vs LTHR (plotted as net heat release rate and scaled by the mass of each zone) of 7 representative zones for the E0 mixture at intake pressure 1.55 bar and intake temperature 390 K](image)

IV. Conclusions:

In this paper, the Low-Temperature Heat Release (LTHR) behavior of gasoline, and gasoline-ethanol blends, was explored in an HCCI engine, RCM, and through zero-dimensional chemical
kinetic modeling. A key focus of these investigations is the transition of a fuel from single-stage to dual-stage heat release in an engine with increased intake pressure. A summary of the key findings of the investigation are presented below:

\(a)\) Engine

1. At low intake pressures, lean mixtures and moderate engine speeds, gasoline exhibits single-stage heat release when burned in an HCCI combustion system.
2. As intake pressure is increased, gasoline begins to exhibit Low Temperature Heat Release.
3. Ethanol addition to gasoline increases the pressure at which the onset of LTHR begins. At low intake pressures at which LTHR does not occur for gasoline, ethanol addition had minimal effect on auto-ignition behavior.
4. The primary reference fuel and FACE A and C gasolines behaved similarly, but not identically, both neat and with ethanol addition.
5. Low Temperature Heat Release significantly changes the intake temperature required to maintain constant combustion phasing. This is both a thermal and a chemical effect.

\(b)\) RCM

6. FACE A, C, and PRF 84 have similar first stage and total ignition delays.
7. PRF 84 is an acceptable chemical surrogate for FACE A and C both neat and with ethanol addition.
c) Kinetic Modeling

8. LTHR, while having both thermal and chemical effects on ignition delay, primarily encourages ignition through the release of chemical energy which raises charge temperatures.

9. Ethanol acts as a radical sink, both reducing LTHR magnitude and delaying ignition.

10. LTHR is not uniform across the combustion chamber due to temperature gradients near TDC. The coolest regions of the combustion chamber exhibit the most LTHR; however, the hottest zones autoignite first and thermally trigger ignition in colder zones.

These results have a number of implications for the operation and simulation of HCCI. Chiefly, ethanol significantly inhibits the low-temperature chain-branching pathways of gasoline, which typically become active at higher pressures for engine-relevant timescales. By inhibiting these chain-branching pathways, the overall auto-ignition process is inhibited under these conditions (although not at lower intake pressure, higher intake temperature conditions), reducing system reactivity. This effect of ethanol addition is important to account for in the operation strategies of Advanced Combustion Engines (ACE’s). In the case of HCCI engines, the shift in reactivity that accompanies the activation of low-temperature chain branching drastically changes the intake conditions required to hold combustion phasing constant. Thus, this effect is critical for the design and operation of an HCCI engine (or similar type of ACE) that must run on commercially available gasoline which has varying levels of ethanol. The results of these investigations are also relevant, although not directly applicable, to GCI and PPC engines. These types of engines typically use
gasoline fuels similar to the type tested in this study, and achieve autoignition of the fuel through compression, as in the HCCI engine, although due to the non-fully-premixed nature of GCI and PPCI engines, the equivalence ratio of the autoigniting mixture is much higher for these engines. Nonetheless, when examining the operating strategy of these engines, such as [50] and [51], challenges achieving autoignition exist at low loads (and low intake pressure), while at high loads (and higher intake pressure) fuel reactivity must commonly be suppressed with exhaust gas recirculation (which reduces oxygen concentration). This behavior is reflective of the behavior observed in the HCCI engine, which is unsurprising, considering the general similarities between these engines. Therefore, ethanol content in a fuel may have similar effects on fuel reactivity in a GCI or PPCI engine as have been observed here. This may have particularly strong effects on low-load operation of these engines, where strong low-temperature chemistry may help achieve autoignition with low intake temperatures, but which ethanol could inhibit. This hypothesis will be investigated in future work. Another combustion system to which these results may be relevant is the stoichiometric Spark Ignition (SI) system, which is limited by autoignition of the fuel-oxidizer end-gas. It has been demonstrated the LTHR is important for the autoignition process of this end-gas [52]. It has further been demonstrated that ethanol provides significant anti-knock qualities in gasoline in SI engines, especially at elevated intake pressure [13]. The results in this paper hint at the kinetic portions of the ethanol blending effects. The inhibition of the low-temperature chain branching pathway, which is still not well captured by kinetic mechanisms, significantly alters the operating range of turbocharged SI engines, as shown in [13]. The operating range of an engine is critical to understand when designing modern SI engines, as it effects sizing of all key components, and thus the underlying kinetics of ethanol addition are important to understand and quantify for this application, in addition to other forms of advanced engines.
Finally, the variation in LTHR observed across the multi-zone model, with lower temperature zones yielding higher rates of heat release than higher temperature zones, has implications for analysis of experimental data and understanding of fuel specific behavior. Engine experiments which use cylinder pressure as the primary diagnostic must analyze the bulk heat release behavior, and in HCCI engines this is assumed to be relative uniform due to the well-mixed fuel. However, the modeling shows that zones of different temperatures may yield magnitudes of LTHR which vary by a factor of six, leading to reduced temperature stratification across the combustion chamber. This may have effects on autoignition, with less heat release in higher temperature zones delaying autoignition relative to what would be expected if uniform heat release occurred, on combustion duration, with more uniform zone temperature distributions yielding more uniform autoignition and shorter combustion duration, and on ringing intensity, with shorter combustion duration and more rapid heat release causing an increase in cylinder pressure rise rates and oscillations.

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VI. References:


