Full Length Article

Experimental investigation of laminar flame speeds of propane in O_2/CO_2 atmosphere and kinetic simulation

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ABSTRACT

In this paper, the laminar flame speeds of C_3H_8 in O_2/CO_2 atmosphere were investigated experimentally and numerically. The laminar flame speeds of $C_3H_8/O_2/CO_2$ were measured using a Bunsen flame under the condition of different equivalent ratios and O_2 concentrations at ordinary pressure and temperature. It was found that the laminar flame speed gradually increased with the increase of O_2 concentration. The equivalent ratio of the highest laminar flame speed is between 1.0 and 1.1 under each fixed oxygen concentration. The high concentration CO_2 reduces the laminar flame propagation velocity of C_3H_8, which is due to thermal, radiative and chemical properties of CO_2. The calculations were performed to investigate the effects of CO_2 on the laminar flame speed. Results show that the thermal effect of CO_2 is the determining factor, the chemical effect is the second factor and radiative effect is the last one. Reaction $H + O_2 = O + OH$ is the most important chain reaction for the oxidation of C_3H_8. In addition to this, the third body effect in reaction $H + O_2 + M = HO_2 + M$ changed the laminar flame speed significantly in the condition of very low equivalent ratio and O_2 concentration.

1. Introduction

Recent years, the carbon capture and storage (CCS) technology is the most widely used method for greenhouse gas abatement [1,2]. Oxy-fuel combustion is regarded as one of most promising CCS technologies. In the traditional combustion, air is used for auxiliary combustion. In the oxy-fuel combustion, air is replaced by pure oxygen and recycled flue gas mixture, which highly increases the CO_2 concentration and decreases the volume of flue gas. The higher CO_2 concentration can significantly reduce the cost of CO_2 capture. In order to improve the application of oxy-fuel combustion, recent research focus on the flame characteristics of oxy-fuels mixture, such as the laminar flame speed [3,4]. The laminar flame speed is a fundamental parameter characterizing combustion. It is also an important indicator of the chemical reaction rate, mass transfer characteristics and heat release of the combustion mixture. Compared to conventional combustion, high concentration CO_2 changes the laminar flame propagation velocity of the fuel in O_2/CO_2 atmosphere.

There are various influence factors of the laminar flame propagation velocity of fuels. These factors include O_2 concentration, equivalent ratio, initial temperature and pressure. The laminar flame speeds of CH_4 [4-7], C_2H_6 [8] and C_3H_6 [9] have been measured in the condition of various O_2 concentration and equivalent ratios in O_2/CO_2 atmosphere.

The effects of CO_2 on the laminar flame speeds of syngas (CO/H_2) were studied by J. Natarajan et al. [10,11], Ai et al. [12] and Weng et al. [3]. Results show that the laminar flame speed of fuels increases with the raising O_2 concentration, and increases first then decreases with the increase of the equivalent ratio. Compared with the laminar flame speed in O_2/N_2 atmosphere, the laminar flame speed of fuel in O_2/CO_2 atmosphere is much lower. This is because CO_2 significantly reduces the flame temperature and the combustion chemical reaction rate.

In fact, CO_2 participates in chemical reactions directly, which is one of the main reasons for reducing the flame propagation velocity. Liu et al. thought that CO_2 directly participates in several elementary reactions and reduces the laminar flame speed. The main reason is that the most important elemental reaction $OH + CO <=> H + CO_2$ competes for H radicals with the chain decomposition reaction $H_2 + O <=> H + OH$. This leads to a decrease of global combustion chemical reaction rate [13]. Abián et al. studied the chemical effect of CO_2 on CO oxidation process and found that the effect of the third body reaction of CO_2 on the oxidation process is mainly related to the equivalent ratio and the flame temperature [14]. Watanabe et al. [15] believed that the third-body effect of CO_2 has a limited impact on the combustion process. These studies show that the effect of CO_2 participation in elemental reactions on laminar flame speed is not negligible, but the effect is related to the equivalent ratio and O_2 concentration.

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Generally, these studies have proved the influence of CO_2 on the laminar flame propagation velocity of gaseous fuel in O_2/CO_2 atmosphere, but the effect of the physical and chemical properties of CO_2 on the laminar flame speed of gas mixture in O_2/CO_2 atmosphere is unclear.

Propane and LPG are common gaseous fuels in industrial and residential applications [16]. Comparing with petrol or diesel, the CO_2 and NO emission from propane combustion is lower [17]. In order to improve the application of oxy-propane combustion, it is necessary to study the laminar flame speed of propane in O_2/CO_2 atmosphere and investigate the effect of CO_2 on the laminar flame speed of oxy-propane mixture.

There is only some research focused on the laminar flame speed of propane-air mixtures diluted by CO_2. Akram M et al. studied the effects of CO_2 and N_2 on the laminar burning velocity of propane-air mixtures at elevated temperature. Results show that CO_2 significantly reduces the laminar flame speed of propane [18]. Nair A et al. found the laminar flame of LPG-air mixture diluted by CO_2 decreased with an increase of dilution rate [19]. Ajay T et al. studied the effect of CO_2 on the laminar flame speed of LPG-air mixtures using the orifice burner and cylindrical tube method. Results show that the maximum laminar flame speed decreases from 57.5 cm/s to 35.5 cm/s as the CO_2 concentration increases from 0 to 60% [20]. Yelishala et al. investigated the effects of CO_2 on the laminar flame speed of C_3H_8 using a spherically expanding flame. They found the the laminar flame speed decreased with the dilution CO_2 fraction [21]. They reviewed the studies on the effect of CO_2 on the laminar burning velocity of propane-air [22]. Both the experimental and calculated results show that the maximum laminar burning speed shifts toward stoichiometric mixture as CO_2 concentration increases. However, there is little research about the laminar flame speed of propane in O_2/CO_2 atmosphere. In order to study the effects of CO_2 on the laminar flame propagation velocity of $C_3H_8/O_2/CO_2$ mixture, the laminar burning velocity of propane was measured using a Bunsen burner in the condition of various equivalence ratios and O_2 concentrations in O_2/CO_2 atmosphere in the present work. Then, the discussions were performed on the thermal, chemical and radiative effects of CO_2 on the laminar flame speed of $C_3H_8/O_2/CO_2$ mixture.

2. Experimental measurements and kinetic simulations

2.1. Experimental method

Fig. 1 shows the schematic of the experimental device, which consists of a thermostatic waterbath, a gas supply system, a Bunsen burner, three mass flow controller (MFC) and a digital single lens reflect (DSLR) camera (Canon 80D). C_3H_8, O_2 and CO_2 were mixed in a pipe after passing through the MFC. After fully mixing, the gas mixture flowed

Fig. 1. Schematic of the experimental setup.

through 2 m long copper tube into the Bunsen burner. Both the copper tube and the Bunsen burner were immersed in the thermostatic waterbath to ensure that the temperature of the gas mixture is constant. The DSLR camera was employed to capture the flame images. The Bunsen burner is made of a stainless-steel tube and its inner diameter is 6 mm. The tube length is 800 mm. The length of the burner is at least 50 times the diameter to ensure that the gas flow is laminar and fully developed [14].

According to the law of conservation of mass, the flow rate of gas mixture is equal to that of gas mixture consumed by combustion, so

$$A_f \cdot S_L = A_0 \cdot S_0 = Q \qquad (1)$$

where A_f is the area of the reaction zone, S_L is the laminar flame propagation velocity, A_0 is the exit area of the burner, S_0 is the average flow velocity at the exit of the burner and Q is the total volume flow of unburned gas mixture. Thus,

$$S_L = \frac{Q}{A_f} \qquad (2)$$

The value of Q was obtained from the MFC and A_f was calculated using the flame images. In the present work, the shape of Bunsen flame is not strict cone. In order to get the accurate calculation of the flame surface area, the flame contour should be located precisely. In the reaction zone, the location of the highest OH concentration is often the highest temperature position which is approximately to be the boundary of the flame surface. The brightest spots on the flame image are corresponding to the highest temperature positions. A MATLAB program was used to capture the brightest spots in the flame image.

The O_2 concentration in the mixture was defined as follows:

$$X_{O_2} = \frac{O_2}{CO_2 + O_2} \times 100\% \qquad (3)$$

2.2. Uncertainty analysis

There are three main sources of the experimental errors in the measurements. The first one is from the MFC. Based on the information from the manufactory of MFC, the error of the total flow rate (E_q) caused by the MFC is less than 2%. The second one is from the Bunsen method (E_a), including the flame image resolution and the approximation error. The value of E_a is about 3%. The last one is caused by the initial temperature of the mixture (E_t). In this experiment, the temperature fluctuation is less than 3 K, and the value of E_t is less than 1%. Thus, the overall error of the measurement in this paper can be estimated by equation 4.

$$E = \sqrt{E_a^2 + E_q^2 + E_t^2} = 3.74\% \qquad (4)$$

2.3. Numerical methods

In this paper, a free propagating one-dimensional premixed flame of $C_3H_8/O_2/CO_2$ mixture was studied under ordinary conditions (1 bar, 300 K). The CHEMKIN-PRO simulation software with PREMIX model was employed to predict the laminar flame speed of $C_3H_8/O_2/CO_2$ mixtures. In PREMIX code, the values of GRAD and CURV (grid points based on gradient and curvature) determine the number of grid points. Both the GRAD and CURV were set to 0.01 through the grid independence analysis of the laminar flame speed. The length of the calculation domain was 10 cm to ensure the completion of all combustion reactions. The kinetic simulation was performed using the detailed reaction mechanism of C_3 fuel combustion [23]. This detailed mechanism was usually used to describe the combustion process of propene, propyne, allene and propane [19]. In order to evaluate the effect of radiation on the laminar flame speed, an optical thin model was used to estimate the heat loss from radiation. As the CO_2 is a participating medium in heat radiation, the latest modified weighted
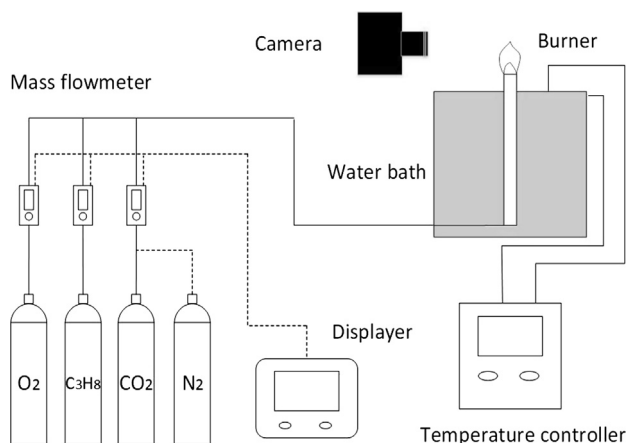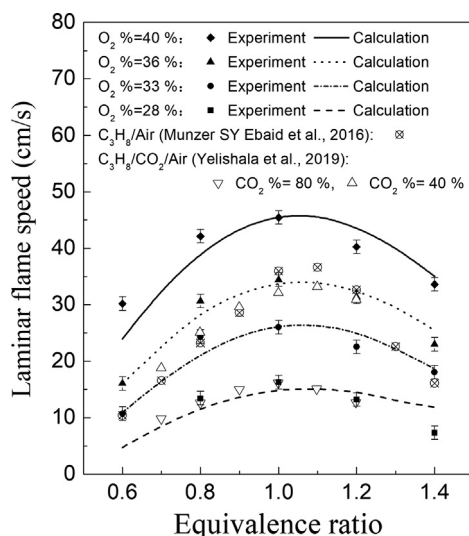
Fig. 2. The change of experimental and calculated laminar flame speeds of C_3H_8 with equivalent ratios in the condition of different oxygen concentrations.

gray gas model [24] was used as a subroutine of the PREMIX code [25].

3. Results and discussion

3.1. Effects of equivalent ratio and O_2 concentration

Fig. 2 shows the experimental and calculated laminar flame speeds of $C_3H_8/O_2/CO_2$ in the condition of various oxygen concentrations (28%, 33%, 36%, 40%) and equivalent ratios (from 0.6 to 1.4). Experimental results show that the laminar flame speed first increased and then decreased with the increase of equivalent ratio. The laminar flame speed reached the maximum near the stoichiometric ratio point. Results show that the calculated values were closed to the experimental results. The maximum calculated value of laminar flame speed appeared within the range of equivalent ratio from 1.0 to 1.1. The change trends of the laminar flame speed of $C_3H_8/O_2/CO_2$ mixture is similar to those of other hydrocarbon fuels, such as CH_4 [4,25,26] and Dimethyl Ether [27,28]. This is because both the fuel and oxygen are completely burned near the stoichiometric ratio point. The corresponding flame temperature and the concentration of high-energy radicals O and OH reach the maximum, so the maximum flame speed appeared near the stoichiometric ratio point.

For comparison, the measured laminar flame speeds of C_3H_8-air [29] mixture and C_3H_8/CO_2/air [22] mixture were presented in Fig. 2. Results show that the changes of the laminar flame speeds of C_3H_8-air and C_3H_8/CO_2/air mixture are similar to those of $C_3H_8/O_2/CO_2$ mixture, which indicates the measurements of the laminar flame speeds in the present works are reliable. In addition, the laminar flame speeds of C_3H_8/CO_2/air mixture at 80% CO_2 concentration are very closed to those of $C_3H_8/O_2/CO_2$ mixture at 28% O_2 concentration. It is noted that the CO_2 concentration in literature [22] is the CO_2 percentage of C_3H_8/CO_2 mixture.

With the increase of oxygen concentration, laminar flame speed gradually increased. The maximum values are 10.0 cm/s, 19.5 cm/s, 31.5 cm/s, 45.8 cm/s and 62.2 cm/s in the condition of increasing O_2 concentration (from 25% to 45%). Fig. 3 shows the corresponding flame images of $C_3H_8/O_2/CO_2$ mixtures at the stoichiometric ratio. Result shows that the higher oxygen concentration, the brighter the flame contour and the stronger combustion reaction rate.

Fig. 4 shows the change of laminar flame speeds with O_2 concentrations. The laminar flame speed increased nonlinearly with O_2 concentration. It is found that an approximately quadratic function relation existed between the laminar flame speeds and the O_2

concentrations by fitting the experimental data. On one hand, the increase of O_2 concentration increased some free radical concentrations (such as O radical) and enhanced the probabilities of free radical collision in the reaction zone, which generates more new chain reactions. On the other hand, the heat released from combustion is also enhanced by O_2, because the C_3H_8 and O_2 concentrations increase with raising O_2 concentration. In addition, the specific heat capacity of CO_2 is higher than that of O_2. The CO_2 concentration and the heat absorbed by CO_2 are reduced by the increase of O_2 concentration. Thus, the flame temperature increases with the raising O_2 concentration. The higher flame temperature significantly increases the concentrations of free radicals, especially the high-energy radicals such as O, H and OH in the combustion reaction zone. Higher concentration free radicals accelerate the chemical reaction rate and increase the laminar flame propagation speeds.

3.2. The thermal, chemical and radiative effects of CO_2

Due to the thermal, chemical and radiative properties of CO_2, the combustion characteristics of C_3H_8 changed in the O_2/CO_2 atmosphere. In order to distinguish the chemical influence of CO_2 on the flame speed, a virtual substance FCO_2 was used in the kinetic simulation [13,30]. The thermophysical properties FCO_2 and CO_2 are the same, but FCO_2 does not participate in any chemical reactions that CO_2 participates in. The main combustion products of $C_3H_8/O_2/FCO_2$ mixture are CO_2, H_2O and FCO_2. It should be pointed out that the FCO_2 is a diluent and the total amount of FCO_2 remains unchanged before and after combustion. For $C_3H_8/O_2/CO_2$ mixture, the main products are CO_2 and H_2O. For $C_3H_8/O_2/N_2$ mixture, N_2 is approximately regarded as an inert gas, since the NO_x formation is generally rather small.

The effects of thermal, chemical and radiative properties of CO_2 on laminar flame speed were calculated by Eqs. (4–6) respectively.

$$\Delta S_{L,therm} = S_{L,N2} - S_{L,FCO2} \tag{4}$$

$$\Delta S_{L,chem} = S_{L,FCO2} - S_{L,CO2} \tag{5}$$

$$\Delta S_{L,radi} = S_{L,CO2} - S_{L,nonadia}; \tag{6}$$

where $\Delta S_{L,therm}$ is the influence of thermal properties of CO_2, $\Delta S_{L,chem}$ is the influence of chemical reactivity of CO_2 and $\Delta S_{L,radi}$ is the influence of radiation properties of CO_2. $S_{L,N2}$ is the laminar flame speed of $C_3H_8/O_2/N_2$. $S_{L,FCO2}$ is the laminar flame speed of C_3H_8 in O_2/FCO_2 atmosphere. $S_{L,CO2}$ is the laminar flame speed of $C_3H_8/O_2/CO_2$ mixture and $S_{L,nonadia}$ is the laminar flame speed of $C_3H_8/O_2/CO_2$ without radiation heat loss.

3.2.1. The thermal effect of CO_2

Fig. 5 shows the changes of $\Delta S_{L,therm}$, $\Delta S_{L,chem}$ and $\Delta S_{L,radi}$ with the increase of O_2 concentration at the stoichiometric ratio. The thermal property of CO_2 has the greatest influence on the flame speeds. The effect of chemical reactivity is the second factor and the radiative characteristics have little effect.

Fig. 6 shows the changes of the specify heat capacity of $C_3H_8/O_2/N_2$ and $C_3H_8/O_2/CO_2$ mixtures versus O_2 concentration. Fig. 7 shows the adiabatic flame temperature of $C_3H_8/O_2/N_2$, $C_3H_8/O_2/FCO_2$ and $C_3H_8/O_2/CO_2$ mixtures in the condition of various O_2 concentration. The specify heat capacity of $C_3H_8/O_2/CO_2$ mixtures decreased with the increasing O_2 concentration, while the specify heat capacity of $C_3H_8/O_2/N_2$ mixtures increased as the O_2 concentration increased. The values of the specify heat capacity of $C_3H_8/O_2/CO_2$ are larger than those of $C_3H_8/O_2/N_2$ mixture, which is due to the higher specify heat capacity of CO_2. So, the adiabatic flame temperature of $C_3H_8/O_2/CO_2$ is lower than that of $C_3H_8/O_2/N_2$ mixture (shown in Fig. 7). Comparing with the $C_3H_8/O_2/N_2$ mixture, the laminar flame speed of $C_3H_8/O_2/CO_2$ was reduced by the lower adiabatic flame temperature. With the increase of the O_2 concentration, the difference of the specify heat capacity
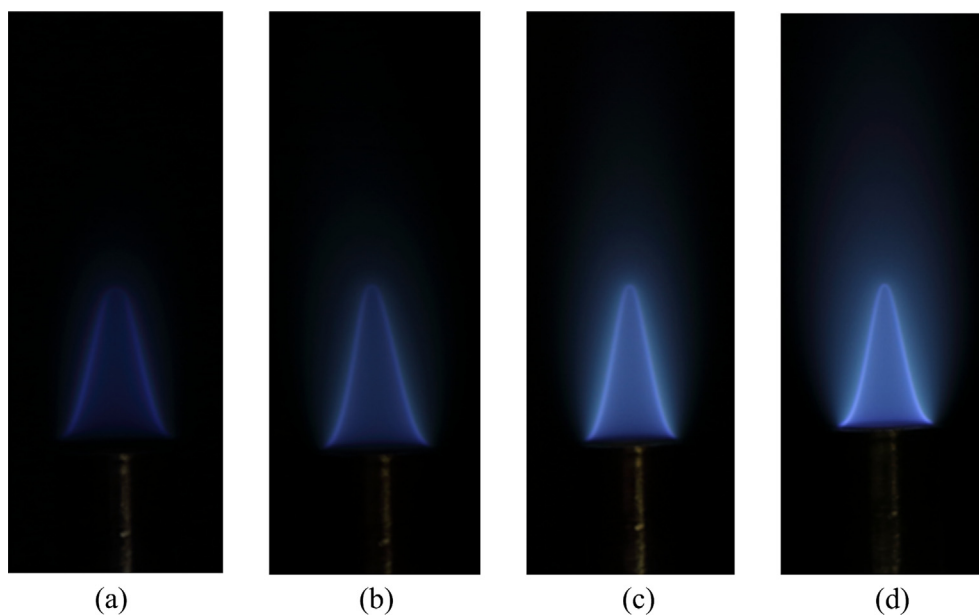
Fig. 3. The flame images of $C_3H_8/O_2/CO_2$ mixtures at the stoichiometric ratio in the condition of different oxygen concentrations: (a) 28%; (b) 33%; (c) 36%; (d) 40%.
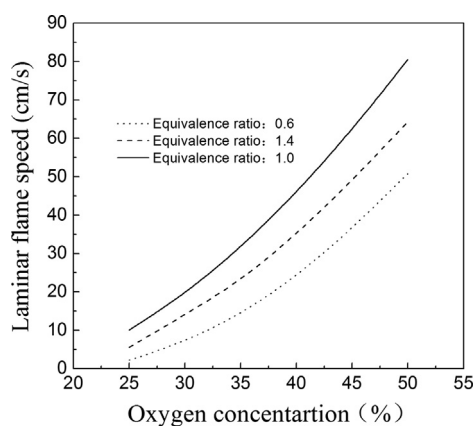

Fig. 4. The change of laminar flame speeds with O_2 concentrations in the condition of different equivalent ratios.
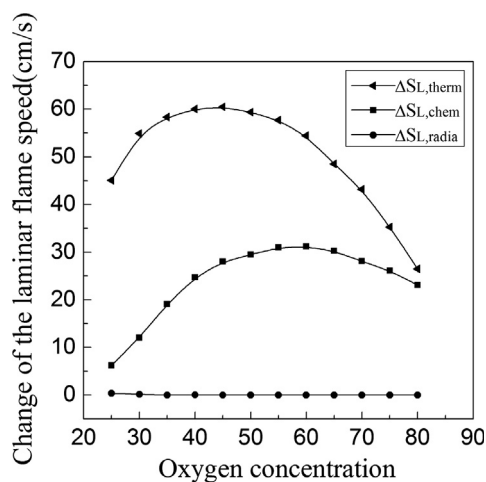

Fig. 5. The changes of $\Delta S_{L,therm}$, $\Delta S_{L,chem}$ and $\Delta S_{L,radi}$ with the O_2 concentration at the stoichiometric ratio.
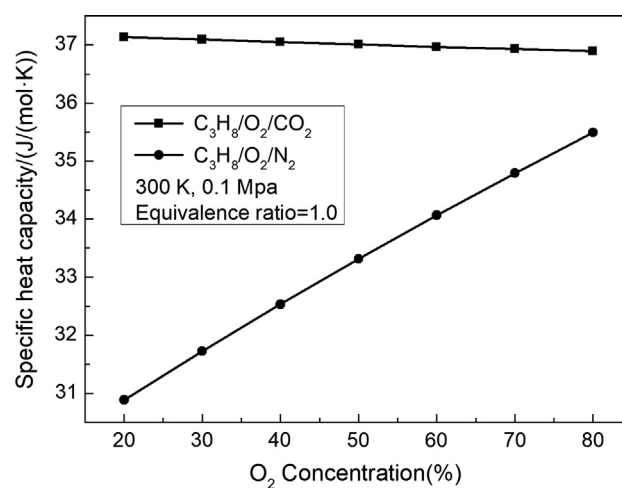

Fig. 6. The changes of the specify heat capacity of $C_3H_8/O_2/N_2$ and $C_3H_8/O_2/CO_2$ mixtures versus O_2 concentration.
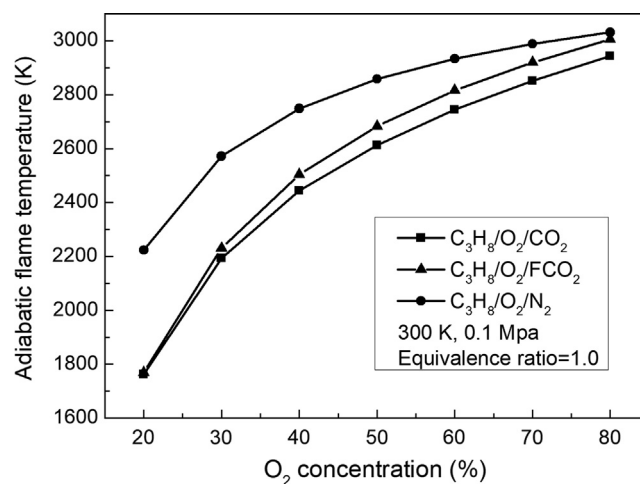

Fig. 7. The adiabatic flame temperature of $C_3H_8/O_2/N_2$, $C_3H_8/O_2/FCO_2$ and $C_3H_8/O_2/CO_2$ mixtures in the condition of various O_2 concentration.
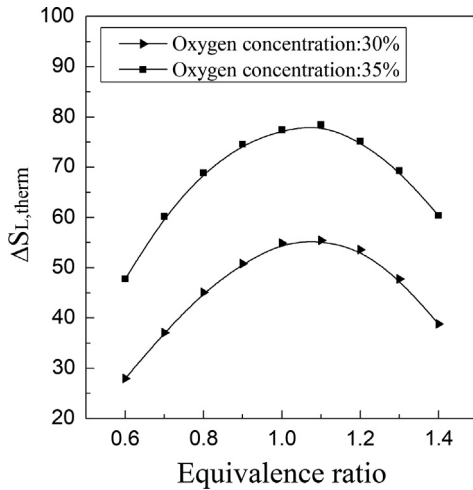
Fig. 8. The change of $\Delta S_{L,therm}$ with the equivalent ratios in the condition of different O_2 concentrations (30% and 35%).

between $C_3H_8/O_2/N_2$ mixture and $C_3H_8/O_2/CO_2$ decreased, which is due to the decreased dilution gas concentration. The adiabatic flame temperature of $C_3H_8/O_2/FCO_2$ is very closed to that of $C_3H_8/O_2/CO_2$ in the condition of low O_2 concentration (e.g. O_2 % = 20%). As O_2 concentration increases, the value of the adiabatic flame temperature of $C_3H_8/O_2/FCO_2$ grew faster than that of $C_3H_8/O_2/CO_2$ and got closer to that of $C_3H_8/O_2/N_2$ in the condition of high O_2 concentration (e.g. O_2 % = 80%). The adiabatic flame temperature increased with increasing O_2 concentration. More and more CO was produced with the increased flame temperature, which is due to the chemical effect of CO_2. Thus, the difference of the adiabatic flame temperature between $C_3H_8/O_2/FCO_2$ and $C_3H_8/O_2/CO_2$ increased with the raising O_2 concentration.

With the increase of O_2 concentration, the value of $\Delta S_{L,therm}$ first increases and then decreases, and the maximum values appears around 42% O_2 concentration. The value of $\Delta S_{L,therm}$ increased with raising O_2 concentration, which indicates that the changes of the laminar flame speed with the thermal effect is enhanced by the adiabatic flame temperature in the condition of low O_2 concentration. As the O_2 concentration continues to increase, the CO_2 concentration gradually decreases, and the influence of the thermal effect of CO_2 is reduced.

Fig. 8 shows the change of $\Delta S_{L,therm}$ with the equivalent ratios in the condition of different O_2 concentrations (30% and 35%). $\Delta S_{L,therm}$ first increased and then decreased with the increase of equivalent ratios. $\Delta S_{L,therm}$ reached the maximum near the stoichiometric ratio. This indicate that the thermal effect of CO_2 is closely related to the adiabatic flame temperature, because the adiabatic flame temperature generally reaches the highest value near the stoichiometric ratio (shown in Fig. 11).

3.2.2. The radiative effect of CO_2

It can be seen in Fig. 5 that the effect of the radiative properties of CO_2 on the laminar flame speed is very small compared with the thermal property and chemical reactivity of CO_2. The radiative effect is also affected by the equivalent ratio and O_2 concentration. Fig. 9 shows the change of laminar flame speeds of $C_3H_8/O_2/CO_2$ mixture with equivalent ratios under adiabatic and non-adiabatic conditions. The calculated laminar flame speeds under non-adiabatic condition are lower than that under adiabatic condition. It is found that $\Delta S_{L,radi}$ increased as the decreased oxygen concentration. $\Delta S_{L,radi}$ decreases first and then increases with the increase of the equivalent ratio, and it reached the lowest point around the stoichiometric ratio. In the condition of equivalence ratios which are far away from 1.0 and lower oxygen concentration, the amount of heat released by chemical reactions during combustion is smaller, thus the proportion of radiative heat loss becomes larger. This enhances the radiative effects of CO_2.

According to Yu's study [31], the radiation effect of CO_2 depends on the value of laminar flame speed. The smaller the laminar flame speed, the stronger the radiation effect. In the present work, the radiation effect on the smallest laminar flame speed was studied. It is found that the smallest laminar flame speed appeared at 28% O_2 concentration and 1.4 equivalence ratio (shown in Fig. 2). In order to evaluate the radiation effect, the reduction rate of the laminar flame speed with the radiation effect was calculated by equation 7.

$$R = 1 - \frac{S_u}{S_u^0} \times 100\% \tag{7}$$

where R is the reduction of the laminar flame speed with the radiation effect, S_u is the calculated laminar flame speed with the radiation heat loss and S_u^0 is the calculated laminar flame speed without radiation heat loss. The calculated value of R is 4.93% at the smallest laminar flame speed point. Based on the results from Yu's study [31], the values of R in other conditions are lower than 4.93%. In other words, the reduction rate of the laminar flame speed with the radiation effect is within 4.93% in the present work.

3.2.3. The chemical effect of CO_2

Fig. 5 shows that the influence of CO_2 reactivity first increases and then decreases with the increase of O_2 concentration and the maximum value of $\Delta S_{L,chem}$ appears around 55% O_2 concentration. When O_2 concentration is low, the CO_2 concentration is high. The chemical reactions are inhibited by high concentration CO_2. As high concentration of CO_2 intensifies the competition of H radical between elementary reaction $CO_2 + H = CO + OH$ and $H + O_2 = O + OH$. Fig. 10 shows the mole fraction of O, H and OH radicals in the condition of various O_2 concentration. Result shows that the O, H and OH concentrations were enhanced by the increased O_2 concentration. The higher radical concentration also increased the chemical effects of CO_2. Thus, the chemical effect of CO_2 increased with the increasing O_2 concentration. However, with a further increase of O_2 concentration, chemical reactions are inhibited owing to the lack of C_3H_8.

Fig. 11 shows the change of $\Delta S_{L,chem}$ with the equivalent ratio under a fixed O_2 concentration (30%). As the equivalent ratio increases, $\Delta S_{L,chem}$ increases first and then decreases, reaching the maximum within the range of equivalent ratio 1.0–1.05. The chemical reaction rate is mainly affected by the flame temperature. Fig. 11 shows the change of adiabatic flame temperature with the equivalent ratio. Result shows that the higher the flame temperature, the faster the reaction rate. If the flame temperature is too low, the chemical reaction will be inhibited. The variation trend of adiabatic flame temperature is the same as that of $\Delta S_{L,chem}$. The chemical reaction rate and $\Delta S_{L,chem}$ are affected directly by the adiabatic flame temperature.
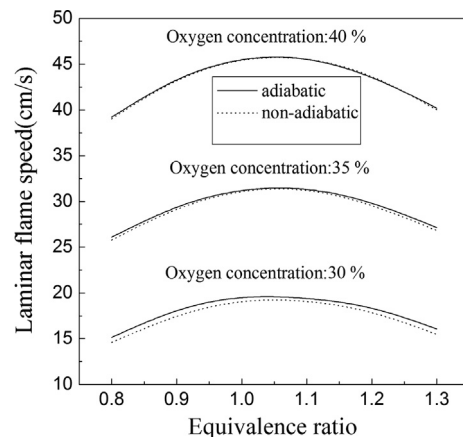

Fig. 9. The change of laminar flame speeds of $C_3H_8/O_2/CO_2$ mixture with equivalent ratios under adiabatic and non-adiabatic conditions.
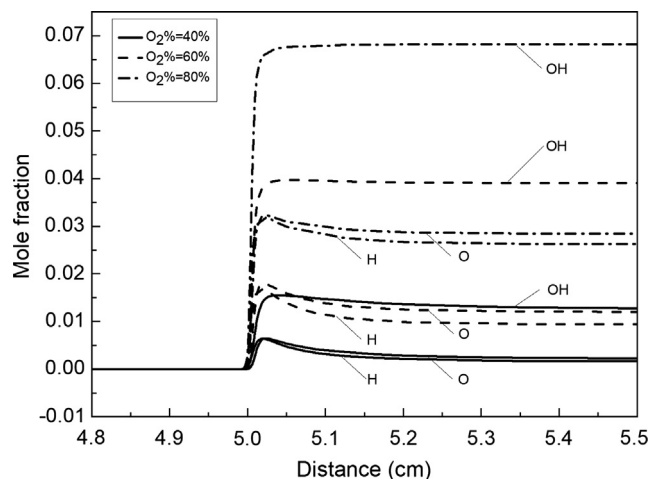
Fig. 10. The mole fractions of O, H and OH in the condition of various O_2 concentration.
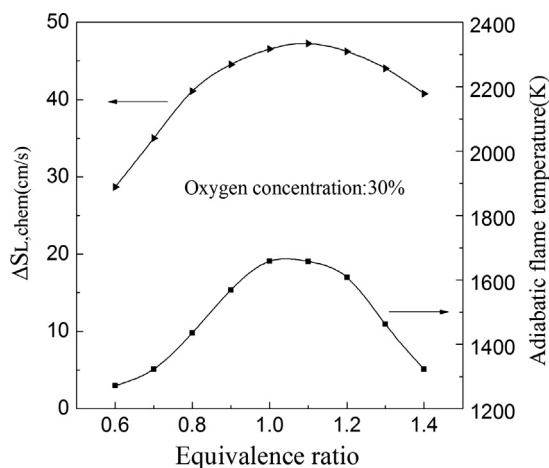

Fig. 11. The changes of $\Delta S_{L,chem}$ and adiabatic flame temperature with the equivalent ratios in the condition of a fixed O_2 concentration (30%).
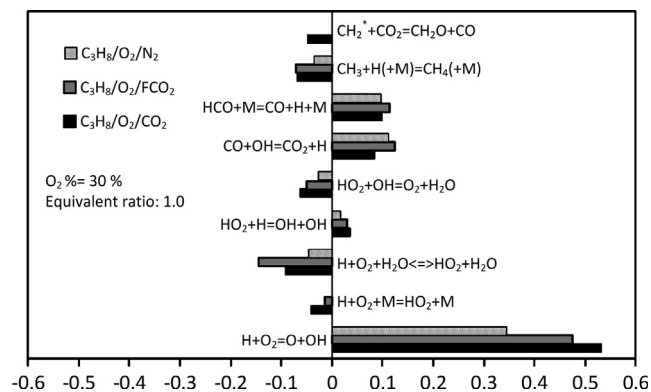

Fig. 12. The sensitivity coefficients of the main chain reactions to the laminar flame speed.

The influence of CO_2 reactivity is due to the element reactions which CO_2 participate in. The sensitivity analysis was performed to present the import reactions which affect the laminar flame speed [26]. In order to investigate the discrepancies of the laminar flame speeds among the $C_3H_8/O_2/CO_2$, $C_3H_8/O_2/FCO_2$ and $C_3H_8/O_2/N_2$. The sensitivity coefficients of the flow rate of gas mixture were calculated to emphasis the most important reactions which change the laminar flame speeds of C_3H_8 diluted by CO_2, FCO_2 and N_2。Fig. 12 shows the

sensitivity coefficients of the main element reactions to the laminar flame speeds. Through the comparison, $H + O_2 = O + OH$ is the most important chain reaction for the oxidation of C_3H_8. In O_2/CO_2 atmosphere, the sensitivity coefficient of $H + O_2 = O + OH$ is larger than that in O_2/FCO_2 and O_2/N_2 atmosphere. The importance of reaction $H + O_2 = O + OH$ was increased by the high CO_2 concentration in O_2/CO_2 atmosphere. Reaction $CO + OH = CO_2 + H$ is the main pathway for CO conversion to CO_2 and also the most important reaction which CO_2 participates in. The high CO_2 concentration decreases the forward reaction rate and sensitivity coefficient of chain reaction $CO + OH = CO_2 + H$, which reduces the heat release from the oxidation of CO. Except reaction $H + O_2 = O + OH$ and $CO + OH = CO_2 + H$, $HCO + M = CO + H + M$ is also an import radical reaction for increasing the laminar flame speed of C_3H_8 and the sensitivity coefficients are nearly the same for $C_3H_8/O_2/CO_2$ and $C_3H_8/O_2/N_2$ mixture. $H + O_2 + H_2O = HO_2 + H_2O$ and $CH_3 + H + M = CH_4 + M$ are the major reactions for reducing the laminar flame speed, especially for $C_3H_8/O_2/FCO_2$ mixture. Because the two reactions compete H radical with reaction $H + O_2 = O + OH$ and reduce the H radical concentration. There are three three-body recombination reactions in Fig. 12 among the main chain reactions which affect the laminar flame speed significantly. Thus, it is necessary to investigate the third body effect of CO_2 on the laminar flame speeds. Zhang et al pointed that the third body effect in the three-body recombination reaction $H + O_2 + M = HO_2 + M$ is very important [32]. In the following paragraph, the third body effect in reaction $H + O_2 + M = HO_2 + M$ was studied using the kinetic calculation.

Another virtual substance XCO_2 was used to distinguish the third body effect in reaction $H + O_2 + M = HO_2 + M$. The physical and chemical properties of XCO_2 are the same with CO_2 but the XCO_2 does not act as a three-body and the three-body coefficient of CO_2 is changed to be zero in reaction $H + O_2 + M = HO_2 + M$. The third body effect of CO_2 on the laminar flame speed was calculated by equation 8.

$$T = \frac{S_u^x - S_u}{S_u} \times 100\%$$

(8)

where T is the change rate of the laminar flame speed with the third body effect of CO_2 in reaction $H + O_2 + M = HO_2 + M$. S_u^x is the laminar flame speed of $C_3H_8/O_2/XCO_2$ and S_u is the laminar flame speed of $C_3H_8/O_2/CO_2$.

Fig. 13 shows the change rate of the laminar flame speed versus the equivalent ratios with the third body effect of CO_2 in the condition of various O_2 concentration. The value of T decreased with the increase of
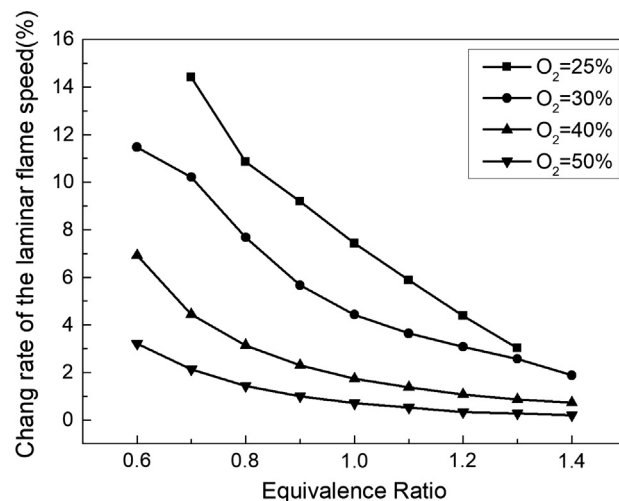

Fig. 13. The change rates of the laminar flame speed versus the equivalent ratios with the third body effect of CO_2 in the condition of various O_2 concentration.

equivalence ratio from fuel-lean side to fuel-rich side. For fuel-lean gas mixture, O_2 is excess and H is not rich. The global reaction rate is decreased by the third body effect of CO_2 because of the competition of H radical between elementary reaction $H + O_2 + M = HO_2 + M$ and $H + O_2 = O + OH$. Fig. 13 indicates that the change rate of the laminar flame speed increased with the decrease of O_2 concentration for fuel-lean gas mixture. The lower O_2 concentration and equivalence ratio, the higher the third body effect of CO_2 on the laminar flame speed. Zhang et al. [32] found that the dilution limit was mainly changed by CO_2 involved in the three-body recombination reaction. The dilution limit point of gas mixture is a very low equivalent ratio and O_2 concentration case.

4. Conclusions

In this paper, the laminar flame speeds of C_3H_8 in O_2/CO_2 atmosphere were studied. It is approximately a quadratic function between the laminar flame speeds and oxygen concentrations. The optimal equivalent ratio is in the range of 1.0–1.1. The maximum laminar flame speeds of $C_3H_8/O_2/CO_2$ mixtures are 10.0 cm/s, 19.5 cm/s, 31.5 cm/s, 45.8 cm/s and 62.2 cm/s in the condition of corresponding 25%, 30%, 35%, 40% and 45% O_2 concentration. The decrease of the laminar flame speed of C_3H_8 caused by CO_2 is mainly owing to thermal properties of CO_2. The chemical property is the second factor and the radiative property is the last one. The third body effect of CO_2 in reaction $H + O_2 + M = HO_2 + M$ cannot be ignored in the condition of very low equivalent ratio and O_2 concentration.

CRediT authorship contribution statement

Xianzhong Hu: Conceptualization, Methodology, Investigation, Writing - original draft. **Wei:** Writing - review & editing.

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