Soot Characteristics of High-Reactivity Gasoline under Compression-Ignition Conditions

Using a Gasoline Direct Injection (GDI) Piezoelectric Fuel Injector

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Abstract

Gasoline compression ignition (GCI) engine technology has become one of the promising alternative solutions to achieve better fuel economy and meet emission requirement. Higher reactivity gasoline-like fuels are more desirable in GCI engines. This study investigates the soot processes under autoignition combustion of high-reactivity gasoline (HRG) with an outwardly opening piezo gasoline direct injection (GDI) fuel injector. HRG fuels are mixtures of refinery streams with RON of 50-80 and they can potentially yield better fuel economy and emissions in GCI engines. Five ambient oxygen concentrations varying from 10% to 21% and three different ambient temperature combinations were selected to simulate various ambient environments. A two-color pyrometry was applied to measure flame temperature and soot concentration (i.e., KL factor). In general, HRG flame temperatures range from 1500-2400 K under selected conditions. HRG flames have relatively low KL factor for all selected experiment conditions. High KL factors are only observed at the flame periphery where flame temperatures are lower than 1800 K. Accumulated KL factor was calculated to evaluate overall soot amount. Flames at 800 K ambient temperature always have the highest accumulated KL factor. The soot and soot temperature trade-
off is also discussed. The desired condition needs to approach a moderate soot temperature with a relative low integrated KL factor level. The conditions of 800 K with 15% O₂, 1000 K with 10% O₂ and 1000 K with 12% O₂ shows better results. The findings can help facilitate the application of high reactivity gasoline fuels in next generation clean combustion engines.

**Keywords:** two-color pyrometry; auto-ignition; soot; high-reactivity gasoline; gasoline direct injection engine

1. Introduction

The legislative requirements aimed at reducing tailpipe emissions, improving vehicle efficiency and mitigating the impact of transportation on CO₂ emissions are the main drivers when it comes to changes in the transportation landscape. Those legislative requirements, along with consumer demands for vehicles with improved efficiency, drivability, and affordability, are pushing automakers to explore many aspects of engine designs, combustion control and after-treatment systems that simultaneously reduce fuel consumption and emissions.

Gasoline compression ignition (GCI) engine technology is one of the promising alternative solutions. Compared to diesel fuels, gasoline has longer ignition delay time and better volatility which allows it to better mix with in-cylinder air resulting in relatively leaner air-fuel mixtures and hence lower soot emissions [1-2]. Experimental study has shown that stable GCI operation can be achieved down to idle speed and load on a multi-cylinder engine [3]. The utilization of gasoline in compression ignition (CI) engines can lead to diesel-like efficiency while producing less emissions, simultaneously [4-6].

Two compression-ignition combustion modes, premixed charge compression ignition (PCCI) and homogenous charge compression ignition (HCCI), are extensively studied in published research activities. Both combustion modes can potentially achieve low-NOx and low-smoke in a compression ignition engine when using fuels that have gasoline-like volatility and reactivity compared to market diesel fuels [7-8]. Compared with HCCI combustion, PCCI combustion does not require the mixture to be homogeneous and is relatively easy to be implemented in real engines. PCCI engine combustion was experimentally evaluated in terms of fuel economy and NOx reduction in 1990s by Aoyama and co-workers with a compression ratio of 17.4 [9]. This combustion mode is mainly driven by spontaneous auto-ignition at random locations. By using a
single-cylinder light-duty compression ignition engine with PCCI combustion mode, Hildingsson, et al. [10] investigated the necessity of high volatility fuels to achieve more premixed combustion with low NOx and soot emissions. They demonstrated that in partially premixed CI (PPCI) combustion, ignition quality (resistance to autoignition of a fuel) is far more important than volatility or composition. Kalghatgi and co-workers [11] used a similar experimental setup and studied auto-ignition quality of gasoline fuels at different operation conditions. They proposed that a good surrogate for gasoline in PPCI engines is a mixture of toluene, iso-octane, and n-heptane with the same research octane number (RON) and motor octane number (MON). Both experimental and numerical parametrical studies were performed with varying EGR, injection timing, and fuel type in a high-speed direct injection diesel engine by Benajes et al. [12]. They confirmed that the use of gasoline yields much longer ignition delay compared to other engine setting using diesel fuel. HCCI is an alternative combustion approach for both the spark-ignition (SI) engine and the compression-ignition (CI) engines and is more widely used than PCCI in current GCI engine studies. Yoshizawa and co-workers [13] studied PCCI mode combustion by performing multi-zone engine cycle simulations and investigated the characteristics of compression ignition combustion in gasoline engines. In general, the air-fuel distribution in an engine cylinder has a large impact on the combustion characteristics. Uncontrolled auto-ignition could be well prevented by creating a fuel rich zone at the center of cylinder even under high load conditions.

The enabling fuels for GCI engine operation are usually within the gasoline boiling range. However, their reactivity spans a very wide range. Different kinds of fuels have been studied previously in GCI engine operation. Those are conventional gasoline [14-18] or diesel [19-22], gasoline-diesel blends [23-25], high-reactivity gasoline (HRG) fuels [26-29] and reference fuel blends (mixtures of n-heptane, iso-octane and toluene) [30]. Compared with conventional gasoline and diesel fuels, HRG which are mixtures of refinery streams with RON of 50-80, can potentially yield better fuel economy and emissions in GCI engines [31-45]. Generally, these fuels have the appropriate chemical specifications (longer ignition delay than diesel) and lower well-to-tank carbon footprint. HRG fuels are mostly paraffinic with relatively low aromatics content [7-8, 37-45]. Subsequently, HRG has low sensitivity (RON-MON) and hence their ignition characteristics are similar to primary reference fuels (PRF) which exhibit negative temperature coefficient (NTC) behavior and two-stage ignition [43-45]. In Hao et al.’s study [31], it was found that the HRG fuel
resulted in a 24.6% power consumption reduction and a 22.8% reduction in greenhouse gas emissions compared to conventional gasoline production. Wang et al. [32] reported that HRG fuels are normally less processed and require 12g/MJ of energy compared to 18g/MJ for market gasolines. In addition, these HRG fuels have lower carbon numbers because they mainly consist of C5 to C11 hydrocarbons [33]. The higher hydrogen/carbon ratio for the HRG fuels results in higher heating values compared to conventional gasoline and diesel fuels. Higher heating values yield lower fuel consumption [34]. Chang et al. [35] showed that significant fuel consumption reduction can be achieved over a wide range of part-load conditions using a HRG fuel. Kolodziej et al. [36] compared engine combustion, performance, and emissions using high-reactivity and E10 gasoline fuels in a second generation single-cylinder GCI engine. They showed that HRG fuels result in lower hydrocarbon and carbon monoxide emissions at low loads. Saudi Aramco's research team has extensively studied GCI engine combustion using HRG fuels [37-45].

In order to characterize the soot formation in combustion engines, different research groups had used several different methods to measure and study the soot distribution quantitatively during spray combustion. Although LII (Laser induced incandescence) was used in measuring soot in both constant volume chamber and optical engines [46-49], the two-color pyrometry was more cost effective and widely employed in soot concentration and temperature measurements [50-54]. Ito and Azetsu [51] investigated the dilution effects of nitrogen and carbon dioxide on intermittent spray combustion in a constant volume chamber using a two-color method. Xuan et al. [55] used the two color technique for soot investigation and compared it with the light extinction method and the two approaches yield good agreement under certain conditions. The effects of fuel properties were investigated in an optical engine for jet fuel and ultra-low sulfur diesel and transient soot and temperature were measured [56]. Generally along the line of sight, the soot concentration gradients might affect the two-color pyrometry method [57], but this method is still a good way to study the downstream soot distribution where most planar or extinction techniques present meaningless results due to high soot opacity. Additionally, the two-color method can obtain two-dimensional transient soot concentration and temperature simultaneously for the entire spray combustion event [58].

In the present study, the soot processes of auto-ignition combustion of high-reactivity gasoline (HRG) were investigated under different ambient conditions. Two-color pyrometry was employed to measure the flame temperature and KL factor distributions. Average flame
temperature, KL and accumulated KL factors were calculated to evaluate the effect of ambient conditions on soot formation characteristics. Time averaged soot characteristics have also been compared. The soot and soot temperature trade-off are also discussed. The results not only demonstrate the low sooting nature of the gasoline compression ignition combustions but also provide useful fundamentals of soot formation and combustion behavior of HRG fuels to help implement these new fuels and clean combustion modes in next generation combustion engines.

2. Experimental Setup

The experiment was carried out in a constant volume chamber in a simulated compression ignition combustion environment. The chamber has six ports where six plugs with different functions are mounted on the chamber. This allows a direct and precise control over certain key parameters in the chamber. Optical access to the chamber volume is provided by a quartz window on one of the six ports. Detailed information can be found in earlier publications of our research group [59]. Figure 1 shows the schematic of the constant volume chamber with a two-color pyrometer setup. The total chamber volume is 0.95 Liter and the window inner diameter is 100 mm. Three different gases were used to formulate the appropriate mixture to achieve the desired simulated ambient temperature and EGR conditions: acetylene, dry air, 50/50 mixture of oxygen and nitrogen by volume. In the beginning of the experiment, the premixed mixture is ignited by a spark plug, producing high temperature and pressure conditions simulating the compression ignition environment right before liquid fuel injection. The transient pressure curve in the chamber is recorded by a pressure transducer at a high frequency (50000 Hz) before and after both the premixed combustion and the spray auto-ignition events. The injector used was an outwardly opening piezo gasoline direct injection fuel injector, and the produced spray is in a hollow-cone shape as shown in Figure 2. A piezo injector driver from National Instruments was used to drive the injector. The trigger signal was generated by an external pulse delay generator or an integrated Labview program via the signal from timing board PCI-6602. Fuel pressure was generated by a gasoline common rail fuel system. More details of the injection system can be found in earlier papers [60-61]. The high pressure pump was controlled by the pressure signal feedback from the fuel rail with a PID loop. The high pressure pump was driven by a 3 Horsepower motor (Marathon G590) which runs at its maximum speed. The highest rail pressure for gasoline fuels is 20 MPa.
In order to implement two-color measurements, a 550 nm and a 650 nm bandpass filters with 10 mm bandwidth were used to capture desired flame emissions at selected wavelengths. Meanwhile, the camera exposure time, aperture and other parameters were set appropriately. Transient combustion band emission images were captured by using a high-speed camera (Phantom V4.3 from Vision Research Inc.). The frame rate was set at 4801 frames per second (fps), and the resolution is 608×200 pixels for spray structure analysis. The camera was triggered simultaneously with fuel injection process by the same pulse delay generator.

In order to evaluate the effect of ambient oxygen concentration and ambient temperature on HRG auto-ignition characteristics, five different ambient oxygen concentrations (10%, 12%, 15%, 18% and 21%) and three ambient temperature conditions (800 K, 1000 K and 1200 K) were selected and investigated. Ambient gas density was maintained at 15 kg/m³. Compositions of premixed mixture are listed in Table 1. High-reactivity gasoline (HRG) was used to investigate the combustion of gasoline-like fuels under compression-ignition environments. HRG used in this study was obtained from Saudi Aramco and had an AKI value of 61. The properties of HRG are shown in Table 2 and Figure 2 shows the spray characteristics and flame structure schematic of this fuel. In all the spray and combustion images shown in this study, the injector is positioned at the right side of the viewing area, and the spray/flame develops from right to left in the viewing area. For all experiments, fuel injection pressure difference (pressure difference between fuel and environment in chamber) was maintained at 10 MPa (100 bar). Fuel injection duration signal was set to be 1.4 ms, and the fuel mass per injection was measured at around 50 mg. It is noted that due to the short ignition delays under the given ambient conditions, the fuel/air mixture is highly stratified with some similarity to diesel spray combustion. To eliminate possible condensation of water generated by the premixed combustion, the whole combustion chamber was kept at 393 K through all experiments. For each condition, five repeatable tests were made and statistical calculations were calculated based on the five runs.

3. Principle of the two color pyrometry

Two-color pyrometry is a technique to obtain flame temperature and soot distribution by measuring flame thermal radiation at two different wavelengths [62-63]. Generally speaking, thermal radiation from a blackbody source at a certain temperature and a given wavelength can be evaluated by the Planck’s equation:
\[ I_{b,\lambda}(T) = \frac{C_1}{\lambda^5 \left[ e^{(C_2/\lambda T)} - 1 \right]} \]  

where \( I_{b,\lambda} \) is the monochromatic emissive intensity of a blackbody at temperature \( T \). \( \lambda \) is the light wavelength, \( C_1 \) and \( C_2 \) are the first Planck’s constant and the second Planck’s constant. For a non-blackbody source, the monochromatic emissivity is defined as:

\[ \varepsilon_{\lambda} = \frac{I_{\lambda}(T)}{I_{b,\lambda}(T)} \]  

where \( I_{\lambda}(T) \) and \( I_{b,\lambda}(T) \) are the monochromatic emissive intensity of a non-black body and a blackbody surface at the same temperature and wavelength, respectively. Hottel and Broughton [64] proposed an empirical correlation for the monochromatic emissivity of soot particles as

\[ \varepsilon_{\lambda} = 1 - e^{-KL/\lambda^\alpha} \]  

where \( K \) is an absorption coefficient that is proportional to soot particle concentration, \( L \) is the geometric thickness of the flame along the optical path. \( \alpha \) is a parameter related to the physical and optical properties of the soot particles. Due to the complicated geometry of a real spray combustion flame, \( KL \) is often treated as a whole called the KL factor to represent the soot concentration in a flame.

Combining Equations (2) and (3), the emissive intensity at the two different wavelengths under a certain temperature is given as:

\[ \left( 1 - e^{-KL/\lambda_a^\alpha} \right) \left( \frac{2C_1}{\lambda_1^5 \left[ e^{(C_2/\lambda_1 T)} - 1 \right]} \right) = I_1 \]  

\[ \left( 1 - e^{-KL/\lambda_b^\alpha} \right) \left( \frac{2C_1}{\lambda_2^5 \left[ e^{(C_2/\lambda_2 T)} - 1 \right]} \right) = I_2 \]

According to equations (4) and (5), the soot (flame) temperature and KL factor can be calculated if the monochromatic emissive intensity is measured at the two given wavelengths. To acquire the relationship between the camera response and the emission intensity, a calibration of the optical system is necessary. In this study, a Halogen Light Sources (LS-1-LL) with a 2800 K bulb was used to calibrate the relationship between image pixel value and the monochromatic emissive power at the selected wavelength. For this work, 550 nm and 650 nm bandpass filters were used.
Signals from this light source were captured at each camera setting that was used in experiments. A linear relationship is demonstrated between the camera exposure time and the image pixel value at all apertures used in this study (shown in Figure 3). The relation between pixel value and emissive power at each pixel could be evaluated by the calibration process. $\alpha$ is a parameter that relates to light wavelength, soot particle size, refractive index of soot and fuel type [63]. In the visible wavelength region, selection of $\alpha$ is less critical on flame temperature evaluation, since flame temperature is not sensitive to $\alpha$. Thus in this study, the difference between $\alpha_1$ and $\alpha_2$ could be negligible. It is recommended to use 1.39 as the value of $\alpha$ with wavelength 550 nm and 650 nm by Yan and Barman [65]. Wavelengths from 550 nm to 650 nm were widely used to implement the two color measurement [66-67].

4. Results and Discussions

In this section, five oxygen concentrations and three ambient temperatures were investigated to evaluate the effects of ambient conditions on HRG auto-ignition characteristics. Transient flame temperature and KL factor distribution under different ambient conditions were calculated and analyzed based on the two-color measurement and a representative set of images was selected and presented in the paper. Average flame temperature and average KL factor at selected time steps were calculated to evaluate temperature and KL factor development during fuel combustion based on the five repeatable runs. In addition, the accumulated (namely, spatially integrated) KL factor under different ambient conditions were also calculated to estimate the total soot signal.

4.1 Flame transient temperature and KL distribution

4.1.1 Low oxygen concentration conditions

Transient flame temperature and KL factor distributions at the 800 K and 10% oxygen condition are shown in Figure 4 (a) and (b). At this condition, fuel combustion process could last for more than 30 ms due to slow reaction. Therefore, one of every ten images with a time interval of 2.091 ms was selected to illustrate the HRG fuel combustion development in this section. As shown in Figure 2, the fuel injector is positioned at the right side of the viewing area, and spray develops from right to left in the viewing area. As seen from Figure 4, fuel auto-ignition appears at a location close to the injector nozzle and the timing is close to the end of fuel injection. The combustion and flame development processes are slow since flame is still visible at 21 ms after
the start of the injection trigger (ASOIT). An obvious flame propagation process from the right to
the left until the end of fuel combustion is noticed after ignition. At 800 K and 10% oxygen
condition, fuel auto-ignition delay is relatively long (longer than the fuel injection duration) and
the flame no longer maintains a hollow-cone shape. Instead, the flame occupies more than half of
the chamber. Flame temperature at this condition ranges from 1500 K to 1800 K. Areas with higher
flame temperature are located at the flame center, and this high temperature area moves to the left
side as time progresses. At each time step, the flame periphery always has a lower temperature.
The soot KL factor distribution at this condition is shown in Figure 4(b). It is found that most parts
of the flame have very low values of KL factor. High KL factor areas are observed at the flame
edges for the first five images. However, after 10.651 ms ASOIT, high KL factor areas gradually
moves inward with time. At 21.101 ms ASOIT high KL factor areas are almost located in the
middle of the flame. Comparing the temperature distribution and locations of high KL factor areas,
it is noted that high KL factor areas are closely related to the temperature gradient. High KL factor
areas mostly are located in an area where temperature changes from high to low levels. Specifically,
at the 800 K and 10% oxygen condition, high KL factor is observed at an area where flame
temperature drops from 1800 K to 1500 K rapidly.

Flame temperature and KL factor distributions at 1000 K and 10% oxygen concentration
are presented in Figure 5 (a) and (b). Compared with the flame at the 800 K and 10% oxygen
condition, flame auto-ignition is still found at a location close to the injector nozzle. However,
several differences in flame development and temperature distributions can be noticed. First, the
flame temperature ranges from 1500 K to around 2000 K, which is higher than the 800 K and 10%
oxygen condition. Second, the fuel combustion process becomes faster at 1000 K. Flame is almost
extinct at 21.101 ms ASOIT, and the flame area is much smaller at this same time step than the
flame at 800 K. The KL factor distribution is shown in Figure 5(b). Compared with the 800 K and
10% oxygen condition, the KL factor at 1000 K condition is negligible before 10.651ms ASOIT.
Only several tiny areas located at the flame front are found with noticeable high KL factor. After
10.651 ms ASOIT, high KL factor areas increase with time, and locations of the high KL factor
areas are found at the flame upstream. For the first five images, areas that with rapid temperature
variation are mostly seen at the downstream. While for the last five images, the flame upstream
has more obvious temperature drop from around 1800 K to 1500 K. These locations are consistent
with the observed high KL factor regions.
Flame temperature and KL factor distributions at 1200 K and 10% oxygen concentration are shown in Figure 6 (a) and (b). Both flame temperature distribution development and KL factor distribution development are quite similar to the flames at 1000 K and 10% oxygen concentration condition. Differences are found at in the flame temperature range and fuel combustion rate. The highest flame temperature at 1200 K and 10% oxygen concentration reaches about 2100 K, which is higher than flames at a lower ambient temperature. Flame disappears at around 18.802 ms ASOIT. This timing is the earliest under the three ambient temperature conditions with 10% oxygen concentration. In addition, flame begins to split to small local regions at around 14.622 ms ASOIT until the end of the combustion, but flame at the downstream still has a higher temperature than the upstream under this condition.

4.1.2 Normal air ambient oxygen concentration (21%) conditions

Low oxygen concentration conditions generally occur in high exhaust gas recirculation (EGR) conditions in engine operations. Under normal engine operation conditions, the ambient oxygen concentration is often at 21%. A conventional environment for diesel-like fuel compression ignition is considered as 1000 K ambient temperature with 21% ambient oxygen concentration. This experimental condition is also selected for HRG auto-ignition experiments. HRG flame temperature and KL factor distribution results at different timings are presented in Figure 7 (c) and (d). Under this condition, the flame peak temperature reaches more than 2300 K, and the flame temperature of most parts is higher than 2000 K before 8.651 ms ASOIT. Meanwhile, the inner side of flame has a higher temperature than the flame periphery, and the lowest flame temperature is found at the flame upstream. After 8.651 ms ASOIT, the flame temperature decreases until the end of fuel combustion. Compared with the 1000 K and 10% oxygen concentration condition, fuel under this condition has much higher combustion rate. Flame begins to shrink at 8.651 ms ASOIT, and disappears at 12.741 ms ASOIT. Besides this, flame under this condition can only spread to around 55 mm horizontally from the injector nozzle (located on the wall of the chamber at right side), while flame at 10% oxygen concentration with the same ambient temperature reaches more than 85 mm. Moreover, a confined hollow-cone shape of flame is observed at the first two images. This is believed to be caused by the faster fuel reaction rate under this ambient condition. A faster fuel combustion rate leaves shorter time for fuel mixture to penetrate, and also leads to a faster mixture burning rate. Both factors help shorten the flame spread areas. The KL factor distributions at 1000 K and 21% oxygen concentration are presented in Figure
7 (d). The KL factor distributions at 1000 K and 21% oxygen concentration condition are consistent with the flame at 1000 K and 10% oxygen concentration. The KL factor over the whole flame is negligibly low until 10.651 ms ASOIT. Only a few discrete areas are found with a high KL factor by the end of combustion. In addition, flame temperatures at areas that have high KL factors are lower than 1800 K. Combined with the findings of the KL factor distribution before that high KL factors appear at an area with a rapid temperature drop from 1500 K to 1800 K, it may indicate soot is more likely to survive at an environment with a temperature lower than 1800 K due to a slow soot oxidation process.

4.1.3 Effect of ambient oxygen concentration

Five ambient oxygen concentration conditions ranging from 10% to 21% were selected to explore the effect of oxygen concentration on flame temperature and KL factor distribution. Results of flames at 1000 K ambient temperature with different oxygen concentrations are illustrated in Figure 8 (a) – (e). Several flame features could be observed. Firstly, a higher flame peak temperature could be found at a high oxygen concentration condition for all investigated experiment conditions. For example, peak flame temperature at 21%, 15% and 10% oxygen concentrations are around 2300 K, 2100 K and 2000 K, respectively. Second, higher flame temperature areas are mostly located at inner side of the flame until the end of fuel combustion. By the end of fuel combustion, flame downstream generally has higher temperature than flame upstream, which is believed to be caused by the cooling effects of fuel evaporation near the fuel injector. It should be noted that the timing of the end of fuel combustion varies at different oxygen concentrations. At 10% oxygen concentration combustion lasts more than 21 ms, but at 21% oxygen concentration condition this period reduces to less than 13 ms. This indicates that a higher oxygen concentration could accelerate fuel combustion rate at selected ambient temperature range. At last, a more confined flame structure could be observed under a higher oxygen concentration condition. At 6.741 ms ASOIT, flame structures at 10%, 12% and 15% oxygen concentrations are irregular. For 18% and 21% oxygen concentration conditions, flames gradually present an oval shape. KL factor distributions at 1000 K with different oxygen concentrations are presented in Figure 9. Flames at different oxygen concentrations have quite similar KL factor distributions and developments. KL factor are maintained at low level for the whole flame until the end of combustion. By the end of combustion, high KL factors could be noticed once flame begins to
shrink and extinct. Most high value KL factors are located at the region that has rapid temperature drop with temperature lower than 1800 K.

4.2 Time resolved results

4.2.1 Averaged flame temperature

In order to evaluate the effect of ambient temperature conditions on flame development, average flame temperature at each time step is calculated for all selected ambient conditions. The average flame temperature at a time step is defined as the accumulated temperature over the flame area. Results of average flame temperature at each oxygen concentration with different ambient temperatures are presented in Figure 10. Developments of average flame temperature are quite similar. For each experimental condition, the average flame temperature first increases monotonically for the first half of combustion process, then decreases until the end of combustion. Differences are found with average temperature value at each time step, the timing for each flame to reach temperature peak, and temperature drop rate. In the start of combustion phase, a higher ambient temperature results in a higher average flame temperature at the same time step. However, average flame temperature drops faster for flames at a higher ambient temperature than a lower ambient temperature condition. Moreover, flame at a higher ambient temperature reaches the peak average temperature earlier. This is caused by the faster fuel combustion rate at higher ambient temperature conditions. Comparison of average flame temperatures at different ambient temperature conditions are shown in Figure 11. Oxygen concentration has similar effect as ambient temperature. At each ambient temperature, a higher ambient oxygen concentration leads to a higher flame average temperature at the same time step during the monotonically increasing stage, and a faster temperature drop rate after the temperature peak. Meanwhile, flame at a higher oxygen concentration reaches the peak flame average temperature earlier.

4.2.2 Averaged KL factor

Average KL factor at each ambient condition is calculated to evaluate the soot density during the combustion process. The average KL factor is defined as the summation of the KL factor of the entire soot area divided by the total soot area at a frame (time step), which is also called pixel average KL factor. Comparisons of average KL factor development at different ambient temperature for each oxygen concentration are shown in Figure 12. In general, an “M” shape development pattern is noticed for flames at each ambient condition. At the beginning of
fuel combustion, average KL factor is relatively high for all flames. Then the average KL factor continuing decreasing until the half stage of the whole combustion. In the second half stage of combustion, KL factor first increase rapidly and then drop to around zero by the end of combustion. This second peak of KL factor is believed due to the less soot oxidation close to the end of combustion with low flame temperature (well below 1800 K as shown in Fig. 10) and less available oxygen in the flame regions. For each oxygen concentration, the effect of ambient temperature on average KL factor is different in different time period. For the first half of combustion process, a higher average KL factor is observed under a lower ambient temperature condition for each selected time step. However, for the second half of combustion process, a higher ambient temperature on the contrary leads to a higher average KL factor. Comparison of average KL factor at different oxygen concentration for each ambient temperature is illustrated in Figure 13. The effect of ambient oxygen concentration on average KL factor development is similar as the effect of ambient temperature. The two-stage effect of ambient oxygen concentration is still observed for all investigated ambient temperatures. A higher ambient oxygen concentration results in a lower average KL factor for the first stage of fuel combustion, while a lower ambient oxygen centration leads to a lower average KL factor in the second stage. However, it should be noted that ambient oxygen concentration has little effect on average KL factor peak. For each ambient temperature condition, the highest average KL factor value are close under different ambient oxygen concentrations. For each ambient temperature, flame under a higher ambient oxygen concentration reaches the peak value earlier than flames under a lower ambient oxygen concentration.

4.2.3 Spatially integrated KL factor

In order to evaluate soot formation during the combustion process, accumulated KL factors are calculated for each ambient condition. Accumulated KL factor is defined as the spatial sum of KL factors of the entire flame at each time step. In general, accumulated could be regarded as an indicator of amount of soot formation during the combustion. Results of accumulated KL factor at different ambient temperatures under each oxygen concentration are shown in Figure 14. It is seen that the M pattern development is only found with flames at 800 K ambient temperature and 10% or 12% ambient oxygen concentration. For flames at other experiment conditions, the accumulated KL factors are all first increasing and then decreasing until the end of combustion. Flames at 800 K ambient temperature always has the highest accumulated KL factor for all selected ambient
oxygen concentration conditions. Lowest accumulated KL factors are observed with flames at 1000 K ambient temperature when the ambient oxygen concentration is 10% or 12%. However, when the oxygen concentration is higher than 12%, flames at 1200 K then have the lowest accumulated KL factor for all selected time steps.

Comparison of accumulated KL factor development at different oxygen concentration for each ambient temperature is presented in Figure 15. The effect of ambient oxygen concentration on accumulated KL factor is consistent at different ambient temperature conditions. A lower oxygen concentration always results in a higher accumulated KL factor for most part of the combustion process. Meanwhile, it is noticed that at 1000 K ambient temperature, accumulated KL factor at different oxygen concentration are quite close, especially before 10 ms ASOIT. However, for 800 K and 1200 K ambient temperature conditions, accumulated KL factors of flames at 10% and 12% ambient oxygen concentrations are much higher than flames under an ambient oxygen concentration that is higher than 12%. This may indicate that a lower oxygen concentration could promote soot formation due to less soot oxidation, and this promotion is more significant at 800 K and 1200 K.

4.3 Further discussion on HRG soot and temperature

4.3.1 Ambient effects on soot temperature

In this part, we want to evaluate the effect of ambient temperature conditions on time-averaged flame temperature and peak flame temperature. The time averaged flame temperature is the averaged value across an entire flame development event under one certain condition.

Figure 16 shows the time averaged flame temperature under different ambient oxygen concentration and temperature conditions. It is clear that with increased ambient oxygen concentration the time averaged flame temperature is increasing. The time averaged flame temperature is also increasing with increased ambient temperature.

The peak flame temperature, shown in Figure 17, has similar character. The peak flame temperature increases with increased ambient oxygen concentration and increased ambient temperature. One difference between Figure 17 and Figure 16 is that for the peak flame temperature, the temperature difference between three lines (three ambient temperature conditions) becomes smaller as the ambient oxygen concentration goes higher, while for the time averaged flame temperature, the temperature difference between three lines does not change much with
changing ambient oxygen concentration. This indicates that when the ambient oxygen concentration is at a higher level, the effect of ambient temperature on the peak flame temperature becomes less significant.

4.3.2. Ambient effects on KL factor

The effects of ambient conditions on KL factor can be analyzed based on the time averaged KL and time averaged integrated KL. The time averaged KL is the averaged value of KL (at one time frame of the combustion event) across the entire combustion event, while the time averaged integrated KL is the averaged value of the integrated KL (at one time frame of the combustion event) across the entire combustion event. Figure 18 shows the time averaged KL under different ambient oxygen concentration and temperature conditions. Figure 19 shows the time averaged integrated KL. It can be seen that generally the KL factor decreases with increasing ambient temperature and increasing ambient oxygen concentration. One thing to note is about the two conditions of 10% and 12% oxygen concentration under 800 K. Their time averaged KL are slightly higher than those of the other two temperature conditions, but their time averaged integrated KL are significantly higher than those of the other two temperature conditions at same ambient oxygen concentration. This is caused by a larger flame area with similar average KL value, which contributes to a larger integrated value.

4.3.3 Temperature and KL trade-off

In order to compare the potential trend of forming soot and NOx under all the conditions, the time averaged integrated KL factor and time averaged flame temperature are plotted in Fig. 20. The blue, green, red points are 800 K, 1000 K, 1200 K ambient temperature conditions, respectively. The lower ambient temperature and lower O₂ concentration condition leads to a higher integrated KL factor with a lower flame temperature, which is to the upper left direction. A higher ambient temperature with a higher O₂ concentration has a lower integrated KL factor but higher average flame temperature, which is to the lower right direction. The desired region needs to approach the lower left corner, which can achieve a moderate soot temperature with a relative low integrated KL factor level. It can be seen that the conditions of 800 K with 15% O₂, 1000 K with 10% O₂ and 1000 K with 12% O₂ shows desired results.
6. Conclusions

In this study, two-color measurements were conducted for HRG auto-ignition experiments under different ambient conditions. The effects of both ambient temperature and oxygen concentration on soot temperature and KL factor were investigated. This is one of the few works on soot measurements for auto-ignition combustion of HRG in the literature. Major conclusions are summarized as follows:

1. HRG auto-ignition is observed at all selected experiment conditions. The HRG flame temperature ranges from 1500 K to 2400 K for the investigated conditions. For each ambient condition, high flame temperature areas are found at flame center or flame downstream during most parts of combustion, and high temperature areas gradually moves downstream with flame. Flame upstream always has lower temperature than other flame regions.

2. For each experiment condition, the average flame temperature first increases then decreases with time. After the temperature peak, the average flame temperature at a higher ambient temperature or a higher ambient oxygen concentration drops faster.

3. HRG flames have low KL factor values for all selected experiment conditions. High KL factors are observed at flame periphery where the flame temperature is lower than 1800 K and has strong temperature variation. Locations of high KL factor areas are isolated. The average KL factor shows an “M” shape development pattern in this study. A higher ambient oxygen concentration or a higher ambient temperature results in a lower average KL factor for the first half combustion process, while a lower ambient oxygen concentration or a lower ambient temperature leads to a lower average KL factor in the second stage.

4. Flames at 800 K ambient temperature always have the highest accumulated KL factor. Lowest accumulated KL factors are found with flames at 1000 K ambient temperature when the ambient oxygen concentration is 10% or 12%. When the oxygen concentration is higher than 12%, flames at 1200 K then have the lowest accumulated KL factor for all selected time steps.

Acknowledgement

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Aramco and KAUST intended to address the fundamental aspects of hydrocarbon fuel combustion in engines, and develop fuel/engine design tools suitable for advanced combustion modes.

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Table 1. Composition of the premixed combustion reactants.

<table>
<thead>
<tr>
<th>NO.</th>
<th>Fuel</th>
<th>Ambient Oxygen (V%)</th>
<th>C$_2$H$_2$ (V%)</th>
<th>O$_2$/N$_2$ (V%)</th>
<th>Air (V%)</th>
<th>MW (g/mol)</th>
<th>Density (kg/m$^3$)</th>
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<tbody>
<tr>
<td>1</td>
<td>HRG</td>
<td>10%</td>
<td>4.85</td>
<td>8.63</td>
<td>81.82</td>
<td>28.85</td>
<td>15.06</td>
</tr>
<tr>
<td>2</td>
<td>HRG</td>
<td>12%</td>
<td>4.81</td>
<td>13.37</td>
<td>81.82</td>
<td>28.85</td>
<td>15.06</td>
</tr>
<tr>
<td>3</td>
<td>HRG</td>
<td>15%</td>
<td>4.83</td>
<td>24.19</td>
<td>70.96</td>
<td>28.97</td>
<td>15.04</td>
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<tr>
<td>4</td>
<td>HRG</td>
<td>18%</td>
<td>4.86</td>
<td>35.13</td>
<td>60.01</td>
<td>29.09</td>
<td>15.03</td>
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<tr>
<td>4</td>
<td>HRG</td>
<td>21%</td>
<td>4.89</td>
<td>45.65</td>
<td>49.46</td>
<td>29.21</td>
<td>15.01</td>
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Table 2. Selected fuel properties of HRG.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Density (gm/liter at 25°C)</th>
<th>Viscosity (mPa/s at 25°C)</th>
<th>Surface tension (dyn/cm)</th>
<th>Boiling Point (°C, initial/final)</th>
<th>RON</th>
<th>MON</th>
</tr>
</thead>
<tbody>
<tr>
<td>HRG</td>
<td>637</td>
<td>0.28</td>
<td>16.4</td>
<td>50-73</td>
<td>62</td>
<td>60</td>
</tr>
</tbody>
</table>
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(a) Pixel intensity with 2.8 aperture  
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