Study of the Effect of Research Octane Number on the Auto-Ignition of Lubricant Oil Surrogates (n-Hexadecane)

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ABSTRACT: Engine oil is considered one of the sources for pre-ignition in downsized boosted direct injection spark-ignited engines. When interacting with fuel sprayed in the combustion chamber, engine oil forms an ignitable mixture and can cause an ignition event before firing the spark plug. Because high research octane number (RON) fuels are difficult to auto-ignite and tend to suppress the knock in an internal combustion engine, studying their interaction with engine oil is essential. Hence, in the current study, a suitable lubricant oil surrogate, namely, n-hexadecane, is mixed with iso-octane and n-heptane at different concentrations to investigate the auto-ignition behavior at elevated pressures. Five sets of fuels (PRF0, PRF20, PRF50, PRF80, and PRF100) were prepared to get a wide range of RONs and blended with n-hexadecane at 15, 25, 35, and 45% mixture concentrations (vol %). These experiments were conducted in a constant volume combustion chamber, keeping the initial temperature constant at 300 °C. A single droplet of the mixture was suspended on a thermocouple bead to record the droplet’s lifetime temperature. It was observed that hexadecane mixed with PRF0, PRF20, PRF50, and PRF80 showed similar auto-ignition behaviors. The time of ignition (TI) for these mixtures initially increased until 25% concentration of the fuel in n-hexadecane, and further addition of fuels to 35% and higher concentrations showed a gradual decrease in TI. Ignition of mixtures with 35% and 45% fuel concentrations is attributed to n-heptane, as its low temperature chemistry is the dominant factor in its high reactivity compared to iso-octane. TI increased with the increasing concentration of PRF100 mixtures in hexadecane, unlike other PRF fuels tested in this study. This is because iso-octane is a high RON fuel with a higher auto-ignition temperature, making it challenging to auto-ignite.

INTRODUCTION

Lubricant oil in highly boosted spark ignition engines is believed to be a significant cause of pre-ignition. Hence, several study groups are paying particular attention to engine lubricants’ effect on the occurrence of pre-ignition. Lubricant oil is diluted by fuel sprays from direct fuel injection directed toward a wall, leading to a local reduction in the surface tension and viscosity of the oil. As the piston decelerates close to the top dead center, decreased surface tension allows the oil–fuel mixture to escape in the combustion chamber. The fuel–oil mixing has a critical ratio that provides the mixture with sufficient physical properties to make its way into the combustion chamber. A large oil fraction would have a high surface tension or viscosity, making it difficult to shape individual droplets, whereas a higher fuel fraction would result in a high delay time of ignition (TI), as the research octane number (RON) is high in gasoline. In addition, under regular engine-running conditions, the ignition delay of the fuel is usually higher than what would cause it to auto-ignite. Lubricant base oil, however, is long-chain hydrocarbons with very short ignition delays. The addition of small quantities of oil to gasoline substantially decreases the delay in the ignition time.

Dahnz et al. studied pre-ignition occurrences both experimentally and numerically in highly supercharged SI engines and confirmed that the release of lubricant oil droplets from the cylinder liner might be the most likely cause for the occurrence of pre-ignition. Kuboyama et al. visually analyzed the pre-ignition phenomenon induced by oil droplets in a highly boosted spark ignition engine. They reported that the lubricant oil and fuel mixture accumulates in the piston crevice area, igniting under low oxygen conditions. The effect of fuel compounds on pre-ignition in high-temperature and high-pressure environments was studied by Toyota Motors and JX

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Nippon Oil and Energy Company.\textsuperscript{15} Their study reported that the pre-ignition temperature decreased for fuels with long-chain olefins and paraffin and unsaturated naphthenes. In addition, they stated that the pre-ignition temperature, relative to RON, showed a stronger association with MON and AIT. However, in their study,\textsuperscript{15} the complete process of the fuel reaction was not identified. Another Toyota Motors research found that temperature and pressure strongly affected the pre-ignition occurrence.\textsuperscript{16} General Motors developed a series of test fuels to examine the effect of octane number on the pre-ignition occurrence in a turbocharged direct-injection engine. A wide variety of pre-ignition event responses were seen for the fuels.\textsuperscript{17} It differed from no incidents to a very high number of cases. Their outcome showed no significant links with the sensitivity, RON, motor octane number (MON), or anti-knock index (AKI) of these fuels.

Amann et al.\textsuperscript{18} also found that the chemical composition of the fuel had an apparent effect on the pre-ignition frequency. Their analysis found that the increased level of aromatics in fuel blends increased the frequency of pre-ignition. Conversely, oxygenated fuels and low aromatic blends diminished the pre-ignition occurrences. In addition, the various knock and auto-ignition characteristics of the test fuels in the DISI engine were observed, even though the fuels had identical RON and MON ratings. Their results and prior research proposed that the critical cause of pre-ignition was the lubricant or fuel-based hydrocarbon layer on the piston crevices.

Jatana et al. compared the pre-ignition count of neat Haltermann gasoline and three fuel blends consisting of 75% Haltermann gasoline and 25% ketone, alcohol, and aromatic by a mass fraction in a turbocharged downsized direct-injection engine. They reported that the fuel blends with similar boiling points and octane numbers showed higher pre-ignition events than neat Haltermann.\textsuperscript{19} Other studies show that high-RON fuels increased the anti-knock quality of an AVL single-cylinder four-stroke DISI engine\textsuperscript{20} and increased power and reduced fuel consumption.\textsuperscript{21} However, the impact of these high-octane fuels when diluted in lubricant oil and their role occurrence of pre-ignition have not been discussed.

The effect of lubricants’ reactivity has yet to be thoroughly investigated,\textsuperscript{22} and owing to its unpredictability, the phenomenon has not yet been completely understood, and the difficulty of the mixture in the engine cylinder makes the study difficult.\textsuperscript{4} Therefore, a constant volume combustion chamber (CVCC), where temperature and pressure could be controlled independently, is used to study the effect of RON on the auto-ignition of the lubricant oil surrogate. Previous studies have shown hexadecane to be a suitable surrogate for lubricant oil as it shows similar ignition characteristics.\textsuperscript{3,12,23} Hence, hexadecane has been considered as a surrogate for lubricant oil in this study. Previously, Mitsudharmadi et al.\textsuperscript{24} investigated the effect of RON of different fuels by mixing FACE I, PRF91, PRF95, and toluene with hexadecane by 25 vol % in pre-ignition occurrences. Their investigation showed that the effect of RON did not affect the auto-ignition of the mixtures for pressures above 20 bar. However, their study focused only on mixing 25 vol % of fuels with hexadecane. Hence, in this study, a wide range of PRFs are mixed with hexadecane at 15, 25, 35, and 45 vol % to investigate their effect on the auto-ignition of the mixtures at high temperatures and pressures.

**EXPERIMENTAL SETUP**

The auto-ignition of hexadecane mixed with PRFs under various concentrations and pressures conditions was investigated in a CVCC. The experimental configuration schematic is shown in Figure 1. The CVCC with a volume of 4 L is well suited for researching single droplet ignition phenomena at elevated temperatures and pressures. It is built of 316 L stainless steel material with 320 mm outer diameter and 30 mm wall thickness. In the CVCC, three orthogonal pairs of quartz windows are fitted that provide excellent optical access to allow photographic droplet combustion diagnostics. To heat the CVCC, an in-line heater (Watlow) with a power rating of 3 kW and four heating tapes (Omega STH052-100) with a power rating of 0.738 kW each were installed.

At an initial temperature of 300 ± 4 °C and initial pressures ranging from 4 to 22 bar, the experiments described here are carried out in an air environment. This temperature was chosen because it was above the auto-ignition temperature of the surrogate oil (hexadecane) but below the auto-ignition temperature of the various diluting fuels. A single droplet injection system was integrated in the chamber. A capillary tube resides with an actuator device inside a cooling chamber assembly that is water-cooled at 10 °C and prevents the droplet from evaporating or igniting until it is suspended on the k-type thermocouple bead. Thus, the temperature of the droplet life span can be tracked from its suspension time until it is consumed entirely. A syringe pump (Harvard Apparatus PHD 2000) delivers the hexadecane/fuel mixture to the capillary channel. The piston’s movement is regulated by pneumatic solenoid valves (Peter Paul Electronics Co. EH22H90CCH6) within the actuator cylinder. Further experimental details can be found in ref 24.

A shadowgraph technique is used to record the auto-ignition of the mixture droplet, and the images are captured using a high-speed camera (PCO, Imager Pro HS, 4 M) at 500 fps. In addition, LabVIEW-based software is employed to synchronize the activation of the syringe pump to inject the mixture, the extension and retraction of the piston of the actuator holding the capillary tube, the camera trigger, and the acquisition of temperature data.

The data collected from at least 10 tests for each running condition are averaged in combination with the established automation system to record the data and monitor the injected
fuel quantity. This contributes to solid repeatability and high precision in producing the quantity of the mixture being injected. Therefore, the TI reported from any test is based on the same volume of the injected mixture, despite the droplet’s shape. To find the correct location of the thermocouple relative to the injection needle to suspend the droplet on the thermocouple bead, several preliminary tests were performed. The angle of inclination of the thermocouple was set such that the quantity of the injected mixture was adequate to form a droplet very similar to the shape of the sphere. The droplet will not be suspended if the volume of the injected mixture is too small, as the volume of the mixture produces a thin layer on the wire of the thermocouple. On the other hand, the droplet would not be suspended if the volume of the mixture injected is too much because it will drop automatically because of its weight. Because of this, it is important to carefully identify the combination of the thermocouple wire’s inclination angle and the volume of the fuel mixture injected to suspend the droplet on the thermocouple bead.

**Investigated Fuel Mixtures and Test Matrix.** To study the interaction between the oil and fuel mixture, hexadecane was mixed with n-heptane and iso-octane at different concentrations. First, hexadecane was mixed with n-heptane at 15, 25, 35, and 45% (vol %) concentrations to form PRF0 mixtures. Similarly, hexadecane was mixed with n-heptane and iso-octane at the previously mentioned concentrations to form PRF20, PRF50, and PRF80 mixtures. Finally, iso-octane was blended with hexadecane to form PRF100 mixtures. The physical properties are listed in Table 1.

![Table 1. Properties of n-Hexadecane, n-Heptane, and Iso-octane](https://doi.org/10.1021/acsomega.1c05535)

| properties          | units     | hexadecane | PRF0 n-heptane | PRF100 iso-octane |
|---------------------|-----------|------------|----------------|-------------------|
| molecular formula   |           | C₁₆H₃₄    | C₇H₁₆          | C₈H₁₈             |
| molecular weight    | g/mol     | 226.44     | 100.20         | 114.23            |
| boiling point       | °C        | 286.9      | 98.5           | 99.0              |
| auto-ignition       | °C        | 202        | 215            | 418               |
| flash point         | °C        | 135.0      | −1.0           | 4.5               |
| density             | kg/m³     | 770        | 680            | 690               |
| heat of combustion  | (LHV)     | 43.9       | 44.9           | 44.7              |
| heat of vaporization| kJ/kg     | 359        | 317            | 283               |

The tests were carried out for different pressures while keeping the initial temperature constant at 300 ± 4 °C. The experiment matrix and the derived cetane number (DCN) of each fuel and mixtures are shown in Table 2. An ignition quality tester (IQT) was used to get the DCN of the mixtures following the ASTM D6980 method. The RON of the fuels can be then calculated by using the correlation between RON and DCN proposed by Naser et al. and is given below

$$\text{RON} = -293 \left( \frac{\text{DCN}}{100} \right)^2 - 52 \left( \frac{\text{DCN}}{100} \right) + 114.1$$

**Defining TI.** A National Instrument c-RIO-9038 chassis is programmed to monitor and record the temperature and pressure in each of the experimental cases. The temperature data for each case are saved in the .tdms format. To read and post-process the temperature data, a MATLAB script is built. Because the PI vessel is not a standard vessel, it is essential to specify the TI for the current investigation of droplet ignition. The temperature record of hexC₂₅_PRF5₀₂₅ at an initial temperature of 300 °C and 10 bar pressure is shown in Figure 2. The thick black line reflects 10 experiments’ average temperature in an air environment, while the gray vertical fringe defines the standard deviation of these experiments. Additionally, the blue dotted line defines the evaporation of the mixture droplet in a nitrogen environment. The size of the suspended droplet is 1.1 ± 0.2 mm throughout the study.

As shown in Figure 2, before the mixture is pumped into the thermocouple bead, the thermocouple reads the actual temperature of the ambient air. The actual droplet temperature is much lower than that of the ambient air temperature within the tube because the mixture remains inside a cooling chamber before the moment of injection. When the droplet falls into contact with the bead of the thermocouple, it will observe a slight decrease in temperature. The thermocouple now measures its internal temperature when the droplet is suspended effectively, and a steeper decrease in temperature is tracked before it approaches a minimum temperature (A). This trend is observed for both the air and nitrogen environment cases.

For the air environment case, point A denotes time zero. Due to evaporation on the surface, the size of the droplet shrinks. Owing to inner conduction, heat is transmitted from the atmosphere to the internal core of the droplet. The internal droplet temperature also rises with a growing evaporation rate until it ignites (B), caused by the combustion of the ignitable vapor around the droplet. This is accompanied by a significant rise in temperature until the droplet is wholly absorbed, achieving a saturation point. During this phase, the temperature steadily falls to the actual ambient air temperature.

On the other hand, for the nitrogen environment case, the droplet evaporates until it completely vaporizes. With the superposition of the air and nitrogen environment temperature profiles, it can be observed that the slope diverges after it passes through point B. This indicates that the droplet in the air environment ignited at point B. TI is therefore specified as the time interval between the minimum local temperature (A) and the time when the droplet ignition first occurs (B). The massive spike in dT/dt observed from the history of the temperature demonstrates this.

### RESULTS AND DISCUSSION

**Effect of Concentration of PRFs in Hexadecane.** Initially, pure hexadecane was mixed with n-heptane and iso-octane individually at various concentrations and investigated at different initial pressure conditions keeping the initial temperature constant at 300 °C. First, the data obtained from PRF0 and hexadecane mixtures are analyzed. The results for TI at 300 °C at varying pressures are shown in Figure 3. A gradual increase in TI is observed with the increasing n-heptane concentration until it reaches a maximum at 25%, after which further addition of n-heptane in the mixture results in a decrease in TI.

Second, the data obtained from PRF100 and hexadecane mixtures are analyzed. As shown in Figure 4, the TI increased with the increasing concentration of iso-octane in the mixture. This trend is expected because iso-octane is a high-RON fuel and has a more vital ability to consume the OH radical, causing it to be less reactive and thus difficult to auto-ignite. Therefore, this trend narrowed down the possibility of iso-
octane to play a significant role in early ignition observed at 35% or higher concentration PRFs in hexadecane.

The temperature profiles for Hex75_PRF020, Hex65_PRF035, and Hex55_PRF045 at 10 bar and 300 °C are shown in Figure 5. For the Hex75_PRF020 mixture (3), the cooling effect is much higher compared to the Hex65_PRF035 (1) and Hex55_PRF045 (2) mixtures. In the Hex75_PRF035 mixture, the ignitable mixture around the droplet is formed slower, and hence, we observe an increased TI. It was interesting to observe why this phenomenon does not occur for Hex65_PRF035 and Hex55_PRF045 mixtures. The DCN of the mixtures decreases (see Table 2) as the concentration of PRFs in hexadecane increases, implying that the RON increases. Therefore, it was an unexpected trend for Hex65_PRF035 and Hex55_PRF045 mixtures because the TI is supposed to increase with the addition of higher RON fuels.

Table 2. Test Matrix and DCN of Mixtures as Measured in IQT

| Fuels   | Mixture Concentration | Hexadecane Vol % | n-Heptane Vol % | iso-Octane Vol % | DCN  |
|---------|-----------------------|------------------|-----------------|------------------|------|
| Hex100  | 0                     | 100              | 0               | 0                | 106.2|
| Hex85_PRF015 | 15                   | 85               | 15              | 0                | 101.1|
| Hex85_PRF020 | 25                   | 75               | 25              | 0                | 96.6 |
| Hex85_PRF025 | 35                   | 65               | 35              | 0                | 89.2 |
| Hex85_PRF030 | 45                   | 55               | 45              | 0                | 85.6 |
| Hex85_PRF035 | 15                   | 85               | 12              | 3                | 101.1|
| Hex85_PRF040 | 25                   | 75               | 20              | 5                | 93.8 |
| Hex85_PRF045 | 35                   | 65               | 28              | 7                | 87.8 |
| Hex85_PRF050 | 45                   | 55               | 36              | 9                | 82.3 |
| Hex85_PRF055 | 15                   | 85               | 7.5             | 7.5              | 95.4 |
| Hex85_PRF060 | 25                   | 75               | 12.5            | 12.5             | 88.4 |
| Hex85_PRF065 | 35                   | 65               | 17.5            | 17.5             | 82.4 |
| Hex85_PRF070 | 45                   | 55               | 22.5            | 22.5             | 76.7 |
| Hex85_PRF075 | 15                   | 85               | 3               | 12               | 98.7 |
| Hex85_PRF080 | 25                   | 75               | 5               | 20               | 88.1 |
| Hex85_PRF085 | 35                   | 65               | 7               | 28               | 79.1 |
| Hex85_PRF090 | 45                   | 55               | 9               | 36               | 72.6 |
| Hex85_PRF100 | 15                   | 85               | 0               | 15               | 92.7 |
| Hex85_PRF105 | 25                   | 75               | 0               | 25               | 84.8 |
| Hex85_PRF110 | 35                   | 65               | 0               | 35               | 77.8 |
| Hex85_PRF115 | 45                   | 55               | 0               | 45               | 70.7 |

Figure 2. Defining TI for 75 vol % hexadecane mixed with 25 vol % PRF50. The blue dotted lines represent the temperature profile for the experiment conducted in a nitrogen environment, while the black line represents the experiment conducted in an air environment. The TI is defined from point (A) (minimum temperature) to point (B) (steeper change in gradient).

Figure 3. TI for PRF0 mixed with hexadecane at different concentrations for a wide pressure range. Maximum TI is observed at 25 vol % mixtures for all tested cases.

Figure 4. TI for PRF100 mixed with hexadecane at different concentrations for a wide pressure range. TI increased with the increasing concentration of PRF100 in hexadecane.
It is also observed that for the Hex75_PRF2025 mixture, the droplet core temperature read by the thermocouple had to exceed the boiling point of hexadecane (see Table 1) before getting an ignition event. However, for Hex65_PRF2035 and Hex55_PRF2045 cases, the ignition occurred at a much lower temperature before the droplet’s core temperature reached the boiling point of hexadecane. Hence, it is suspected that n-heptane (PRF0) played an essential role in triggering the ignition and that there is a trade-off between the chemical and physical properties of these mixtures, which impacts their TI.

The ignition sequence of the Hex75_PRF2025 mixture at 4 bar pressure and 300 °C is shown in Figure 6.

To further investigate this phenomenon, the ignition temperature is plotted against the concentration of PRFs in the mixture at 4 bar pressure and 300 °C, shown in Figure 7.

As shown in Table 1, the auto-ignition temperatures of n-heptane and hexadecane are much lower than the ambient test temperature of 300 °C. On the other hand, the auto-ignition temperature of iso-octane is relatively higher despite having a lower boiling point. The fuel mixture droplet resides in a cooling chamber, and hence when introduced in the hot environment, the initial reading of the droplet’s core temperature is around 200 ± 10 °C, which is about a 100 °C lower than the ambient temperature. As the fuel mixture droplet is successfully suspended, it starts to vaporize, reducing the droplet size over time. Because evaporation occurs on the surface of the droplet, the particles on the surface of the droplet carry away some of the droplets’ kinetic energy in order to break their liquid bonds and to convert into gas. Because of this endothermic process, the overall thermal energy of the droplet decreases, and it cools down. The boiling point and the auto-ignition temperature of n-heptane are both lower. Once the fuel mixture lacks sufficient amount of hexadecane to drive the ignition, n-heptane plays a crucial role in the occurrence of the ignition. With an increasing concentration in the mixture, the amount of n-heptane increases as well. Hence, the flammability region is reached faster with the increasing amount of n-heptane in the mixtures. Ruling out iso-octane’s contribution in getting an early ignition can also be justified by observing the PRF100 trend in Figure 4. Iso-octane being a high-RON fuel, the fuel mixture gets difficult to auto-ignite with its increasing concentration and hence requires a higher temperature at a higher concentration of mixtures.

To support the hypothesis, PRF20, PRF50, and PRF80 were mixed with hexadecane at different concentrations to investigate the ignition behavior of the mixtures. Figures 8 and 9 show the TI for PRF20 and PRF80 mixtures, respectively, at 300 °C. For both the cases, the TI initially increased with the increasing concentration of PRFs in hexadecane. However, it reached its maxima at 25% concentration and started to decline with further increase in the PRF concentration. It can also be observed that the TI for

Figure 5. Temperature profile for PRF20 mixed with hexadecane at different concentrations for 10 bar pressure. Mixtures with 25 vol % (1) of PRF20 in hexadecane showed longer TI, while 35 vol % (1) and 45 vol % (2) had shorter TI.

Figure 6. Ignition sequence of the Hex75_PRF2025 mixture at 4 bar pressure and 300 °C.

Figure 7. Ignition temperature of PRFs mixed with hexadecane at different concentrations. The ignition temperature was maximum for PRF0 and PRF50 at 25 vol % concentration.

Figure 8. TI for PRF20 mixed with hexadecane at different concentrations at 300 °C. The maximum TI is observed at 25 vol % concentration of PRF20 mixed with 75 vol % hexadecane.
PRF80 (Figure 9) is much longer compared to the TI for PRF20 (Figure 8) because the amount of iso-octane in the mixture is increasing. As previously discussed, it is attributed to RON and hence yields a longer TI. Nevertheless, the fuel blends consisting of PRF0 (n-heptane) exhibited a similar trend for all tested pressure and concentration cases. Hence, it can be concluded that the ignition of PRF0, PRF20, PRF50, and PRF80 at 35 and 45% concentration is driven by the presence of n-heptane (PRF0) in the mixture. To further validate the hypothesis of n-heptane playing a key role in the ignition of mixtures at 35 and 45% concentrations, TI and pressure are plotted for hexadecane and PRFs mixtures at 25, 35, and 45% concentration and are shown in Figures 10−12 respectively. From Figure 10, it can be observed that the TI for the Hex75_PRF025 mixture is higher compared to that for pure hexadecane for all the tested pressures. This implies that for 25% concentration of fuels, hexadecane initiates the ignition event.

On the other hand, in Figure 11, the TI for Hex75_PRF035 mixtures is almost the same as the TI for pure hexadecane. The difference in the TI for Hex75_PRF025 and Hex65_PRF035 is significant. This implies that n-heptane has now started playing a role in initiating the ignition event. This phenomenon is more evident in Hex65_PRF035, which is shown in Figure 12. The TI for Hex65_PRF035 is now faster than that for pure hexadecane, supporting the hypothesis of n-heptane playing a significant role at a higher concentration of fuels mixed with hexadecane. Therefore, the TI for the mixtures does not increase with the increasing concentration of PRFs in hexadecane but rather increases until it reaches a maximum point, and with the further addition of fuel, it gradually starts to decrease.

Effect of Pressure on the Ignition of the Mixtures. In order to study the effect of pressure, hexadecane was mixed with different PRFs at different concentrations. The experiments were conducted at pressures 4, 10, 16, and 22 bar and at 300 °C initial temperature. Figure 13 shows the results for hexadecane mixed with PRF0 and PRF80 individually at different concentrations at an ambient temperature of 300 °C. The TI decreases with increasing pressure because the reactivity of the mixtures increases with increasing pressure. The TI distribution is sparse for PRF0 mixtures at lower pressures, whereas it gets denser at higher pressures. With further increase in pressure, it can be deduced that the TI will show asymptotic behavior. However, the change in the TI for the Hex65_PRF035 mixture, represented in Figure 12 by black dotted lines, is very small compared to that in other tested PRF0 mixtures. PRF0 mixtures ignited the fastest because the auto-ignition and boiling temperatures of n-heptane are much lower compared to those of iso-octane. On the contrary, PRF80 mixtures yielded a longer TI since iso-octane has a very high auto-ignition temperature, and as discussed previously, it
CONCLUSIONS

The effect of RON in the ignition of lubricant surrogate n-heptadecane was investigated in this study to determine how RON will play a role in the occurrence of the pre-ignition phenomenon. Experiments were carried out in a 4 L CVCC to investigate the ignition characteristics of hexadecane mixed with different PRFs at different concentrations. The test temperature was set at 300 °C, and the test pressures were varied from 4 to 22 bar at 6 bar intervals. The key findings are summarized below:

- Hexadecane mixed with PRF0, PRF20, PRF50, and PRF80 all showed a similar trend for getting TI. The TI for these mixtures initially increased until 25% concentration, after which it reached its maxima. Further addition of fuels with 35% and higher concentrations showed a gradual decrease in the TI.
- Mixtures at 25% concentration ignited only after the droplet core temperature reached higher than the boiling temperature of hexadecane.
- Ignition for mixtures with 35 and 45% concentrations is attributed to n-heptane as it has a lower boiling and auto-ignition temperature.
- As the hexadecane was mixed with PRFs in an increasing amount from PRF0 to PRF100, the TI was observed to be longer. This is because the amount of iso-octane in the mixture increases as we move from PRF20 to PRF100 and iso-octane is a high-RON fuel and has a higher auto-ignition temperature, which makes it difficult to auto-ignite.
- The TI get longer as the RON of the fuel gets higher. However, it heavily depends on the composition of the fuel. PRF80 has a RON of 80, yet the TI of this fuel, when mixed with hexadecane higher than 35%, yielded a shorter TI. Therefore, the physical properties of fuels play an important role.

Hence, the findings of this work show that the fuel’s RON and the mixture concentration (fuel and oil) both show potential implications for pre-ignition occurrence in downsized boosted SI engines. Additionally, this work provides further insights into studying the complex pre-ignition phenomena.

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Notes
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NOMENCLATURE

- CVCC: constant volume combustion chamber
- DCN: derived cetane number
- RON: research octane number
- PRF: primary reference fuel
- IQT: ignition quality tester
- PRF0: n-heptane
- PRF100: iso-octane
- TI: time of Ignition (s)
- T: temperature (°C)
- P: pressure (bar)

REFERENCES

(1) Singh, E.; Hlaing, P.; Shi, H.; Dibble, R. W. Effect of Different Fluids on Injection Strategies to Suppress Pre-Ignition. SAE Technical Paper, 2019.
(2) Zaccardi, J.-M.; Escudié, D. Overview of the main mechanisms triggering low-speed pre-ignition in spark-ignition engines. Int. J. Engine Res. 2015, 16, 152–165.
(3) Dahm, C.; Spicher, U. Irregular combustion in supercharged spark ignition engines—pre-ignition and other phenomena. Int. J. Engine Res. 2010, 11, 485–498.
(4) Ohtomo, M.; Miyagawa, H.; Koihe, M.; Yokoo, N.; Nakata, K. Pre-ignition of gasoline-air mixture triggered by a lubricant oil droplet. SAE Int. J. Fuels Lubr. 2014, 7, 673–682.
(5) Takeuchi, K.; Fujimoto, K.; Hirano, S.; Yamashita, M. Investigation of engine oil effect on abnormal combustion in turbocharged direct injection-spark ignition engines. SAE Int. J. Fuels Lubr. 2012, 5, 1017–1024.
(6) Maharjan, S.; Qahtani, Y.; Roberts, W.; Elbaz, A. The Effect of Pressure, Temperature and Additives on Droplet Ignition of Lubricant Oil and Its Surrogate. SAE Technical Paper, 2018.
(7) Dahoz, C.; Han, K.-M.; Spicher, U.; Magar, M.; Schiessl, R.; Maas, U. Investigations on pre-ignition in highly supercharged SI engines. SAE Int. J. Engines 2010, 3, 214−224.
(8) Maharjan, S.; Elbaz, A.; Mitsudharmadi, H.; Roberts, W. Studying Ignition Delay Time of Lubricant Oil Mixed with Alcohols, Water and Toluene in IQT and CVCC; 0148-7191. SAE Technical Paper, 2020.
(9) Singh, E.; Dibble, R. Mechanism Triggering Pre-Ignition in a Turbo-Charged Engine; 0148-7191. SAE Technical Paper, 2019.
(10) Kalghatgi, G. T.; Bradley, D. Pre-ignition and super-knock in turbo-charged spark-ignition engines. Int. J. Engine Res. 2012, 13, 399−414.
(11) Singh, E.; Morganti, K.; Dibble, R. Dual-fuel operation of gasoline and natural gas in a turbocharged engine. Fuel 2019, 237, 694−706.
(12) Kuti, O. A.; Yang, S. Y.; Hourani, N.; Naser, N.; Roberts, W. L.; Chung, S. H.; Sarathy, S. M. A fundamental investigation into the relationship between lubricant composition and fuel ignition quality. Fuel 2015, 160, 605−613.
(13) Singh, E.; Ali, M. J. M.; Ichim, A.; Morganti, K.; Dibble, R. Effect of mixture formation and injection strategies on stochastic pre-ignition; 0148-7191. SAE Technical Paper, 2018.
(14) Kuboyama, T.; Moriyoshi, Y.; Morikawa, K. Visualization and analysis of LSPI mechanism caused by oil droplet, particle and deposit in highly boosted SI combustion in low speed range. SAE Int. J. Engines 2015, 8, 529−537.
(15) Sasaki, N.; Nakata, K.; Kawatake, K.; Sagawa, S.; Watanabe, M.; Sone, T. The Effect of Fuel Compounds on Pre-ignition under High Temperature and High Pressure Condition; 0148-7191. SAE Technical Paper, 2011.
(16) Sasaki, N.; Nakata, K. Effect of fuel components on engine abnormal combustion; 0148-7191. SAE Technical Paper, 2012.
(17) Chapman, E.; Davis, R. S.; Studzinski, W.; Geng, P. Fuel octane and volatility effects on the stochastic pre-ignition behavior of a 2.0 L gasoline turbocharged DI engine. SAE Int. J. Fuels Lubr. 2014, 7, 379−389.
(18) Amann, M.; Mehta, D.; Alger, T. Engine operating condition and gasoline fuel composition effects on low-speed pre-ignition in high-performance spark ignited gasoline engines. SAE Int. J. Engines 2011, 4, 274−285.
(19) Jatana, G. S.; Splitter, D. A.; Kaul, B. J.; Szybist, J. P. Fuel property effects on low-speed pre-ignition. Fuel 2018, 230, 474−482.
(20) Wang, C.; Janssen, A.; Prakash, A.; Cracknell, R.; Xu, H. Splash blended ethanol in a spark ignition engine—Effect of RON, octane sensitivity and charge cooling. Fuel 2017, 196, 21−31.
(21) Rodríguez-Fernández, J.; Ramos, A.; Barba, J.; Cárdenas, D.; Delgado, J. Improving Fuel Economy and Engine Performance through Gasoline Fuel Octane Rating. Energies 2020, 13, 3499.
(22) Amann, M.; Alger, T. Lubricant Reactivity Effects on Gasoline Spark Ignition Engine Knock. SAE Int. J. Fuels Lubr. 2012, 5, 760−771.
(23) Distaso, E.; Amirante, R.; Calò, G.; Palma, P. D.; Tamburrano, P.; Reitz, R. D. Investigation of lubricant oil influence on ignition of gasoline-like fuels by a detailed reaction mechanism. Energy Proc. 2018, 148, 663−670.
(24) Mitsudharmadi, H.; Maharjan, S.; Elbaz, A. M.; Qahtani, Y. A.; Roberts, W. L. Auto-Ignition of a Hexadecane Droplet Mixed with Different Octane Number Fuels at Elevated Pressures To Investigate the Pre-Ignition Behavior. Energy Fuels 2019, 34, 806−816.
(25) McAllister, S.; Chen, J.-Y.; Fernandez-Pello, A. C. Thermodynamics of Combustion. Fundamentals of Combustion Processes; Springer New York: New York, NY, 2011; pp 15−47.
(26) Sandia, N. T. A. E. S. o. https://ecn.sandia.gov/diesel-spray-combustion/sandia-cv/fuels/ (accessed on Dec 14, 2021).
(27) Naser, N.; Yang, S. Y.; Kalghatgi, G.; Chung, S. H. Relating the octane numbers of fuels to ignition delay times measured in an ignition quality tester (IQT). Fuel 2017, 187, 117−127.
(28) Fan, Q.; Wang, Z.; Qb, Y.; Wang, Y. Investigating auto-ignition behavior of n-heptane/iso-octane/ethanol mixtures for gasoline surrogates through rapid compression machine measurement and chemical kinetics analysis. Fuel 2019, 241, 1095−1108.