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Auto-ignition and stabilization mechanism of diluted H_2 jet flame[*]

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Abstract: The controllable active thermo-atmosphere combustor (CATAC) has become a utilizable and effective facility because it benefits the optical diagnostics and modeling. This paper presents the modeling research of the auto-ignition and flames of the H_2/N_2 ($H_2/CH_4/N_2$, or $H_2/H_2O_2/N_2$) mixture on a CATAC, and shows curves varying with temperatures of auto-ignition delay, the height of the site of auto-ignition of lifted flames, and flame lift-off height. The results of auto-ignition delay and the lift-off height are compared the experimental results to validate the model. A turning point can be seen on each curve, identified with criterion temperature. It can be concluded that when the co-flow temperature is higher than the criterion temperature, the auto-ignition and lifted flame of the mixture are not stable. Conversely, below the criterion temperature, the mixture will auto-ignite in a stable fashion. Stabilization mechanisms of auto-ignition and lifted flames are analyzed in terms of the criterion temperature.

Key words: Simulation, Combustor, Auto-ignition, Jet flame, Stabilization mechanism
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1 Introduction

Studies of the auto-ignition and stabilization mechanism of jet fuel are among the most important research efforts concerning improving combustion (Chen and Bilger, 2002). However, the complexity of the combustion process and limitations of testing methods, especially due to limited references and simulations based on experiments, have left unanswered questions. The controllable active thermo-atmosphere combustor (CATAC) has been used for investigating auto-ignition and stabilization mechanisms of fuels because it has a stable thermo/oxygen atmosphere, a simple structure, and stable temperature/velocity fields. Researchers have carried out a large number of investigations using the CATAC (Cabra *et al*., 2001; 2005; Wu *et al*., 2003; 2005; Gordon *et al*., 2007a; Patwardhan and Lakshmisha, 2008; Gkagkas and Lindstedt, 2009; Lawn, 2009). Among them, Wu *et al*. (2003; 2005) studied the lift-off height of H_2/N_2 in two typical experimental conditions using a high-speed imaging system and laser measurement. Cabra *et al*. (2001) conducted experiments and numerical analyses of H_2/N_2 turbulent jet flame by means of CATAC.

Many investigations of the stabilization mechanism of turbulent lifted flames have been carried out (Chen and Bilger, 2002; Kim, 2002; Joedicke *et al*., 2005; Won *et al*., 2005; Gordon *et al*., 2007b; Lyons, 2007; Duwig and Fuchs, 2008; Lu *et al*., 2008; Kerkemeier *et al*., 2009; Navarro-Martinez and Kronenburg, 2009). Won *et al*. (2005) investigated the stabilization mechanism of lifted flames in the near field of co-flow jets experimentally and numerically for methane fuel diluted with nitrogen. They found the stabilization mechanism to be due to the variation

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of the propagation speed of the lifted flame edge with axial distance from the nozzle in the near field of the co-flow, as compared to the local flow velocity variation at the edge. Joedicke *et al.* (2005) investigated the structure and stabilization mechanism of turbulent lifted non-premixed hydrocarbon flames using combined laser imaging techniques. They measured the geometrical structure of multi-reaction zones and the flow field at the stabilization region in 16 hydrocarbon flames, and revealed the existence of triple flame structure at the stabilization region of turbulent lifted flames.

Our group (Deng, 2007) found a turning point on the diesel oil auto-ignition flame curve, and defined it as the criterion temperature according to a great amount of experiments conducted on CATAC. The lifted flame is not stable when the thermo-atmosphere temperature is lower than the criterion temperature; in the converse condition, it is stable. This paper investigates the auto-ignition and stabilization mechanisms of N_2-diluted H_2 in the thermo-atmosphere in view of the criterion temperature. The curves varying with temperatures of the auto-ignition delay, the height of the site of auto-ignition, the OH mass fraction at the site of auto-ignition, and the lifted height of turbulent flame were attained, the criterion temperature was found by means of numerical simulation, and the mechanism based on criterion temperature was analyzed as well. Furthermore, the same fraction of CH_4 and H_2O_2 was added into the diluted H_2 mixture separately to discuss the criterion temperature and stabilization mechanism.

2 Modeling

The code STAR-CD 3.26 (CDAJ, China) was used for simulation. The 150 mm high space above the perforated plate is the region for this study. The grid model is four times the radial and axial space, so it can be regarded as infinite space above the perforated plate. In addition, one twelfth of the entire circle is built as the grid model due to the axisymmetric structure of the perforated plate (Fig. 1). The total number of grids is 9564. The boundary interfacing with the atmosphere was set as pressure boundary with the outer space being air.

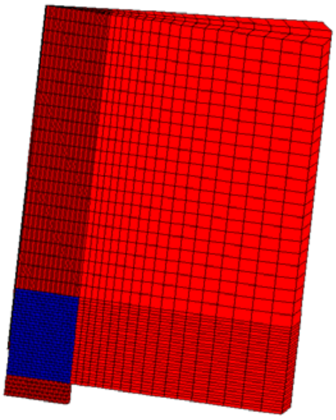


Fig. 1 Meshed model of simulation

The typical experimental conditions were adopted as boundary conditions (Table 1) (Wu *et al.*, 2003). Pressure boundaries were applied on the top surface and circumferential surface for simulating open space. The k-ε high Reynolds number model was set as the turbulent model. The combustion model adopted the complex chemical reaction model, and the reaction of H_2/N_2 mixture used a 20-step reaction mechanism of H_2 (Ó Conaire *et al.*, 2004).

3 Results and discussion

The auto-ignition delay is defined as the time between the injection of fuel and the temperature rising to 1200 K when the auto-ignition happens. The time step for this period is set to 0.01 ms. That is to say, the calculation error is adopted as 0.01 ms. The

Table 1 Typical experimental conditions (Wu *et al.*, 2003)

Condition	Jet flow					Co-flow					Lift-off height (mm)
	Q_{H_2} (L/min)	Q_{N_2} (L/min)	T (K)	V (m/s)	Re	Q_{H_2} (L/min)	Q_{air} (L/min)	T (K)	V (m/s)	Re	
A	25	75	317.5	110	25 760	190.1	1720	1044	4	18 965	~25
B	25	75	317.5	110	25 760	185.2	1720	1013	4	19 200	~100

Q_{H_2}, Q_{N_2}, and Q_{air} are the flow rates of H_2, N_2, and the air; T: temperature; V: velocity site of auto-ignition is the corresponding position with the highest temperature as auto-ignition happens. After auto-ignition, the heat will promote the combustion, so the flame will come back until steady around a specific height, this height being called the lift-off height. The lift-off height is defined as the distance of the lowest location of the 1200 K contour from the nozzle. Fig. 2 is the temperature field contour of the stable flame of H_2/N_2 mixture in the typical condition A after auto-ignition. As marked in the figure, the lift-off height is 20 mm. The lift-off height under condition B has been calculated as well, with the result being 110 mm, which indicates that the flame lift-off height in a low temperature environment is much higher than that in a high temperature environment.

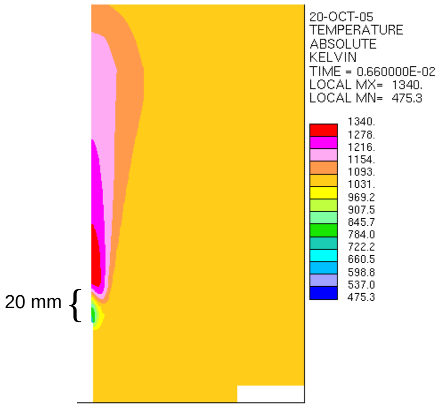
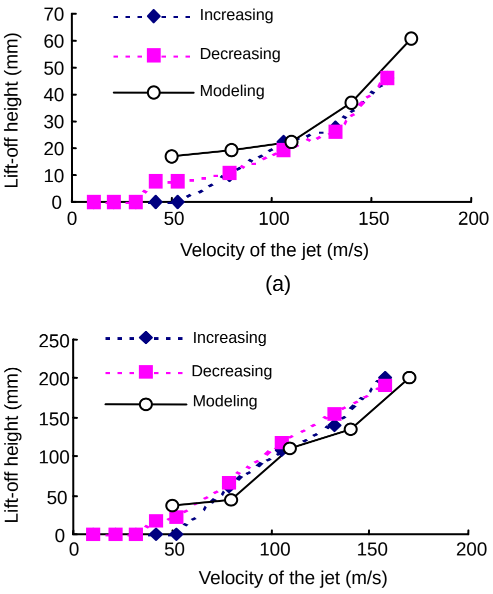


Fig. 2 Sketch map of the lift-off height of condition A

3.1 Model validation

The mole ratio for H_2:N_2 of 1:3 is used for calculations. The lift-off heights under two typical conditions (Table 1) are attained, and compared with the experimental results.

Fig. 3 presents the curves of the lift-off height with increasing/decreasing velocities of the jet flow with the co-flow velocity fixed. There is little difference between these two results. The results of calculation are in good agreement with those of experiments. The height of H_2/N_2 lifted flame increases with the increasing velocity of the jet flow whether in a high or low temperature atmosphere. In the experiment, when the velocity of the jet flow is less than 50 m/s, the bottom of the flame is just at the exit of the tube; that is, the lift-off height is 0 mm. These conditions were not included in calculation. After validating, more simulations could be made. The following results are all obtained from simulation.



(a)

(b)

Fig. 3 Variation of the lift-off heights with jet velocities in the typical conditions A (a) and B (b)

Increasing/Decreasing: fix the co-flow, start from the low/high velocity of the jet flow, and increase/decrease it step-by-step

3.2 Results and analysis

3.2.1 Auto-ignition and flame stabilization of H_2/N_2 mixture

The jet fuel is the mixture of H_2/N_2 with a mole ratio of 1:2, and other conditions are shown in Table 1. It can be attained from calculation that the auto-ignition delay is 1.7 ms, and the site of auto-ignition is 66 mm from the injector in the condition A, while the auto-ignition delay is 7.4 ms, and the site of auto-ignition is 189 mm from the injector in the condition B. Therefore, it can be concluded that temperature has an important influence on auto-ignition. The auto-ignition delay in low temperature conditions is much longer than that for high temperatures, and the site of auto-ignition for low temperatures is also higher than that for high temperature conditions.

Fig. 4 shows the calculation results of auto-ignition delay in different co-flow temperatures and jet velocities under typical conditions.

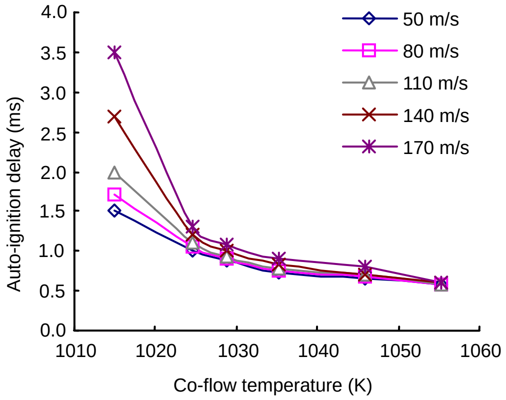


Fig. 4 Variation of auto-ignition delay of H_2/N_2 mixture with co-flow temperature of various velocities of the jet flow

There is a relationship between auto-ignition delay and co-flow temperature, and apparent turning points exist in the curves around 1026 K for various jet flows (Fig. 4). The slopes of these curves are very steep with the temperatures lower than 1026 K; and on the other side, the slopes are gentle. The higher the jet flow velocity, the more significant the phenomenon. The region with temperatures lower than this temperature is defined as 1, and the other side is defined as 2 with $\frac{\mathrm{d}t_1}{\mathrm{d}T_1} >> \frac{\mathrm{d}t_2}{\mathrm{d}T_2}$ (t: the auto-ignition delay; T: the co-flow temperature). The temperature of the turning point is defined as the criterion temperature (Deng, 2007). The region with temperatures below the criterion temperature is defined as the low temperature thermo-atmosphere region, while the region above the criterion temperature is defined as the high temperature thermo-atmosphere region. When the auto-ignition happens in the high temperature thermo-atmosphere region, the variation of the auto-ignition delay is less than 0.3 ms, which indicates that the velocity of the jet flow influences the auto-ignition delay slightly. The auto-ignition delay is influenced little by the velocity of jet flow when the temperature is high enough, and the chemical preparation time is shortened. When the temperature of the co-flow is lower than the criterion temperature, the auto-ignition delay increases sharply when the temperature decreases, being more than 400% of that in the high temperature environment. Moreover, the influence of the velocity of the jet flow becomes evident. In the research range of jet flow velocity, the auto-ignition delay of the highest jet flow velocity is more than two times of that of the lowest one, which indicates that auto-ignition is able to take place in a stable fashion only in high temperature thermo-atmosphere regions.

Fig. 5 shows the height of the site of auto-ignition of H_2/N_2 with different temperatures of co-flow and different velocities of the jet flow. The velocity of jet flow has a stronger influence on the site of auto-ignition than on auto-ignition delay. The higher the velocity of the jet flow, the higher the site of auto-ignition. Because for the same auto-ignition delay, the faster the jet flow is, the farther distance the jet flow passes. As shown in Fig. 5, the maximum height of the site of auto-ignition in the low temperature atmosphere is three times of that in the high temperature atmosphere. Thermo-atmosphere influences the site of auto-ignition as well, although it is not as evident as with the auto-ignition delay, especially when the jet flow velocity is below 50 m/s. Turning points similar to those varying with temperatures on the auto-ignition delay curve can be found on the curves, and these are considered as the criterion temperature, around 1028 K, close to the criterion temperature of the auto-ignition delay. The site of auto-ignition in the low temperature region varies more severely with temperature than in high temperature region. If the low temperature region on the left of 1028 K is defined as 1, and the right region is defined as 2, it comes that $\frac{\mathrm{d}H_1}{\mathrm{d}T_1} >> \frac{\mathrm{d}H_2}{\mathrm{d}T_2}$, where H is the height of the site of auto-ignition. The higher the jet flow velocity, the more significant this tendency.

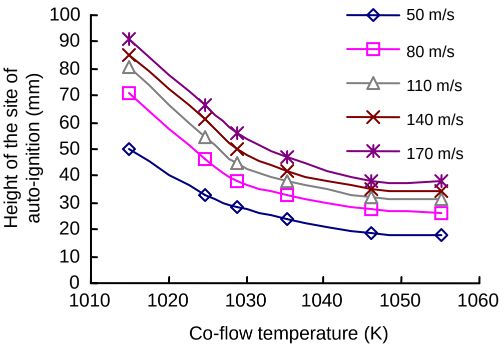


Fig. 5 Variation of the height of the site of auto-ignition of H_2/N_2 mixture with co-flow temperature of various velocities of the jet flow

The auto-ignition of diluted H_2 was investigated above. Stable lifted flame is formed after auto-ignition. The stabilization mechanism is studied from the viewpoint of the lift-off heights of lifted flame as follows.

Fig. 6 shows the lift-off height curves of the jet flow with different temperatures and velocities of the jet flow. The jet flow is still mixed with the mole ratio of 1:2. It can be inferred that the variation of the lift-off heights with the velocity of the jet flow is not affected by co-flow temperatures, but is slowly increased by an increase of the velocity of the jet flow, whether in the high or low temperature regions. The lift-off height decreases with an increase in the co-flow temperature, with the influence being more significant in the low temperature region than the high temperature region. The slopes are steeper in the low thermo-atmosphere region than those in the high thermo-atmosphere region. That is, $\frac{dh_1}{dT_1} >> \frac{dh_2}{dT_2}$, where h is the lift-off height. It infers that, for the stabilization mechanism of lifted flames, the definition of the criterion temperature is also useful. The lifted flame is stable when the temperature is higher than the criterion temperature, while in the converse condition, the lift-off height changes considerably with slight variations in temperature. A turning point is also found on the temperature curve, being around 1027 K, and near to the criterion temperature, which determines the stability of auto-ignition. Hence, when the lifted flame of the H_2/N_2 mixture with a mole ratio of 1:2 is stable, the criterion temperature of the thermo-atmosphere is around 1027 K. With the increase of the jet flow velocity, the criterion temperature increases very little, less than 1 K.

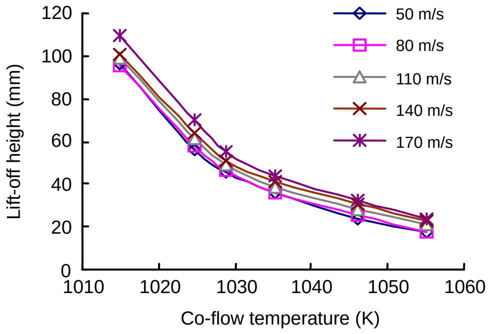


Fig. 6 Variation of the lift-off heights of H_2/N_2 mixture with co-flow temperature of various velocities of the jet flow

3.2.2 Auto-ignition and flame stabilization of $H_2/CH_4/N_2$ mixture

In this section, CH_4 was added into the H_2/N_2 mixture with a mole ratio of the combustible gas to N_2 still 1:2, and other conditions are shown in Table 1. With the addition of CH_4, the auto-ignition delay increased on the order of a few times that of the original condition, and the height of the site of auto-ignition and the lift-off height became larger. Under typical conditions, with the thermo-atmosphere temperature being 1046 K, and the mole proportion of $H_2:CH_4:N_2$ being 0.9:0.1:2, the auto-ignition delay, the height of the site of auto-ignition, and the lift-off height are 1.14 ms, 47.3 mm, and 10.7 mm, respectively. Whereas, when the proportion changes to 0.8:0.2:2, these three parameters increase to 4.70 ms, 126.1 mm, and 103.7 mm, respectively, indicating that the addition of CH_4 influences auto-ignition and stabilization. That is, the greater the proportion of CH_4, the longer the auto-ignition delay. The larger the heights of the site of auto-ignition and the lift-off heights, the more significant the changes. The following results and discussion mainly focus on the condition with the mole ratio of $H_2:CH_4:N_2$ being 0.9:0.1:2. Because the variations are not so apparent, when the velocity of the jet flow is slow, only the high velocity conditions (110, 140, and 170 m/s) are considered.

Figs. 7–9 are the curves of the auto-ignition delay, the height of the site of auto-ignition, and the lift-off height varying with temperature in various velocities of the jet flow. With the addition of CH_4, the trend of the lift-off height and auto-ignition delay is similar to that of the H_2/N_2 mixture except that the lift-off height is affected a little by co-flow at high temperatures. The higher the co-flow temperature, the less the influence. The criterion temperatures are around 1026 K.

In terms of the site of auto-ignition, its trend with co-flow temperature is not as similar as diluted H_2 in the low-temperature thermo-atmosphere region, although it also becomes higher with an increasing velocity of the jet flow. It does not increase sharply like that of the H_2/N_2 mixture with decreases in the co-flow temperature. The lower the temperature is, the longer the time for chemical preparation. The auto-ignition delay is longer after adding CH_4, which makes the time for chemical preparation longer, and makes the auto-ignition unstable. Therefore, auto-ignition was not strongly affected by the velocity of the jet flow.

The velocity of the jet flow is one of the main factors influencing the site of auto-ignition. When the thermo-atmosphere temperature is low, the chemical preparation time is much longer than the physical one, so the site of auto-ignition is influenced by the jet flow velocity, and the increase in the height of the site of auto-ignition is close to the limit if the velocity of the jet flow is not high enough. As a result, the increment of the height of the site of auto-ignition is associated with a smaller decrease in the co-flow temperature. That is, the slope of the curve is smaller. The slope increases with increasing velocity of the jet flow. In the low temperature thermo-atmosphere region, the slope of the height of the site of auto-ignition with the thermo-atmosphere temperature is larger when the jet flow velocity is 170 m/s compared to the slope when the jet flow velocity is 110 or 140 m/s. In the high temperature thermo-atmosphere region, the chemical preparation time is much shorter. The site of auto-ignition becomes higher with the increases in the velocity of the jet flow. Hence, there are still turning points, that is, a criterion temperature, around 1026 K. The slope of the height of the site of auto-ignition with the temperature of co-flow in the low temperature thermo-atmosphere region is lower than that in the high temperature region.

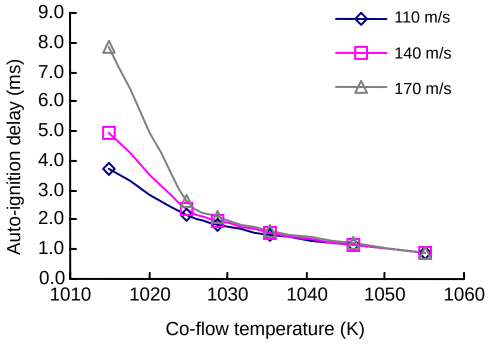


Fig. 7 Variation of auto-ignition delay of $H_2/CH_4/N_2$ mixture with co-flow temperature of various velocities of the jet flow

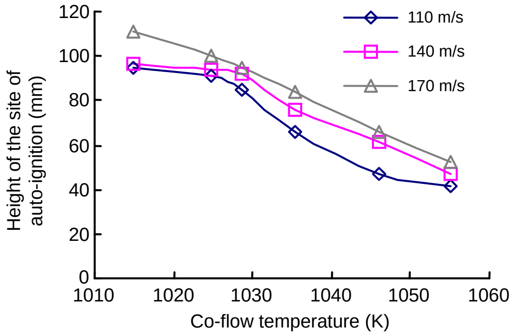


Fig. 8 Variation of the height of the site of auto-ignition of $H_2/CH_4/N_2$ mixture with co-flow temperature of various velocities of the jet flow

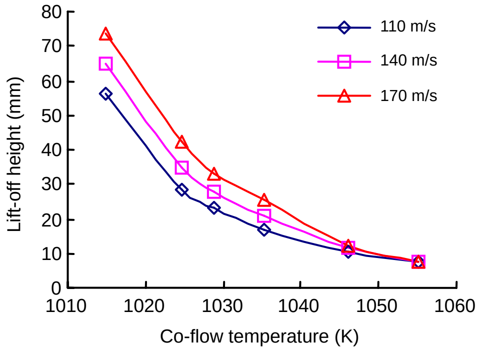


Fig. 9 Variation of the lift-off heights of $H_2/CH_4/N_2$ mixture with co-flow temperature of various velocities of the jet flow

3.2.3 Auto-ignition and flame stabilization of $H_2/H_2O_2/N_2$ mixture

In this section, the additive is changed into H_2O_2 from CH_4, with other conditions unchanged, and it is not able to promote the auto-ignition. H_2O_2 makes the auto-ignition delay a little larger than that for the original mixture. Correspondingly, other parameters, such as the height of the site of auto-ignition, and the lift-off height also increase. The more the mass fraction of H_2O_2, the larger the parameters are. When the mole proportion of H_2:H_2O_2:N_2 is 0.9:0.1:2, the auto-ignition delay, the height of the site of auto-ignition, and lift-off height at the auto-ignition site are 0.90 ms, 35.1 mm, and 14.2 mm, respectively, which are much smaller than those in the condition as CH_4 is added.

Figs. 10–12 are the curves of the auto-ignition delay, the height of the site of auto-ignition, and the lift-off height in various jet flow velocities. Mole proportions were 0.9:0.1:2 for the H_2:H_2O_2:N_2, and the velocities of jet flow are 110, 140, and 170 m/s, respectively.

The trends of auto-ignition delay and the lift-off height in the high co-flow temperature region are just like those of the H_2/N_2 mixture. The trend of auto-ignition delay in the low temperature region is also similar to that of the H_2/N_2 mixture. The criterion temperature is about 1026 K. However, the trend of the site of auto-ignition with the co-flow temperature is not regular. As the velocity of the jet flow is 170 m/s, the site of auto-ignition becomes rapidly higher with decreases in temperature, while the site of auto-ignition increases a little when the jet flow velocity is 110 m/s. The criterion temperature is 1026 K.

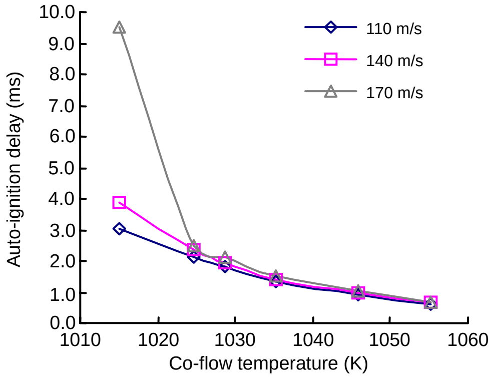


Fig. 10 Variation of auto-ignition delay of $H_2/H_2O_2/N_2$ mixture with co-flow temperature of various velocities of the jet flow

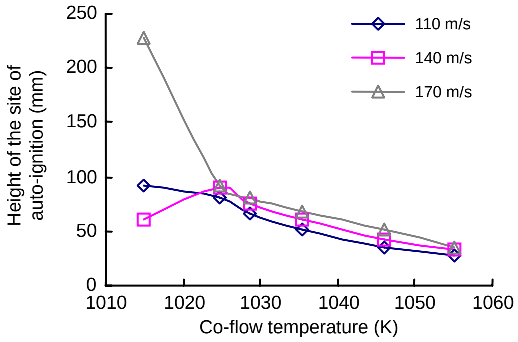


Fig. 11 Variation of the height of the site of auto-ignition of $H_2/H_2O_2/N_2$ mixture with co-flow temperature of various velocities of the jet flow

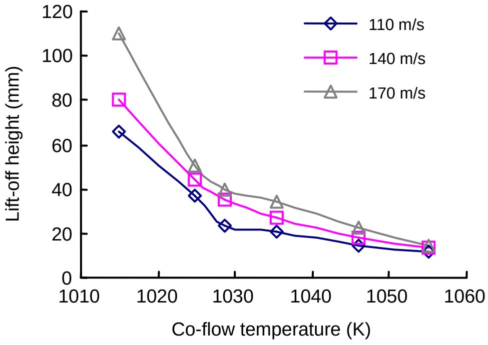


Fig. 12 Variation of the lift-off heights of $H_2/H_2O_2/N_2$ mixture with co-flow temperature of various velocities of the jet flow

The shapes of the lift-off height curves are similar to those of the $H_2/CH_4/N_2$ mixture, although the trend of an increase with increases in the jet flow velocity is more evident. The criterion temperature is 1028 K.

4 Conclusions

The auto-ignition and lifted flames of H_2/N_2, $H_2/CH_4/N_2$, and $H_2/H_2O_2/N_2$ mixtures in the thermo-atmosphere were simulated in this paper. The regularities of the auto-ignition delay, the height of the site of auto-ignition, and the lift-off height were analyzed. The auto-ignition and lifted flame stabilization mechanism of gaseous fuels were concluded as follows:

1. There are criterion temperatures for auto-ignition and lifted flame which can be used to decide whether stable auto-ignition is formed, and whether the lifted flame is stable.

2. Generally, when the thermo-atmosphere temperature is lower than the criterion temperature, auto-ignition delay is longer and influenced significantly by the thermo-atmosphere temperature or jet flow velocity. The site of auto-ignition and the lift-off height are very high, and both vary distinctly in different thermo-atmospheres. Neither the auto-ignition nor the lifted flame is stable.

3. When the thermo-atmosphere temperature is higher than the criterion temperature, the auto-ignition delay is short, ignition happens not far from the nozzle, and the flame is stable near the injector. The auto-ignition delay, the height of the site of auto-ignition, and the lift-off height decrease with increases in temperature and with decreases in the jet flow velocity. The auto-ignition and the lifted flame of jet flow are stable and easily controlled.

4. The parameters of the auto-ignition delay, the height of the site of auto-ignition, and the lift-off height increase sharply when CH_4 is added to the mixture. They increased slightly when H_2O_2 is added to the mixture. The more H_2O_2 added, the more significant the change is, and the lower the criterion temperature. The auto-ignition delay of the $H_2/H_2O_2/N_2$ mixture becomes shorter, and the criterion temperature becomes lower in comparison to the $H_2/CH_4/N_2$ mixture.

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