On the relevance of octane sensitivity in heavily downsized spark-ignited engines.

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Abstract

Over the years, spark-ignition engine operation has changed significantly, driven by many factors including changes in operating conditions. The variation in operating conditions impacts the state of the end-gas, and therefore, its auto-ignition. This can be quantified in terms of K-factor, which weights the relative contribution of Research Octane Number (RON) and Motor Octane Number (MON) to knocking tendency at any operating condition. The current study investigates the fuel requirements when operating an engine at increasing intake air pressures. A model engine was operated at varying intake air pressure in GT-Power software, from naturally aspirated intake air to heavily boosted intake air pressure of 4 bar absolute. The pressure-temperature information from the GT-Power model was used to calculate ignition delay times of the unburnt endgas composed of a sensitive and a non-sensitive fuel in ChemKin software. The results show that high octane sensitivity is desired at negative K values (operating at high intake air pressures). In contrast, zero octane sensitivity fuel performed best at low load operation (positive K). Interestingly, the maximum benefit for using a sensitive fuel was achieved at an intake air pressure of 1.75 bar with diminishing returns at higher intake air pressure for 1000 rpm and at lower intake pressures, as engine speed increased. The pressure effect on auto-ignition tendency was also investigated over existing HCCI data. The auto-ignition tendency was found to be sensitive to octane index in a region of low K value (K~0). This region lies in the negative temperature coefficient (NTC) region, where Primary Reference Fuels (PRFs) shown an increased sensitivity to pressure variation.

Introduction:

Spark-ignition (SI) engines power most passenger cars around the globe. Due to their dominance in road transport, improving the efficiency of SI engines forms a key part of achieving climate mitigation targets. At high load operation, their efficiency is limited by knock, which refers to the auto-ignition of end-gas ahead of a spark-initiated flame front [1]. Increase in compression ratio improves engine efficiency, but also increases the likelihood of knock occurrence.

Knocking is governed by processes related to the engine (design, operating condition, fluid flow, heat transfer etc.) and characteristics of the fuel in use (chemical auto-ignition delay and latent heat of vaporization). Interestingly, the fuel’s inherent tendency to knock (or auto-ignite) also varies with operating condition. Two different operating conditions are used to measure Research Octane Number (RON) and Motor Octane Number (MON). The Octane Numbers are reflective of fuel’s knock resistance [2, 3]. RON tests operate a Cooperative Fuel Research (CFR) engine at 600 rpm, 52 C intake air temperature and a fixed spark timing of -13 CAD aTDC. MON tests operate at 900 rpm, 38 C intake air temperature, 149 C intake charge (fuel+air) temperature and spark timing that varies with compression ratio [4]. Both octane ratings are measured relative to standard fuels known as Primary Reference Fuel (PRF), which corresponds to the representative volume of iso-octane in iso-octane-n-heptane blend. For example, PRF80 refers to 80 %(v/v) iso-octane and 20 %(v/v) n-heptane.

As the spark-initiated flame propagates, the end-gas gets compressed and heated. The resistance of the end-gas to auto-ignite, as its temperature and pressure is raised by the oncoming flame, is indicative of its octane rating. A fuel-air mixture exhibiting a longer ignition delay time would avoid auto-ignition before the end-gas is engulfed by the propagating flame, and thereby avoid knock. Paraffinic fuels exhibit low-temperature heat release that increases the temperature of the end-gas, further accelerating the auto-ignition and likelihood of knock. These fuels exhibit a representative negative temperature coefficient (NTC), where auto-ignition tendency of the fuel and, hence, auto-ignition delays do not decrease monotonically with an increase in temperature. Due to low-temperature chemistry, paraffinic fuels exhibit lower (and often negative) sensitivity to temperature differences between RON and MON tests. Fuels exhibiting smaller low temperature chemistry show a faster decay in auto-ignition resistance, as engine operation shifts from RON to MON. This leads to a disparity in the two fuel types, which is reflected in terms of octane sensitivity (OS = RON-MON) [5].

Modern engines often operate at conditions which are not aptly reflected in RON and MON tests. The engine speed is often higher, in-cylinder temperatures lower and intake pressure higher for modern turbocharged engines. These deviations from standard CFR tests also change the state of the end-gas and, hence, auto-ignition behavior. Naturally, RON and MON may not be suitable for measuring the knock resistance in such operating conditions. Octane Index (OI), which uses a K-factor to reflect variation in operating conditions, might be a more appropriate measure of knocking tendencies of the fuel [6-9]. Octane Index is given by:

\[ OI = RON - K \cdot OS \]  \hspace{1cm} (1)

where OS is the measure of Octane Sensitivity (given by RON-MON). K is equal to 0 and 1 for RON and MON tests, respectively. Looking at Eq. 1, at negative K value (where modern turbocharged SI engines operate), a high OI (and knock resistance) may be achieved from a high RON and OS. An arbitrarily defined metric OS can be correlated with fundamental chemical auto-ignition propensity of fuel in low and intermediate temperatures [4]. More specifically, fuels exhibiting pronounced NTC behavior have low OS, while a more Arrhenius-type behavior is typical of high OS fuels.
There are numerous studies on importance of OS in turbocharged engines [10-18]. Several researchers have looked at the physical and chemical underpinnings of OS i.e., contribution of low temperature reactivity [5, 18, 19] and latent heat of vaporization [16, 20] in determining the OS. Recently, we have also investigated the role of intermediate temperature heat release in OS of toluene/n-heptane/iso-octane blends [4]. It is generally accepted that negative K value of modern turbocharged SI engines decreases further as intake air pressure increases (higher boost pressure). Engine downsizing benefits from reduced pumping loss at low-load operation by operating at throttled intake for lesser time [21-24]. The demand for peak power is met by operating at higher (than atmospheric) intake air pressure (powered by turbochargers driven by exhaust energy). Considering an extremely downsized engine, a 2-cylinder engine running in a small-sized car; the engine would ideally operate at four-times the air to produce the same power as an 8-cylinder engine [25]. However, as the intake pressure increases, knocking tendency also increases, forcing a retarded spark-timing at such high loads. This translates to reduced gains in engine efficiency at knock-limited, high-load operation. To continue high-efficiency operation, engine knock must be avoided at such extremely boosted conditions. Fuel properties to delay auto-ignition (and suppress knock) need further assessment. This will enable fuel design for development of extremely downsized and turbocharged engines.

The current study focuses on the operation of such extremely downsized engine at intake pressure up to 4 bar. The importance of OS is investigated at high intake pressure scenarios. Gopujkar et al. [26] suggested that as intake pressure increases, the role of OS becomes more critical as K becomes more negative. The current study questions this assumption owing to the effects associated with the NTC behavior of a typical gasoline fuel. It is hypothesized that the OS becomes less critical to engine knock beyond a critical intake air pressure (load). The hypothesis is based on the operation falling outside of NTC regime at such intake conditions.

**Methodology:**

A modern engine architecture based on AVL 5401 Pre-ignition engine is used for building a GT-Power model. The AVL 5401 engine has been used by the researcher in previous work and details can be found in [27, 28]. The GT-Power model is used to simulate the engine with intake pressure ranging from 1 bar (abs) to 4 bar (abs). The engine is operated at increasing engine speed (from 1000 to 3000 rpm) with a fixed spark timing of -18 CAD aTDC. As an output from the GT-model, pressure traces for all the intake air pressure cases are deduced. These conditions do not consider knock calculations and are used only to obtain the pressure-time histories. The pressure histories are, in turn, used as an input to chemical kinetic simulation performed in ChemKin. For the chemical kinetic simulation, a homogeneous constant volume batch reactor module with constrained pressure, is employed to model the end-gas auto-ignition in highly boosted engines. Instead of commonly used fixed initial temperature-pressure condition, the pressure-time data from the GT-Power model calculations is imposed into the ChemKin model [29]. Time = 0 was defined at the instant when the calculated unburnt mixture temperature is 500 K. The initial temperature 500 K is chosen for time = 0, as negligible chemical reactions occur at lower temperature within the residence time applicable for this study. Moreover, studies have shown least uncertainty in measured pressure data for this temperature range [30]. For time > 0, pressure was imposed from the GT-Power output and temperature was calculated based on the imposed pressure values and the heat released from chemical reactions. The boundary conditions refer to the state of the end-gas as the spark-initiated flame propagation compresses the end-gas and heats it, therefore these simulations capture both the effects of piston motion and flame propagation on the end-gas. The ignition delay time in such simulations is similar to the onset of knock for the specific operating condition. A reactant mixture in the ChemKin simulations is a fuel-air mixture at equivalence ratio of 1, which is representative of modern spark-ignition engines constrained with using a three-way catalyst. Two fuels are used for the study. Fuel # 1 is a primary reference fuel (PRF90): molar fractions 0.111 n-heptane and 0.889 iso-octane. Fuel # 2 is a toluene reference fuel (TRF90): molar fractions of 0.750 toluene and 0.250 n-heptane. Fuel # 2 showed similar knocking resistance to Fuel # 1 in RON conditions in CFR tests [4] and has an octane sensitivity of 10.55, i.e. both Fuel # 1 and Fuel # 2 have RON 90, while Fuel # 2 has MON of 89.45. By definition, the PRF mixture have OS of zero. These two fuels were selected because they represent the two extremes of OS achievable with mixtures of iso-octane, n-heptane and toluene. The choice of the fuels is also based on chemical kinetic simulation results discussed next.

RON and MON pressure traces were extracted from [15] and a peak-knock lambda from [31, 32] was used to match the ignition delay time of TRF90 with that of PRF90. PRF90 auto-ignited (onset of knock) at 5.25 CAD aTDC at RON condition. Thereafter, Fuel # 2, which had the same onset of auto-ignition, was found iteratively. The initial guess for the TRF composition was taken from [33, 34]. These TRFs have the same RON, which are experimentally measured in a CFR engine. However, these fuels do not provide the same ignition delay times in the chemical kinetic model due to various idealizations (including no heat transfer assumption). Hence, the fraction of toluene-n-heptane is varied to achieve the same ignition delay time as for PRF90 at RON condition. The matching TRF has auto-ignition onset at 5.24 CAD aTDC at RON condition. Thereafter, same mixture is modeled at MON condition: PRF90 auto-ignited at 16.82 CAD aTDC, while TRF90 auto-ignited at 15.42 CAD aTDC (earlier than PRF90 due to lower MON).

Once the fuel formulation is fixed, the ignition delay is calculated at operating conditions other than RON and MON at equivalence ratio 1. This includes calculation of ignition delay times along the pressure-time trajectories corresponding to increasing intake pressure from 1 bar to 4 bar.

The current study uses chemical kinetic mechanism from [35]. The mechanism has been validated over conventional engine operating conditions, shock tubes, and rapid compression machines [35]. The detailed mechanism consists of 701 species and 16048 reactions.

**Results and Discussions:**

Figure 1 shows the typical temperature and pressure traces from a fixed spark timing of -18 CAD aTDC, not limited by knock or peak pressure.
Operating at such advanced spark timing is not possible in a real engine because knock can severely damage the engine. Hence, the pressure-time trajectories shown in Figure 1 are representative of an engine capable of withstanding peak pressures up to 350 bar without knocking. Note, conventional engines are not designed to withstand such high peak pressures as in Figure 1b (100-350 bar).

The temperature trajectories in Figure 1a are plotted against CAD. The CAD at which T=500K is chosen as the start of chemical kinetic simulation. As it can be seen in Figure 1a, the CAD for time = 0 are not the same for all cases, in-cylinder temperature decreased slightly with increasing intake air pressure (shown by darkening green color). Figure 1b shows the pressure time trajectory, starting from time = 0 marked in Figure 1a, up to the peak pressure. The figure provides the methodology used for the study at 1000 rpm. Similar trajectories were obtained for other engine speeds as well.

The pressure-time trajectories shown in Figure 1b are used as boundary conditions for end-gas modeling in ChemKin. Auto-ignition delay times are calculated for PRF90 and TRF90. The difference in ignition delay times for TRF90 and PRF90 ($\Delta\tau_{id}$) is shown in Figure 2. Since TRF90 has the same RON and low MON compared to PRF90, the difference in ignition delay times between TRF90 and PRF90 is negligible at RON condition and negative at MON condition (TRF90 auto-ignites earlier than PRF90). At intake pressure of 1 bar, the PRF90 performs better than TRF90, exhibiting longer ignition delays and, hence, better knock resistance. This is consistent with experimental observations by Szybist and Splitter [13]. As intake air pressure increases, the engine operates at beyond-RON conditions (i.e., the temperature-pressure trajectory followed by the end-gas before auto-ignition is in higher pressure and lower temperature region compared to that under RON condition), where the suggested value of K is negative. Here, the behavior is reversed and a low MON TRF90 auto-ignites later than PRF90 (resulting in better resistance to knock for TRF90). This is indicated by a positive value of $\Delta\tau_{id}$ for intake pressure greater than 1 bar ($\Delta\tau_{id}$ = $\tau_{id}(TRF90) - \tau_{id}(PRF90)$) longer ignition delay time and higher knock resistance for TRF90 than PRF90). In the region of positive $\Delta\tau_{id}$ TRF90 is preferable over PRF90 for SI engine operation (at increased intake air pressure or negative K), and vice versa. $\Delta\tau_{id}$ reaches a maximum at intake pressure of 1.75 bar. The lowered benefit of TRF90 over PRF90 beyond intake air pressure 1.75 bar may point to a increase in K-factor. However, this (decrease or increase of K-factor) depends on how RON varies with respect to changes in $\tau_{id}$. This aspect is investigated in next section.

Secondly, with increasing engine speed, the $\Delta\tau_{id}$ decreases further. It is widely known that the benefit of using fuels with high OS (TRF90 in this case) stems from the less active low temperature reactivity of such fuels. PRFs show high low temperature reactivity which accelerates the transition to main auto-ignition (in case of SI engine, this leads to knock). The low temperature chemistry however does not scale with the engine speed, and is highly reliant on residence time, which decreases linearly with increasing engine speed. With lesser time for low temperature reactions at higher engine speeds, the PRF90 relative reactivity is not as high, compared to the one at low engine speeds [36]. This is pertinent to conventional octane ratings, RON and MON, wherein the engine is operated at 600 and 900 rpm, respectively. Such low engine speeds allow high residence time for low temperature reactivity to increase the relative reactivity of PRFs, which may not be realized in modern (relatively high speed) engines.

Octane Index refers to the PRF which matches the knocking tendency of the tested fuel at any operating condition. For the operating conditions tested, TRF90 ignites later than PRF90 at beyond-RON conditions. Hence, the PRF which has the same the ignition delay time as TRF90 is calculated to obtain the Octane Index at various operating conditions. Experimentally, at any operating condition the test fuel is
matched with PRF of the same knocking tendency. Traditionally, measuring octane rating of fuels with knock resistance higher than pure iso-octane (Octane Number \( > 100 \)) has required tetra ethyl lead (TEL) addition to iso-octane. For example, adding 1, 2 and 6 ml TEL to pure iso-octane leads to octane number 108.6, 112.8, 120.3 respectively [2, 3]. We propose a novel methodology to calculate OI \( > 100 \) based on ignition delay times of PRFs up to RON 100. In the current methodology, we have used an extrapolation method to get the octane-index of the TRF90 at varying intake air pressure. This method relies on calculating \( \tau_{id} \) for increasing PRF mixture and extrapolating them to achieve target \( \tau_{id} \) of TRF90. Three (or more) \( \tau_{id} \) values are required to provide a polynomial fit of order 2 with high R². The curve fit expression can then be used to find the PRF matching the \( \tau_{id} \) of TRF90 at a given intake air pressure. If ignition delay time for TRF90 is greater than PRF100, then the 2-degree polynomial informs the corresponding OI for the target ignition delay time (of TRF90). The target \( \tau_{id} \) of TRF90 are shown in Table 1 for the case of 1000 rpm. The PRF values used to calculate the octane index are shown in Figure 3. This method provides OI calculated based only on chemical kinetics of the tested blends. A correlation between results obtained from this method and from TEL-method is beyond the scope of the current work.

An example of the methodology is provided for the case of intake air pressure 4.0 bar (abs) and engine speed 1000 rpm. When imposing the pressure trace corresponding to intake air pressure of 4.0 bar, from Figure 1b, the ignition delay time (\( \tau_{id} \)) was calculated to be 7.57 ms for TRF90. For the same boundary condition, the \( \tau_{id} \) for various PRFs is calculated, as shown in Figure 3. The values for 4.0 bar case are also given in Table 2. Based on the \( \tau_{id} \) values in Table 2, the relation between OI and \( \tau_{id} \) of PRF can be found as below:

\[
OI = -119.72*\tau_{id}^2 + 1867.8*\tau_{id} - 7176.1 \nonumber \tag{2}
\]

Using Eq. 2, one can find the PRF corresponding to the ignition delay time of 7.57 ms (target \( \tau_{id} \) of TRF90). This was calculated to be equal to 102.72.

Figure 2: The difference of the ignition delay between the PRF90 and TRF90. Ignition delay times are calculated for the pressure-time condition shown in Figure 1. RON and MON values are shown in blue and magenta dots respectively. Dashed line represents zero \( \Delta \tau_{id} \). As the fuels have matched RON, the \( \Delta \tau_{id} \) at RON condition is ~ 0. With increasing engine speed, the difference decreases further.

The calculated OI, based on the extrapolation method, is shown for the TRF90 mixture at increasing intake air pressure and various engine speeds in Figure 4. As opposed to the \( \Delta \tau_{id} \) trend shown in Figure 2, the OI shows a monotonic increase. The OI values for higher engine speeds are relatively similar, and lower than those at 1000 rpm.

The OI value shown in Figure 4 can be used to calculate K factor for different operating conditions. Using Eq. 1, \( K = \frac{RON-OI}{OS} \) can be calculated. Given OS is 10.55 and RON is 90 for TRF90, OI > RON corresponds to negative K value. The calculated K values are shown in Figure 5. Only at the lowest intake air pressure of 1 bar, K value is positive (\( \Delta \tau_{id} \) in Figure 2 is also negative for this operating condition). As intake air pressure increases, K value decreases to negative values. Corresponding to the OI values in Figure 4, K values for higher engine speeds are higher (i.e., the benefit of using high OS fuel is even lower as engine speed increases).
Figure 3: A 2-order polynomial fit is used to calculate the OI of TRF90 at varying intake air pressure condition. \( \tau_{td} \) is calculated for various PRFs and the target \( \tau_{td} \) of TRF90 is matched with respective PRF, which is the OI at that operating condition. The values are shown only for 1000 rpm case.

Table 1: Ignition delay times (\( \tau_{td} \)) for TRF90 for increasing intake air pressure is shown for engine speed of 1000 rpm. These are the target values to calculate the octane index.

<table>
<thead>
<tr>
<th>Intake Pressure (bar)</th>
<th>( \tau_{td} \text{TRF90} ) (ms)</th>
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<tbody>
<tr>
<td>1</td>
<td>9.46</td>
</tr>
<tr>
<td>1.25</td>
<td>8.90</td>
</tr>
<tr>
<td>1.5</td>
<td>8.63</td>
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<tr>
<td>1.75</td>
<td>8.44</td>
</tr>
<tr>
<td>2</td>
<td>8.12</td>
</tr>
<tr>
<td>2.25</td>
<td>8.00</td>
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<tr>
<td>2.5</td>
<td>7.91</td>
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<tr>
<td>2.75</td>
<td>7.83</td>
</tr>
<tr>
<td>3</td>
<td>7.76</td>
</tr>
<tr>
<td>3.5</td>
<td>7.65</td>
</tr>
<tr>
<td>4</td>
<td>7.57</td>
</tr>
</tbody>
</table>

Table 2: Ignition delay times (\( \tau_{td} \)) for TRF90 for increasing intake air pressure, used as target value to calculate OI.

<table>
<thead>
<tr>
<th>PRF</th>
<th>( \tau_{td} ) (ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>7.53</td>
</tr>
<tr>
<td>98</td>
<td>7.50</td>
</tr>
<tr>
<td>95</td>
<td>7.46</td>
</tr>
<tr>
<td>90</td>
<td>7.40</td>
</tr>
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</table>

Figure 4: OI calculated from interpolation/extrapolation of \( \tau_{td} \) of PRFs in Figure 3 used to match \( \tau_{td} \) of TRF90. At high speed, the OI is further reduced.

Figure 5: K values for the operating conditions considered in the current study are calculated based on OI values in Figure 4 and known RON and OS of TRF90. With increase in engine speed, the K-factor increases (closer to zero).

To summarize, counter-intuitively, OI and K values show a monotonic trend while the \( \Delta \tau_{td} \) values show a local maximum at intake air pressure of 1.75 bar for 1000 rpm and a decreasing trend at higher engine speeds. This observation is investigated further. As intake air pressure increases, the change in RON for a given change in \( \tau_{td} \) increases. Hence, at lower intake air pressure, each increment in PRF (from PRF 90 to 91 to 92 for eg.) leads to more significant difference in \( \tau_{td} \). This is shown in terms of slope of the curves in Figure 3. A linear interpolation of the curves in Figure 2 is used to calculate the slope, which is presented in Figure 6. \( \frac{d\text{RON}_{PRF}}{d\tau_{td}} \) is representative of the sensitivity of PRF octane number to the change in \( \tau_{td} \). When
operating an engine at knock-limited condition at a low intake air pressure, an increase in PRF rating (more iso-octane, higher RON) would lead to a more advanced combustion phasing. At higher intake air pressure, the same increase in PRF rating would lead to a less advanced combustion phasing. As intake pressure increases, the autoignition tendency becomes less sensitive to changes in octave rating of PRFs. The effect is further exaggerated as engine speed increases. The experimental validation to the hypothesis is investigated next, using observations made by researchers in HCCI engine.

In a SI engine, knock occurs from auto-ignition of end-gas ahead of spark-initiated flame front. The auto-ignition phenomenon is often studied in isolation in an HCCI engine, albeit for lean fuel-air mixtures [37]. The reactivity in HCCI operation correlates well with the knocking tendency in SI operation. Operating an HCCI engine at similar K-factor values results in unburnt gas following a similar pressure-temperature trajectory as in corresponding SI engine operation. However, the compression in HCCI occurs entirely due to piston movement, rather than flame propagation in SI engine. In the next section, the impact of OI on auto-ignition phasing for HCCI engines is investigated. An attempt is made to correlate the experimental findings from the existing literature with the pressure dependence of reactivity of PRFs, observed in Figure 6.

**K factor variation and pressure dependence in HCCI engine**

HCCI combustion is a function of innate fuel-air reactivity, which is controlled by intake air temperature and pressure, equivalence ratio and residence time. Kalghati et al. [9] used varying level of equivalence ratio and intake air temperature to operate HCCI engine in a range of conditions, from knock limited to unstable. The data shown in Figure 7 is from various engines, operating conditions with and without exhaust gas recirculation. The y-axis refers to the sensitivity of combustion phasing to octane index, which can be understood as variation of ignition delay time with varying PRF (as shown in Figure 6). Figure 7 shows that the combustion phasing (CA50) in an HCCI engine is highly sensitive to the OI in a narrow range of K [38-41]. At high (and low) K values (corresponding to high intake pressure or intake temperature), combustion phasing showed low sensitivity to variation in PRF mixture in an HCCI operation. The K-factor is near zero for the region where combustion phasing is most sensitive to OI. The fuel effects on auto-ignition tendency are relatively insignificant at the extremes. At large K values (K>1, beyond-MON), fuels exhibit similar high-temperature chemistry, exhibiting similar autoignition tendency. This has been observed previously [4, 5, 37]. Pertinent to the current work, the negative K operations also show low sensitivity to variation in PRF, as was observed in Figure 6.

**Conclusions:**

The current work investigated the fuel requirements in future heavily downsized engines. A GT-Power model was created based on an AVL engine geometry. The operating conditions were selected at excessively high intake air pressure, without knock limit. The resultant pressure traces were extracted from these calculations and imposed in chemical kinetic simulations. Following novel conclusions can be drawn:

1. The benefit of using a sensitive fuel (TRF90) compared to a non-sensitive fuel (PRF90) in terms of ignition delay time, increases with an increase in the intake air pressure. However, a maximum is reached at intake air pressure of 1.75 bar at 1000 rpm and at lower intake air pressures as engine speed increases.
2. A novel methodology is proposed for calculating OI > 100, using extrapolation method. Using this methodology, the OI increased and K-factor decreased monotonically.
3. The contradiction in the two conclusions above is explained by an increase in sensitivity of RON to ignition delay time as intake air pressure increases. This aspect was investigated from HCCI engine experimental observations.

HCCI experiments from previous research works showed a high sensitivity of combustion phasing to the change in PRFs in a narrow range. This narrow range corresponds to the NTC region where the ignition delay is most sensitive to pressure variation for PRFs. At negative K values, the auto-ignition phasing was found to be less sensitive to octane index, corroborating the modeling results further.

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**Definitions/Abbreviations**

- **aTDC**  
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<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
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<tbody>
<tr>
<td>CAD</td>
<td>Crank angle degrees</td>
</tr>
<tr>
<td>DOHC</td>
<td>Direct overhead cam</td>
</tr>
<tr>
<td>CA50</td>
<td>Crank angle of 50% of the total heat released</td>
</tr>
<tr>
<td>RON</td>
<td>Research Octane Number</td>
</tr>
<tr>
<td>MON</td>
<td>Motor Octane Number</td>
</tr>
<tr>
<td>OI</td>
<td>Octane Index</td>
</tr>
<tr>
<td>$t_{id}$</td>
<td>Ignition delay time (ms)</td>
</tr>
<tr>
<td>GHG</td>
<td>Greenhouse Gases</td>
</tr>
<tr>
<td>IDT</td>
<td>Ignition Delay Time</td>
</tr>
<tr>
<td>IMEP</td>
<td>Indicated Mean Effective Pressure</td>
</tr>
<tr>
<td>NTC</td>
<td>Negative Temperature Coefficient</td>
</tr>
<tr>
<td>rpm</td>
<td>Rotations per minute</td>
</tr>
<tr>
<td>SI</td>
<td>Spark Ignition</td>
</tr>
<tr>
<td>KI</td>
<td>Knock Intensity</td>
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</table>
Response to Reviewers

The authors are thankful to the reviewers for their time in helping us to improve the quality of the manuscript. We appreciate the overall positive tone of the reviewers’ comments and have addressed all the comments in order to improve the manuscript for better readability, insight and novelty. The response to the comments are provided below in blue.

Reviewer # 281003

“As an output to the GT-model …” --> “As an output from the GT model…” maybe?

Thank you for pointing this out. This has been changed.

Figure 1. Please show both p and T traces of end-gas calculated by GT-power.

We have added the Temperature trace for the GT simulations (Figure 1a). However, pertinent to our discussion, we only included the instance in the compression stroke, which is relevant to pick the t=0 point in CAD (aTDC). We are thankful for this comment as it makes it simpler for the reader to understand the methodology.

Figure 3. pressure is not apparent. Please add that info to the chart.

The pressure legend has been added to the plot.

The novel methodology for calculating OI > 100 needs to be better explained, with numerical examples

An example on methodology for calculation OI>100 has been added

What is “Tcomp15”, top of the second column page 5? It is said “… when the in-cylinder temperature is 15 bar in compression stroke.” Maybe in-cylinder pressure? Please revise.

Thank you for pointing this out.

What is (a+b) ? not defined at all. You have to consider that the reader of your paper has not to be forced to read all the references as well, so please be considered and put more effort in explaining the steps carried out in your research.

More details have been added for that reference in general. (a+b) has been replaced by slope of CA50 against Octane Index, which is more relatable. Also the x-axis is changed from Tcomp15 to K factor, which readers can easily relate to. Thank you for pointing this out.

Ref. [5] is cited multiple times on page 5 and elsewhere, but it is a self-citation. It would be better if the Authors repeat the main ideas again in this paper.

This was also mentioned by the other reviewer.We have added more references for the readers to follow the work.

The connection between HCCI and SI mode is not well justified. If figure 6 shows a monotone trend, figure 8 has a totally different behavior. I don’t see why Authors find the correspondence for highly boosted engines (low T side). Can you also comment on what happens at 800 K, or above where the equivalent engine is basically naturally aspirated?

Thank you for pointing this out. We were initially hesitant to include the HCCI part of the manuscript. However, this is among the only observation we could find that related ignition delay with pressure effect, experimentally in an engine. We have revised the text now by making the link between the SI modeling part and the HCCI experimental observations better. Also, we have removed the part related to A and n in the later section as it was not relevant to the overall story. We have now stopped the manuscript at the point of HCCI experimental observations corroborating our modeling results of lower sensitivity of ignition delay time to change in PRF at high intake pressures.

I hope the revised plot brings the observations into better perspective. Regarding what happens at high temperature, this is very well known, and shown in previous work [5]. As temperature increases, fuels tend to behave more similarly. At very high temperatures, all fuels would auto-ignite nearly instantaneously (regardless of their RON/MON values). This is very high K factor operation. The details have been discussed in the revised manuscript.
Out of curiosity, what is the likelihood that fuels available at the pump are really going to be changed, according to new proposed formulations or availability? I’ve seen research projects going on for a decade now regarding fuel optimization, but the blends available at the pump are always the same, i.e., RON 95 MON 85 in EU or 92-82 in US, or similar. This is of course not a critique of the paper, but a more general comment. Thank you.

This is an interesting point of discussion. We are showing the evolution of Anti-knock index (used primarily in the US) as a metric for octane rating $[\text{AKI} = (\text{RON}+\text{MON})/2]$. It is widely known that the discovery of Tetraethyl Lead increased the octane rating significantly, even at low dosage. This led to an increase in AKI over the years of increasing TEL dosage in gasoline. However, the oil companies have still managed to keep the Octane rating constant (more or less) even after the banning of TEL. A kind-of steady state has been reached over last few decades. Two things to learn from this, one, the AKI we are using now is not what we have always been using and two, the refiners found additives to keep the octane rating constant without TEL. Now coming to the current scenario, with a stronger push towards decarbonizing transport, downsizing is one of the way forward. This has started a debate on ‘designing the best fuel for the best engine’, i.e. co-optimizing fuel and engines for working together. In this view, it is not completely out of question to foresee a change in AKI/RON in market gasoline in future. If there was no climate crisis, yes this was out of question. Secondly, I would also like to point out that the countries use different metrics to measure octane rating. Some use RON only, some use RON and MON while some use AKI (thereby controlling both RON and MON). With this study we are investigating the impact of RON for varying MON. If the impact is significant, this would be a good reason for countries not using MON as a metric to continue doing so, and others to give up on MON as a metric, or better, use RON and Octane Sensitivity as metrics of knock resistance. I am certainly not aiming for all that changes from this work alone. This work is merely a step in the direction of better fuel design and prescription for higher engine efficiency.

**Reviewer # 281085**

**Overview:** This manuscript provides an interesting investigation that provides some kinetic insight on the octane index correlation. In particular, it strives to understand whether continual increase in intake manifold pressure, which correlates to continual decrease in the K value, continues to shorten ignition delay. One of the major findings was that the ignition delay difference between PRF90 and TRF90 reached a maximum at an intake pressure of 1.75 bar intake manifold pressure. Despite this maximum, the calculated K and OI changed in monotonic ways due to the change in RON with ignition delay.

**Specific comments:**

There are a couple of sections where this paper could use editing. The first couple sentences of the introduction in particular read awkwardly (tense agreement issues)

In the methodology section, I’m not sure that I understand why 500K was chosen as the starting temperature for a constant volume reaction. I certainly agree that not much is occurring below 500K, but on engine timescales, I would think that 650K is a much more realistic starting temperature for LTHR reactions. For that matter, why no use a changing volume model with an imposed pressure to represent a slider-crank mechanism? I’m not asking for the calculations to be re-done, but I do think that some additional explanations and justification for this are necessary.

The reviewer raises some interesting points. Regarding the choice of temperature, the reviewer is correct in the assessment that (considering the residence time available in an engine system), one can choose to go for a higher temperature as a starting point. Temperature calculations can vary significantly on choosing a wrong baseline point in the calculations. A recent publication which investigated the uncertainties in the in-cylinder measurements found that they were minimum in the region (corresponding to ~500K) and start to rise as we move later in the compression stroke. Using this temperature then, allows us to be a little more confident of a similar starting point for all the tested conditions. We apologize for not including the reference in the manuscript and have revised it in the current version.
There’s something wrong with the scaling in Figure 1. You say in the text that the engine is operating at 1000 rpm, which is 120 ms/ cycle (720 CA). The time axis in Figure 1 goes up to 9000 ms. Is this supposed to be micro-seconds?

Indeed. We really appreciate the comment. It was an oversight and has been corrected in the revision.

Figure 3 and Table 1 illustrate the concern that I stated earlier about starting the calculation at 500K. It seems that there is very little distinction between the higher intake pressure ignition delays – but these are not trending toward zero. Instead, they seem to be reaching an asymptote at about 7.5 ms. Why? Is this the amount of time it takes to get from 500 to 650K? I think this analysis could show a lot more sensitivity if it were done on a shorter timescale. For instance, at 1000 rpm, 1 ms is 12 CA. So, anything below about 3-4 ms is irrelevant on engine timescales.

We would refer again to the rationale behind the choice of the ‘cut-off’ temperature. Checking the time 7.5ms it is definitely not the time from 500 K to 650 K. However, a considerable time (4.8ms) is from 500K to 650K. As seen in figure below (taken from our previous work), for a varying number of fuels, the pressure dependance follows a power-law, wherein the change in IDT is smaller with any further increase in pressure. At the conditions we are operating in the current study, we are on the right side of the data shown below, reaching an asymptotic behavior observed in the study.

![Figure 1](image)

There have been numerous studies in the past that have shown that low temperature heat release doesn’t scale with engine speed (e.g., LTHR is dependent on wall-clock time and not crank angle time). Figure 2 makes me think that you’re looking at a situation where the amount of LTHR plateaus. What would the engine speed effect be here? I’m assuming that, as engine speed increases, the amount of LTHR would plateau at a lower magnitude and as a result the change in ignition delay between the two fuels (during an engine cycle) would diminish as engine speed increased. Correct? I would recommend making a statement about the impact of engine speed here.

What began as a mere curiosity (around the operating conditions moving out of NTC region) is now starting to take a better shape because of this specific comment. We really appreciate this insight. We performed more simulations, at higher engine speeds (1500-2000-3000 rpm). This allowed us to look at the impact of residence time and the wall-clock time-dependance of LTHR. As engine speed increases, we see the previous observations getting more prominent, as shown in figure 2 in the revised manuscript. Fewer data points are shown for higher engine speed conditions as the knocking tendency decreases with increase in engine speed, so the fuels do not auto-ignite on the imposed pressure traces. The imposed pressure traces are also different for these high speed cases.

Figure 7 – there are many different types of HCCI combustion, so it may be good if you provided some additional details. For instance, does this represent similar levels of oxygen concentration (or residuals)? Does it represent similar levels of air/fuel equivalence ratio? Mass based equivalence ratio? These are important parameters for kinetics, so some additional descriptions of the HCCI conditions would be good. I know that you cited the reference for them, but a high-level summary here is recommended.

This is true as well. We have now changed figure 7 to reflect the various HCCI engines that were used to achieve the data in the figure. We have also added a high-level summary for the tests.