RESEARCH ARTICLE

Autoignition of light naphtha and its surrogates in a rapid compression machine

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Abstract
Gasoline Compression Ignition (GCI) is a promising combustion mode to improve engine efficiency and reduce emissions. Naphtha has higher ignitability than gasoline and could be a better fuel for GCI. Understanding the autoignition behavior of naphtha is essential for the development of GCI engines. In this study, the ignition delay of light naphtha and its three surrogates, including PRF59 (59% iso-octane and 41% n-heptane in volume) and two three-component surrogates composed of methylcyclohexane, n-heptane, and iso-octane with blending ratios of 33.8%/43.2%/23% (MRF1) and 31.4%/33.3%/35.3% (MRF2) in volume were studied using a rapid compression machine. PRF59 was selected by matching the RON of light naphtha. MRF1 was composited by matching the RON and MON of light naphtha, while MRF2 was composed by matching RON and H/C. The experiments were conducted at equivalence ratio $\Phi = 0.5$ and 1, $P = 10, 20, \text{ and } 30 \text{ bar, and temperature range of } 665-965 \text{ K. It was found that MRF2 best matched the first-stage and total ignition delays of light naphtha, while PRF59 exhibited shorter first-stage ignition delay. Although the ignition delay times of MRF1 and MRF2 were very close to each other, uncertainty analysis showed that matching RON and H/C ratio was a better method in determining the blending ratio. In addition, the MRF experiments were compared with predictions using the detailed mechanism. The mechanism showed good performance in reproducing the total ignition delay at high-pressure conditions, but it underpredicted the ignition delay at low pressure. Also, the mechanism predicted less pronounced NTC behavior.

KEYWORDS
autoignition, ignition delay, methyl-cyclohexane reference fuel, naphtha, rapid compression machine

1 | INTRODUCTION

Homogeneous Charge Compression Ignition (HCCI) has been widely investigated since 1970s. It could achieve high thermal efficiency due to low heat loss and high specific heat ratios. However, HCCI encountered the difficulties in controlling the combustion phasing and the pressure rise rate at high loads. Recently, Gasoline Compression Ignition (GCI), also defined as Partial Fuel Stratification (PFS), Partially Premixed Compression Ignition (PPCI) or Partially Premixed Combustion (PPC), has been proposed and tested by several groups. By introducing fuel through direct injection in the compression stroke or next to the firing top dead center, both the combustion phasing and pressure rise rate can be better...
controlled. Unlike HCCI, the in-cylinder fuel-air mixture of GCI is stratified or partially premixed through multiple injections, thus, the diffusion combustion could exist to some extent.

Regular gasoline could be used in the compression ignition mode, but the additional devices or controlling strategies like rebreathing were required to obtain a stable combustion for the engine cold-start and low load conditions, which might increase the cost. Compared with the traditional high octane number gasoline, low octane number gasoline could be a better fuel for GCI. If the research octane number (RON) of the fuel was too low, the ignition delay time could be too short to achieve PPCI combustion. On the other hand, it was difficult to achieve stable combustion at low loads if RON was too high. In terms of the RON requirement, some researchers chose naphtha as the test fuel for GCI. Due to the high volatility and two-stage ignition behavior, naphtha was firstly tested in the HCCI combustion for load extension. Recently, both light-duty and heavy-duty engine experiments have demonstrated that naphtha compression ignition could achieve superior performance in both thermal efficiency and engine-out emissions. Extremely low NOx and soot emissions were gained as a result of the "enough premixing" and low temperature combustion. Naphtha fuels usually contained very small percentage of aromatics. Therefore, it was not necessary to include aromatics in naphtha surrogate, while toluene was one of the important species in gasoline surrogates. To develop and validate naphtha surrogate, fundamental investigations on naphtha were essential. Ahmed et al. proposed a five-component surrogate for light naphtha. However, this surrogate exhibited shorter ignition delay than naphtha. Javed et al. and Alabbad et al. measured the ignition delays of light naphtha (RON 64.5 and MON 63.5) and straight-run naphtha (RON 60 and MON 58.3), respectively, in a shock tube and a rapid compression machine over a broad range of temperatures, pressures and equivalence ratios. They also compared the ignition delays of primary reference fuel (PRF) surrogates and multi-component surrogates through both experiments and simulations. At high and intermediate temperatures, ignition delays for PRF and multi-component surrogates showed good agreement with naphtha experimental data, however, PRF exhibited higher reactivity at low temperatures (<700 K) compared to naphtha and multi-component surrogates.

In this paper, the ignition delay times of light naphtha, PRF59, and two naphtha surrogates composed of n-heptane, iso-octane, and methylcyclohexane (MCH) were measured at various conditions using an RCM. A detailed comparison in ignition delay was performed along with the predictions using the mechanism developed by Weber et al. Finally, the best method of composing three-component naphtha surrogate was proposed based on the experiment results and uncertainty analysis.

### Light Naphtha and Surrogate Formulation

#### 2.1 Light naphtha

The light naphtha supplied by China National Petroleum Corporation was tested in this study. Table 1 lists its properties and measurement method. It mainly consists of n-alkanes, iso-alkanes, and cyclo-alkanes. The average molecular
formula is $C_{6.57}H_{14.22}$ suggesting shorter hydrocarbon chains than the regular gasoline. It is worth noting that the octane sensitivity of light naphtha is very small, while the sensitivity of a commercial gasoline is typically about 10.

2.2 Surrogate formulation

Pera et al.\textsuperscript{22} and Mehl et al.\textsuperscript{23} proposed methodologies of composing gasoline surrogates. The method can be divided into two parts: the choice of representative compounds and the proportion of each compound to match the selected properties. To formulate naphtha surrogate, the representative compounds should be determined first. As mentioned in the previous section, naphtha mainly contains n-alkanes, iso-alkanes, and cyclo-alkanes. N-heptane and iso-octane known as primary reference fuels are commonly used to represent n-alkanes and iso-alkanes for gasoline. Here, they are also chosen as components of naphtha surrogates. Both of them have similar physical properties to naphtha, such as H/C, lower heating value, and density. Their boiling points are also close to the T50 of naphtha. The RON of PRF can vary from 0 to 100 depending on the iso-octane and n-heptane ratio. Therefore, it is easy to match the RON of the tested naphtha, which is 59. For cyclo-alkanes, cyclohexane and MCH are commonly used as components of gasoline surrogates. Since most of cyclo-alkanes in the naphtha contain branched chains, MCH is selected to represent cyclo-alkanes. The RON and MON of MCH is 74.8 and 71.1, respectively. In summary, n-heptane, iso-octane, and MCH are selected as the compounds for naphtha surrogate, named Methyl-cyclohexane Reference Fuel (MRF).

Secondly, the blending ratio of each component in MRF needs to be determined. In gasoline engines, the auto-ignition propensity is typically evaluated by RON and MON. Kalghatgi et al. found that in PPCI combustion, the combustion phasing and ignition delay had no correlation with MON and a poor correlation with RON but an excellent correlation with Octane Index.\textsuperscript{24} Octane Index is based on both RON and MON values. Thus, RON and MON are both important for auto-ignition. Another key parameter is H/C ratio, which is related to the lower heating value, density, air/fuel ratio, flame speed, and adiabatic flame temperature.\textsuperscript{20} Consequently, RON, MON, and H/C ratio are chosen as the target properties when determining the ratio of the surrogate components. Since MRF only contains three components, only two of the target properties can be matched. In this paper, two MRF surrogates are studied. The first surrogate (MRF1), which consists of 33.8 vol% n-heptane/43.2 vol% iso-octane/23 vol% MCH, is composed by matching the RON and MON of the light naphtha. The second surrogate (MRF2), which consists of 31.4 vol% n-heptane/33.3 vol% iso-octane/35.3 vol% MCH, is composed by matching the RON and H/C ratio. The linear-by-mole blending rule proposed by Knop et al.\textsuperscript{25} was used to calculate RON and MON (Equation 1). This method was demonstrated to be the most accurate one to calculate RON/MON for ternary mixtures of n-heptane, iso-octane and toluene\textsuperscript{25} and used to estimate RON and MON of multi-component naphtha surrogate.\textsuperscript{20}

\[
ON_{MRF} = \sum_i x_i ON_i = x_n\text{-heptane} ON_{n\text{-heptane}} + x_{iso\text{-octane}} ON_{iso\text{-octane}} + x_{MCH} ON_{MCH}
\]

where ON is RON/MON for each species, $x$ is the mole fraction of each species in the mixture.

The T50 of the test naphtha (98.7°C) is very close to the boiling points of n-heptane, iso-octane, and MCH, which are 98.4°C, 99°C, and 101°C, respectively. The lower heating values of MRF1 and MRF2 are 44.16 MJ/kg and 44.08 MJ/kg close to that of naphtha.

3 EXPERIMENTAL METHOD

3.1 Tsinghua University rapid compression machine

All experiments were conducted using the Tsinghua University Rapid Compression Machine (TU-RCM).\textsuperscript{26,27} The TU-RCM was a single piston type, which could be heated up to 150°C. The mixture could be compressed to high pressure and high temperature in less than 30 milliseconds (ms). The compression ratio could be varied between 5 and 16 by adjusting the length of the combustion chamber. A creviced piston was used to effectively capture the cooler gas in the boundary layer scraped from the chamber wall during compression. Pressure history in the combustion chamber was obtained using a piezoelectric pressure transducer (Kistler 6125C) combined with a charge amplifier (Kistler 5018A). The detailed description of the RCM can be found in Di et al.\textsuperscript{26}

3.2 Mixture preparation

The test mixture was prepared in a stainless steel mixing tank at room temperature and then maintained at 80°C for 2-3 hours to ensure homogeneity. The mixture composition was determined based on the partial pressure of the mixture components. Ultrahigh purity grade nitrogen (>99.999%), argon (>99.999%), oxygen (>99.995%), n-heptane(>99%, Sinopharm Chemical Reagent Co., Ltd., Beijing, China), iso-octane (>99.8%, Sinopharm Chemical Reagent Co., Ltd., St. Louis, MO), and MCH (>99%, Sigma-Aldrich CO., LLC.) were used. The partial pressure of each component was controlled below its saturation vapor pressure to prevent condensation.
3.3 | Definition of experimental conditions and ignition delay

Figure 1 shows the typical pressure trace of light naphtha ignition and nonreactive experiments on TU-RCM. The original pressure trace was filtered using a low-pass filter with cut-off frequency of 3000 Hz. A slight pressure oscillation can be found near the end of compression during the final stage of the piston deceleration. The end of compression \( t_0 = 0 \) ms is defined as the first pressure peak during the pressure oscillation for all experiments. The ignition delay time (for single stage ignition) and total ignition delay time (for two-stage ignition) \( \tau \) are defined as the time interval between \( t_0 = 0 \) ms and the time of the maximum pressure rise rate. The first-stage ignition delay \( \tau_1 \) is defined as the time from \( t_0 = 0 \) ms to the first local maxima of the pressure derivative after the end of compression.

For each experiment, the effective pressure \( p_{\text{eff}} \) and effective temperature \( T_{\text{eff}} \) were used to represent the experimental conditions (Equations 2 and 3), which were defined using the same method described in Di et al.\(^{26}\) Note, the specific heat ratio \( (\gamma) \) was calculated based on the first 15 components that contain the most in naphtha. The experimental uncertainties were calculated using the same method as described in.\(^{26,27}\)

\[
p_{\text{eff}} = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} p \, dt \tag{2}
\]

\[
\tau_{\text{df}} = \frac{\gamma}{\gamma - 1} \int_{T_{\text{in}}}^{T_{\text{in}}} \frac{1}{T} \, d\ln T \ln \left( \frac{p_{\text{eff}}}{p_{\text{in}}} \right) \tag{3}
\]

where \( t_0 \) and \( t_1 \) are the time at end of compression and the time of \( p_{\text{min}} \), respectively. \( T_{\text{in}} \) and \( p_{\text{in}} \) are the initial temperature and pressure before compression.

3.4 | Test conditions

For PPCI combustion using gasoline type fuels, the ignition process was very complex. Zhang et al. found the start of combustion occurred at a fuel lean region in their DNS study,\(^{28}\) while Wolk et al. found that the sequential autoignition of the stratified charge occurred in order of increasing equivalence ratio at 1 bar intake pressure and decreasing equivalence ratio at 2 bar intake pressure.\(^{29}\) In the optical engine tests by Tanov et al.,\(^{30}\) the region for initial autoignition was varied according to the injection strategies and timings. Thus, the conditions with different fuel/air equivalence ratios should be measured to understand the ignition behavior of naphtha and its surrogates.

In order to obtain reliable ignition delay times at high temperature and pressure conditions, the lean condition, equivalence ratio of 0.5, was first chosen with three effective pressures 10, 20, and 30 bar in the tests. The test mixture was diluted to avoid short ignition delay or ignition during compression, which could cause difficulty in determining the end of compression. Additionally, the low temperature GCI engine usually operated at diluted conditions, so the current diluted tests mimicked such scenario to some extent. The mole ratio of the buffer gas (\( N_2/Ar = 5.55/1 \)) to \( O_2 \) was maintained at 6:1. The blending buffer gas was chosen in order to provide a reasonable test temperature range as it had higher specific heat ratio than pure \( N_2 \). The initial temperature \( T_{\text{in}} \) was kept at 80°C to prevent naphtha condensation. At each condition, the ignition delays of light naphtha, PRF59, MRF1, and MRF2 were measured. Even though in the real engine tests the combustion might occur at higher pressure conditions (>30 bar, with boosting), it was difficult to avoid the ignition during compression at higher pressures on RCM. Thus, the maximum test pressure was set to 30 bar. The condition with an equivalence ratio of 1 was also tested for naphtha, PRF59, and MRF1, but the maximum test pressure was only 20 bar due to the very short ignition delays.

4 | COMPUTATIONAL METHODS

Computational simulations were performed using the closed 0-D homogeneous batch reactor model in the CHEMKIN-Pro.\(^{31}\) The ignition of MRF was calculated using the mechanism developed by Weber et al.,\(^{21}\) which consists of 1540 species and 6498 reactions. PRF59 combustion was simulated with the detailed gasoline surrogate mechanism developed by Mehl et al.\(^{32}\) A variable volume model was adopted to represent the compression and expansion process of core region in the RCM. The volume time-history was obtained in the same manner as in Di et al.\(^{26}\) and Ji et al.\(^{27}\) and provided as Supplementary Material. For each experiment, a non-reactive experiment was carried out by replacing \( O_2 \) with \( N_2 \).
RESULTS AND DISCUSSION

5.1 Experimental comparison of autoignition characteristics of light naphtha and surrogates

In this study, special attention was paid to compare the difference between PRF59 and MRF2 to show the effect of MCH, as well as the difference between MRF1 and MRF2 to examine the best method in determining the blending ratio of MRF components. The results for the mixture with an equivalence ratio of 0.5 are discussed in this section.

Figure 2 shows the experimental pressure trace comparing Naphtha, MRF1, MRF2, and PRF59 at four selected conditions and representative nonreactive pressure profiles for each condition are also included. Figure 2A–C show the pressure traces at three different pressure but almost the same temperature (746K). Two-stage ignition was clearly observed for all four fuels. PRF59 had shorter first-stage ignition delay, but longer total ignition delay than Naphtha. Both MRF1 and MRF2 matched the first-stage ignition delay of Naphtha well. Among the three surrogates, MRF2 best matched the total ignition of Naphtha. Both MRF1 and MRF2 matched the first-stage ignition delay of Naphtha well. Among the three surrogates, MRF2 best matched the total ignition of Naphtha. Figure 2D shows the pressure traces at $p_{\text{eff}} = 30$ bar and $T_{\text{eff}} = 923$ K. Single-stage ignition was observed for all fuels. PRF59 had shorter ignition delay than Naphtha. MRF2 almost perfectly matched with Naphtha, while MRF1 exhibited slightly longer ignition delay.

Figures 3–5 compare the total ignition delay and the first-stage ignition delay of Naphtha, MRF1, MRF2, PRF59 at $p_{\text{eff}} = 30, 20, \text{ and } 10$ bar, respectively. The first-stage ignition delays of PRF59 were shorter than those of Naphtha and other surrogates for all the test conditions indicating that PRF59 had the highest low temperature reactivity. The higher reactivity of PRF59 might be attributed to the absence of cycloalkanes. Methyl-cyclohexane can scavenge OH radical by H abstraction reactions to form less reactive radicals (MCHR1, MCHR3, and MCHR4). More details are discussed by the chemical kinetic analysis. MRF1 had a slightly longer first-stage ignition delay than Naphtha at 20 and 30 bar, while MRF2 well matched the first-stage ignition delay of Naphtha. It appeared that the surrogate generated by matching either MON or H/C ratio performed well in capturing the naphtha first-stage ignition delay.

Overall, PRF59 exhibited shorter total ignition delay than Naphtha at 30 bar, but it appeared less reactive than Naphtha as the temperature increased at 10 bar (>696 K) and 20 bar (>721 K). Both MRF1 and MRF2 well matched the ignition delay of Naphtha over the entire pressure range investigated, slightly better for MRF2 at low temperature (<747 K) and low pressure (10 and 20 bar) conditions. Two MRF surrogates exhibited slightly more pronounced NTC behavior than Naphtha and PRF59 at 30 bar. The difference of total ignition delay in the NTC regime is less pronounced between PRF59 and MRFs at 10 and 20 bar. The higher reactivity of PRF surrogates compared to naphtha and multi-component surrogates.

FIGURE 2 Comparison of experimental pressure traces of Naphtha, MRF1, MRF2, and PRF59 (The short dash line in each figure is the representative nonreactive pressure trace)
at low temperature regions was also found by Javed et al. and Alabbad et al.\textsuperscript{19,20}

The ignition delays of light naphtha with an equivalence ratio of 0.5 and pressure of 20 bar measured by Javed et al.\textsuperscript{19} are also shown in Figure 4B. The mixture was not diluted in their tests. As expected, the diluted mixtures in this study exhibited longer ignition delay due to the reduction at the concentration of fuel and oxidizer (Note that, RON of naphtha used in the tests of Javed et al. was 5.5 higher than that in the current tests). Similar to the findings of Alabbad et al.\textsuperscript{20} the diluted mixture exhibited more significant NTC behavior. In the NTC region, the ignition delays of the diluted mixture were almost four times longer, while in the low and high temperature regions, the diluted mixture showed about twice longer ignition delays compared to the nondiluted mixture.

The difference in ignition delays between naphtha and MRF1/MRF2 was evaluated according to Equation 4,

\[
\varepsilon_{\text{MRF}} = \frac{\sum \left| \frac{\tau_{\text{naphtha}} - \tau_{\text{MRF}}}{\tau_{\text{naphtha}}} \right| \times 100}{n}
\]

where \(\tau_{\text{naphtha}}\) and \(\tau_{\text{MRF}}\) are the ignition delays of naphtha and surrogates (MRF1/MRF2), \(n\) is the total numbers of tests. \(\varepsilon_{\text{MRF1}}\) was 11.7% and \(\varepsilon_{\text{MRF2}}\) was 17.2%. Thus, from the experimental results of Figures 2–5, it can be concluded that the three-component surrogates composed by matching RON and H/C ratio (MRF2) is the best in emulating the ignition delay and the pressure evolution of Naphtha.
5.2 Chemical kinetic analysis

Figures 6 and 7 illustrate the model predictions along with the experimental results of MRF1 and MRF2 at three tested pressures. The mechanism predicted shorter first-stage ignition delays at all conditions. The mechanism well predicted the total ignition delays at high-pressure conditions (20 and 30 bar). However, it underpredicted the total ignition delay by a factor of 2 at 10 bar. NTC behavior was observed in both the simulation and experimental results. The mechanism predictions exhibited significantly less pronounced NTC behavior. The mechanism better predicted the ignition delay of MRF2 than MRF1. Comparing mechanism predictions and MRF2 experimental results of the total ignition delay at pressure higher than 20 bar, the major deviation was observed at temperature higher than 824 K. The mechanism slightly overpredicted the first-stage ignition delay by 21% on average.

To understand the different ignition behavior between MRF and PRF, a constant volume simulation was performed for the three surrogates with the same mixture composition as the experiments. Figure 8 shows the evolution of OH ad HO2 fraction during the oxidation of the surrogates at 10 bar, 744 K and 30 bar, 679 K. In the early stage of the oxidation, both OH and HO2 grew faster for PRF in the two conditions, resulting in shorter first-stage ignition delay (see Figure 3A and 5A). MRF exhibited earlier OH and HO2 peaks than PRF in the low pressure condition, while earlier OH and HO2 peaks were found for PRF in the high pressure condition, which explains the difference in the ignition delay in Figures 3B and 5B. Note that, MRF1 showed a little faster OH and HO2 increase than MRF2 at 10 bar, but a slightly longer ignition delay was found for MRF1 in Figure 5B.

A rate of production (ROP) analysis of OH was performed for PRF59 and MRF2 under the same condition in Figure 8. The results are shown in Figure S1. ROP was conducted at the time of 5% of total ignition delay for 10 bar and 744 K condition before the first-stage ignition. The pathway for OH formation was dominated by n-heptane in PRF59, while both low temperature reactions of MCH and n-heptane were important for MRF2. The H-abstraction reactions via OH were the main OH consumption pathway and reactions with MCH exhibited higher OH consumption rate than that with n-heptane for MRF2. The ROP of OH production and consumption was almost three orders of magnitude higher in PRF59 compared to MRF2. N-heptane could produce OH radical pool faster than MCH, resulting in a shorter first-stage ignition delay in Figure 5A. The similar dominant reactions were found in the ROP analysis for 30 bar and 679 K at the time of 25% of total ignition delay.

Using the same method with Weber et al., the ignition sensitivity index was calculated for MRF2 to address the effect of MCH chemistry on the ignition behavior. Figure S2 in Supplementary showed the sensitivity index of MRF2 at 30 bar and 751, 864, 962 K with the same mixture in Section 5.1. The negative sensitivity means this reaction prompts the...
ignition, while the positive sensitivity means this reaction inhibits the ignition. The sensitivity to the first-stage ignition was analyzed for 751 K and 864 K due to the single-stage ignition behavior at 962 K. N-heptane had higher reactivity, thus its low temperature reactions exhibited negative sensitivity. Similar with the results of Weber et al., compared with the other isomers (MCHR1, MCHR3, MCHR4), MCHR2 had higher reactivity, resulting in negative sensitivity for the H abstraction reactions and chain propagation reactions of MCHR2. As the temperature increased to 864 K in the NTC region, the production of methylcyclohexene (MCH-ene) became more pronounced because this was a chain termination pathway. Similar important reactions with n-heptane, iso-octane, and MCH were found in the total ignition delay sensitivity analysis, which showed the similar effect on the ignition. Different from the first-stage ignition, the dissociation of $\text{H}_2\text{O}_2$ to form two reactive OH radicals was the most important reaction. $\text{H}_2\text{O}_2$ started to form during the first-stage ignition and decomposed rapidly at temperature of about 1000 K, which provided chain branching.

6 | DISCUSSION

As mentioned above, the test at stoichiometric condition was performed to further evaluate the ignition behavior of naphtha and its surrogates. The ignition delay times were provided in the Supplementary (Figure S3). The mixture was also diluted to maintain the mole ratio of the buffer gas ($\text{N}_2$/Ar = 3.3/1) to $\text{O}_2$ at 6:1. Similar to the results in Section 5.1, PRF59 exhibited lower ignition delays at low temperature regions, while the reactivity of PRF59 and MPR1 was almost same at intermediate and high temperature conditions. Overall, MRF performed better because it matches the ignition delays of naphtha at two equivalence ratios in the test. In some PPC engine tests, apparent diffusion combustion was observed, suggesting that fuel burned in the rich condition. Thus, the ignition behavior of naphtha and its surrogates should also be compared at an equivalence ratio above 1.

The ignition behavior of MRF was associated with the concentration ratio of n-heptane, iso-octane, and methylcyclohexane in the mixture, which was determined by matching the RON and either MON or H/C ratio of naphtha. Thus, the uncertainty of RON, MON, and H/C ratio in the standard ASTM tests was essential to the species concentration and corresponding ignition behavior. RON was used in constructing both MRF1 and MRF2, leading to the same uncertainty from RON measurement for the two surrogates. Thus, only the measurement uncertainties of MON and H/C ratio were analyzed. The measurement uncertainty of MON was 0.9 when MON falls between 80.0 and 90.0 according to the ASTM method. For low octane number fuel like naphtha, the measurement uncertainty of MON was not reported before, but it could be higher. In this study, 0.9 was used as the
uncertainty of MON in the following analysis. The measurement uncertainty of the mass concentration of hydrogen was 0.18% according to the ASTM method.

Figure 9 shows the volume fraction uncertainty of each component in MRF1 and MRF2, when the measurement uncertainties of MON and H/C were considered. The volume fraction range of each species was calculated by using the largest/smallest values of MON or H/C within the uncertainty (e.g. MON: 58 ± 0.9). It is clear that the volume fraction range in MRF2 was smaller than that of MRF1 and the variation in the ignition delay was expected to be smaller. Therefore, matching RON and H/C was more accurate than matching RON and MON. For naphtha with negative sensitivity, the method of matching RON and MON no longer works, because the calculated volume fraction will be negative since all of three species have positive sensitivity. Therefore, in terms of the ignition behavior and the uncertainty in determining blending ratio, it is strongly recommended to match the RON and H/C ratio when constructing MRF surrogate for light naphtha.

7  |  CONCLUSIONS

Autoignition characteristics of light naphtha and its three surrogates (PRF59 and two MRFs) were studied using the TU-RCM at 10, 20, and 30 bar. The RCM experiments showed that MRFs well replicated the ignition behaviors of light naphtha in both first-stage and total ignition delay, while PRF59 exhibited short first-stage ignition. Compared with the method of matching RON and MON, the MRF surrogate constructed by matching RON and H/C ratio better matched the ignition behaviors of the naphtha. Also, matching RON and H/C ratio had smaller uncertainty, making it an overall better method in determining the blending ratio of MRF surrogate. In addition, the MRF experiments were compared with predictions using the surrogate mechanism developed by Weber et al. The mechanism well predicted the total ignition delay at high pressure conditions (20 and 30 bar). However, the mechanism predicted less pronounced NTC behavior and longer ignition delay at low pressure. Future work will be focused on the ignition behavior of naphtha and its surrogates at rich conditions. Also, the combustion and emissions of naphtha and surrogates should be explored on real engines with different combustion modes.

CONFLICTS OF INTEREST
The authors declare no conflict of interest.

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of the article.

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