一氧化碳添加对甲烷/空气贫燃预混火焰的影响

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摘要: 通过对贫燃条件下(燃料与空气化学计量比 $\varphi=0.60-0.80$)的甲烷/一氧化碳/空气火焰结构进行数值模拟, 研究燃料中一氧化碳添加量对层流燃烧速度、氮氧化合物的排放以及熄火拉伸率的影响. 随着燃料中一氧化碳添加量的不断增加, 层流燃烧速度有所下降, 这与燃料中加入氢气产生的现象有所不同. 为了解释这一现象, 本文深入探讨了层流燃烧速度与 $H+OH$ 浓度峰值之间的关系, 结果表明, 一氧化碳的增加导致 $H+OH$ 浓度峰值呈线性下降, 与层流燃烧速度下降趋势完全一致. 随着一氧化碳的增加, 氮氧化物排放量有所下降. 探讨了 NO 的生成机理, 且由敏感性分析得到生成 NO 的重要反应, 分析当一氧化碳量增大时, NO 的浓度以及重要反应的 NO 生成率均下降. 此外, 利用数值模拟求解径向拉伸率, 深入分析燃料中添加一氧化碳时拉伸率对贫燃火焰稳定性的影响. 由计算结果得到熄火拉伸率, 发现燃料中一氧化碳的添加在一定程度上能够增强火焰的稳定性.

关键词: 一氧化碳添加; 层流燃烧速度; 氮氧化物排放; 熄火拉伸率

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Effects of CO Addition on the Lean Premixed CH_4 /Air Flame

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Abstract: A numerical study was carried out to determine the effects of CO addition on the laminar burning velocity, NO_x emission, and extinction strain rate in a premixed CH_4/CO /air flame under the lean condition (equivalence ratio of fuel to air $\varphi=0.60-0.80$). When more CO was added to the fuel, the laminar burning velocity decreased, which is different from that observed for H_2 addition. To explain this, we studied the strong correlation between laminar burning velocity and $H+OH$ peak concentrations. Results showed that the $H+OH$ peak concentrations decreased linearly with an increase in CO content. This tendency is in good agreement with that of the laminar burning velocity. For NO_x , we observed that increments in CO addition led to a remarkable reduction in the NO_x emission. In addition, we investigated the NO formation mechanism and determined the relevant reactions for NO production using a sensitive analysis. The NO concentrations decreased significantly with enrichment by CO and the NO production rate also clearly decreased. We calculated the radial strain rate S_{rad} and discussed the influence of strain rate on lean flame stability with regards to the addition of different CO mole fractions to the fuel. The extinction strain rates indicated that the lean flammability limits were extended by CO addition in some way.

Key Words: CO addition; Laminar burning velocity; NO_x emission; Extinction strain rate

At present, due to energy crisis as well as global environmental threats, lean combustion technology has received great attention in the combustion and other related fields, so lean combustion

has become a popular method to meet increasingly stringent emissions requirements. Some researchers^[1] have pointed that lean combustion can greatly reduce the fuel consumption and emis-

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sions of greenhouse gases and pollutants, including NO_x , soot^[2], and other particle matter, which was mainly the result of the low flame temperatures encountered in the lean conditions^[3-5].

The lean combustion has its special prospects, but has some disadvantages. The most serious one is that at low equivalence ratio, the combustion stability will be affected and the processes of stretching and heat loss may cause extinction^[6]. To solve this problem, the traditional approach is to adopt fuel enrichment and increase the concentration of the fuel. Though this strategy can enhance the overall burning intensity and the flame stability, but the flame temperatures and the NO_x emissions will be increased. Another method is to add a small amount of other fuels, which can solve the stability problem, while, the NO_x emissions can receive substantial reduction. Hereto, some researchers suggest adding reformat gas to ensure the flame stability, which can diminish the quenching distance and extend the flame limits, as well as reduce NO_x formation. It is well known that H_2 is an important component of reformat gas, so hydrogen addition has attracted many scholars' research. And the previous studies have proved that hydrogen addition can widen the lean burn operation and reduce unburned hydrocarbon and carbon dioxide emissions^[7-9]. This method was discussed more by Yu *et al.*^[1], and they measured the fundamental laminar flame speed of CH_4/air flame with H_2 addition by using the counter flow configuration. Rørtveit *et al.*^[9] studied the lean premixed flame utilizing four kinds of burner experimentally and their results revealed that the flame stability with H_2 addition and the NO_x , CO emissions depended largely on the type of burner and the excess air ratio.

Even though this is an attractive proposition, some specialists, such as Ren *et al.*^[5] pointed that we must realize that it is a challenge to make a large number of H_2 into use because it is expensive to produce. In comparison, the production and storage technology of CO has been quite mature. However, the effect of the addition of various additives on the CH_4/air flame has been investigated, such as H_2 , reformat gas^[10-13], astonishingly there is very few information available in the related literature about the influence of CO addition, especially considering the condition of lean burning. As a kind of important component of reformat gas, it is necessary to study the combustion characteristics of CO. Hence, in this case, we investigate the characteristics of the CH_4/air flame with different CO additions under the condition of lean burning (equivalence ratio, $\varphi=0.60-0.80$). It has been thought that the laminar burning velocity is an important parameter of a combustible mixture as it contains fundamental information regarding reactivity, diffusivity, and exothermicity^[14], on which the changes of flame structure and dynamics are found to depend when fuel composition is varying. The control of NO_x emissions has become an essential factor in the design of modern combustion systems^[15] and the extinction strain rate is the main basis of the flame stability judgment. Therefore, we focus on these three most concerning problems to analyze specific changes with different CO mole fractions in the fuel.

1 Modeling details

1.1 Chemical kinetic model

In this paper, we employ the kinetic model of GRI Mech 3.0^[16], which consists of 325 elementary chemical reactions and 53 species, including NO_x kinetics. This kinetic model has been tested and validated extensively for CH_4 and other natural gases combustion over a wide range of pressure and temperature conditions. Guo *et al.*^[17] has investigated the extinction strain rate and the NO_x emissions of the premixed $\text{CH}_4/\text{H}_2/\text{air}$ flame by employing GRI Mech 3.0, whose object has much consistency with ours.

1.2 Computational specification

According to the object of this study, two different flame models are employed. One is freely propagation flame to get the laminar burning velocities and some parameters to analyze the characteristics of NO_x emissions which is calculated using the PREMIX software^[18] and the other is opposed-jet, symmetric, twin-flame to investigate the extinction strain rate by adopting the OPPDIF software^[19]. In the previous work, these two models were used mostly to compare experimentally observed trends with those predicted by the calculations. Moreover, the two softwares, which were applied mostly by scientific researches and validated in practical engineering fields^[20-21], were both developed by Sandia National Laboratories. In the NO_x section, the NO related important reactions was obtained by utilizing the SENKIN package^[22] of CHEMKIN II^[23] to analyze the influence of CO addition thoroughly.

In addition, in this study, there are some parameters as follows: $\text{CH}_4/\text{CO}/\text{air}$ flames with global equivalent ratios $\varphi=0.60-0.80$, and CO mole fraction in CO/CH_4 mixture $\alpha=0.0-0.9$, where φ , α are defined as,

$$\varphi = \frac{\left[\left(\sum_i X_{\text{fuel}_i} \right) / X_{\text{O}_2} \right]_{\text{actual}}}{\left[\left(\sum_i X_{\text{fuel}_i} \right) / X_{\text{O}_2} \right]_{\text{stoich}}}$$

$$\alpha = X_{\text{CO}} / (X_{\text{CO}} + X_{\text{CH}_4})$$

where X_i is the mole fraction of species i in the fuel.

2 Results and discussion

As mentioned above, we investigate the effect of CO fraction on the CH_4/air flames in terms of the laminar burning speed, the extinction strain rate, and the NO_x formation under the circumstance of the lean burning ($\varphi=0.60-0.80$).

2.1 Laminar burning velocity

The calculations of the unstretched laminar burning velocities are performed with an unburned mixture under the normal atmospheric pressure. The temperature and the mass flow rate are set as 400 K, $0.04 \text{ g} \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$, respectively. The adaptive mesh parameters are GRAD=0.2 and GURV=0.6. The absolute and the relative error criteria are ATOL= 1×10^{-9} and RTOL= 1×10^{-4} . Fig.1 shows the laminar burning velocity under various CO ad-

Fig.1 Laminar burning velocity (μ) as a function of equivalence ratio with various CO additions in CH₄/air flames

dition, and equivalence ratios. We can note that (1) the laminar burning velocities reach the maximum at the rich side of stoichiometry; (2) when equivalence ratios are higher than 1, the velocity increases obviously with the increase of CO mole fraction in the fuel mixture. These results are in accord with the researches by Wu *et al.* [21]. However, their studies have been restricted to the velocity changing trends at the overall equivalence ratios and the main positions of the maximum velocity, without aiming at the lean burning condition.

So we calculate the laminar velocities at $\phi=0.65, 0.70, 0.75$ with the changes of CO concentration in the fuel. Fig.2 shows that both the decreases of the equivalence ratio and the increases of the CO mole fraction lead to the reduction of the velocities. The result of Fig.1 is similar to the case of hydrogen addition to the fuel [8], while in Fig.2, we can observe that the result is obviously different from the hydrogen case. Halter *et al.* [24] studied the influence of hydrogen fraction on the laminar burning velocity of CH₄/H₂ flame and the results showed that the laminar burning velocity increased as the increase of hydrogen fraction in the fuel mixture. Hu *et al.* [25] investigated the effects of the radical mole fractions of OH, H on the burning velocity and they proposed that there was a strong correlation between burning velocity and maximum radical mole fractions of OH+H radicals in the reaction zone of the premixed CH₄/air flames. They pointed

Fig.2 Laminar burning velocity as a function of CO addition in CH₄/air flames

Fig.3 Laminar burning velocity and maximum OH+H mole fraction with various CO additions at $\phi=0.65, 0.70, 0.75$

that with the increase of maximum concentration of OH+H, the burning velocity increased and also gave the detailed formulation, the burning velocity $\mu=0.07929+(X_H+X_{OH})_{\max}$, i.e., μ changed linearly with $(X_H+X_{OH})_{\max}$. Fig.3 shows the laminar burning velocity and the maximum mole fraction of OH+H at three different lean equivalence ratios. We can conclude that (1) at three ratios, the change trends of velocity are consistent with the peak mole fraction, that is, linear relationship exists between them, which is verified by the contrast between the simulation results and the fitting results in Fig.4. And the linear relationships can be expressed by the following formulas, respectively,

$$\mu_{0.65}=0.00151+0.99779(X_H+X_{OH})_{\max}$$

$$\mu_{0.70}=0.00215+0.99777(X_H+X_{OH})_{\max}$$

$$\mu_{0.75}=0.00271+0.99628(X_H+X_{OH})_{\max}$$

(2) as more amount CO mole fraction in the fuel, the burning velocity and the maximum OH+H mole fraction decrease remarkably. Actually, the increases of CO addition cause the peak concentration of OH and H radicals to decrease at different lean equivalence ratios which are showed in the Fig.5.

2.2 NO_x emissions

As one of the main sources of the air pollution, NO_x emissions not only have a detrimental effect on human health, but also contribute significantly to the global environmental pollution, which has caused lots of concerning in the combustion and envi-

Fig.4 Laminar burning velocity at various peak H+OH mole fractions

Fig.5 Maximum H and OH mole fractions at different CO mole fractions in the fuel

ronment fields. Plenty of studies have focused on the effect of adding H_2 , CO_2 , H_2O to natural gas on NO_x production^[26]. And in this section, we study the effects on the NO_x emissions index by adding CO, on the other hand, some questions related to the formation mechanisms are discussed. Fig.6 shows the distribution of the typical NO_x (NO , NO_2 , N_2O), and obvious differences are observed between NO and N_2O formation. The NO formation mostly occurs in the high temperature region, while the N_2O is mainly generated in the low temperature zone, while N_2O is consumed in the high temperature region. These mainly depend on the formation mechanisms of NO and N_2O . The mole fraction of NO , which accounts for 90% in the NO_x , is much higher than N_2O and NO_2 , so in the following studies we will take NO for the main research object.

2.2.1 Flame temperature

It has been known that the formation of NO_x has been extremely influenced by the flame temperature. So many researchers, such as Tuzson^[27] and Maughan *et al.*^[28], have proposed to get low NO_x emissions by bringing down the flame temperature. Because the thermal mechanism plays an important role in high temperature, the emissions are strongly depending on the high temperature, moreover in the Fig.7 we can observe that as the raise of the flame temperature, the NO_x concentration will increase. So in a large extent, we can conclude that high temperature indicates the high NO_x concentration. Fig.8 gives

Fig.6 Profiles of mole fractions of NO , NO_2 and N_2O in the premixed CH_4 /air flame

Fig.7 NO and N_2O mole fractions at various temperatures

the profiles of temperature of CH_4 /air flame with different CO additions at $\varphi=0.70$. As CO addition increases, there is a small decrease in the temperature. According to the theory aforementioned, this change indicates that NO_x emissions would achieve significantly reduction.

2.2.2 NO concentrations

In order to get a better investigation about NO_x emissions after adding CO, we calculate NO mole fraction at $\varphi=0.70$, 0.75 , 0.80 with CO addition $\alpha=0.1$, 0.2 , 0.4 , 0.6 , 0.8 , as seen in Fig.9. It can be seen that at three different ratios, CO addition has a positive effect on NO emission reduction, and more CO concentration leads to lower NO mole fraction. Especially at $\varphi=0.70$, 0.75 , the mole fractions reduce almost 65%, while at $\varphi=0.80$, the mole fraction leaves over 40% of the original. In general, the NO emission situation gets a large scale of improvement. We do not calculate N_2O , NO_2 , but due to the mole fraction of NO accounting for about 90% in NO_x , so we can deduce that the total NO_x emissions get a remarkable reduction.

2.2.3 Problems related to NO_x reaction mechanism

There are three major sources of the to NO formed in the combustion: (1) the thermal NO (Zeldovich) mechanism, (2) the prompt NO (Fenimore) mechanism, (3) the $N_2O \rightarrow NO$ intermediate route. The thermal mechanism is that the NO is formed by a set of highly temperature-dependent chemical reactions known as the extended Zeldovich mechanism. The principal reactions

Fig.8 Profiles of temperature of CH_4 /air flame with different CO additions at $\varphi=0.70$

Fig.9 Profiles of NO mole fraction with different values of φ
 φ : (a) 0.70, (b) 0.75, (c) 0.80

governing the formation of thermal NO are as follows: $O+N_2=NO+N$; $N+O_2=O+NO$; $N+OH=NO+H$; $N+NO=O+N_2$. In the previous researches^[29], there were good evidences that prompt NO can be formed in a significant quantity in some combustion environments, such as in low-temperature, fuel-rich conditions. Although we study at the lean condition, to get precise analogue result, we also consider the prompt mechanism. This mechanism consists of the reactions^[30]: $CH+N_2=HCN+N$; $HCN+OH=CN+H_2O$; $CN+O_2=NO+CO$. The final mechanism involved main reaction: $N_2O+O=2NO$. The main reaction ways of NO production and consumption can be obtained from Fig.10, which also shows the primary materials and radicals involved in the reactions clearly. According to information provided in Fig.10, and considering the reactions contained in GRI Mech 3.0, the main 28 steps reactions related NO have been listed in Table 1. Among them, R178, R179, R180 belong to the thermal mechanism, R222 belongs to the prompt route and R182–R189 are the $N_2O \rightarrow NO$ mechanism. We carry the NO concentration sensitivity analysis on these 28 step reactions. Fig.11 shows (1) R178: $N+NO=N_2+O$, R179: $N+O_2=NO+O$, R180: $N+OH=NO+H$, R189: $NO_2+H=NO+OH$, these four reactions play positive roles in the NO production which tallys with the mechanism, (2) R186: $HO_2+NO=NO_2+OH$; R249: $CH_2+NO=H+HNCO$, are the main consumption routes. Fig.12 shows the profiles of the total production rates of NO. It can be observed that at $\varphi=0.70$, with the in-

Fig.10 NO production and consumption ways in CH₄/air combustion

crease of CO addition, the rate changes fluctuate severely much. With the three different CO additions, all the peak values appear at the flame height from 0.15 to 0.20 where the temperature rises to the maximum and the valley values appear at the height from 0.05 to 0.10. Moreover, from the flame height 0.10 to 0.15, the fluctuation is fierce and these regions are precisely the place in which the temperature rises quickest. From $\alpha=0.2$ to $\alpha=0.6$, the peak values reduce by 60%, the valley values rise about 30%.

Fig.13 indicated the profiles of NO production rate of the main

Table 1 Main reactions related to NO production and consumption

Reaction number	Reaction step	Reaction number	Reaction step
R178	$N+NO=N_2+O$	R208	$NNH+O=NH+NO$
R179	$N+O_2=NO+O$	R214	$HNO+H=H_2+NO$
R180	$N+OH=NO+H$	R219	$CN+H_2O=HCN+OH$
R182	$N_2O+O=2NO$	R222	$NCO+O=NO+CO$
R183	$N_2O+H=N_2+OH$	R240	$CH+N_2=HCN+N$
R185	$N_2O(+M)=N_2+O(+M)$	R246	$CH+NO=HCN+O$
R186	$HO_2+NO=NO_2+OH$	R247	$CH+NO=H+NCO$
R188	$NO_2+O=NO+O_2$	R248	$CH+NO=N+HCO$
R189	$NO_2+H=NO+OH$	R249	$CH_2+NO=H+HNCO$
R190	$NH+O=NO+H$	R250	$CH_2+NO=OH+HCN$
R192	$NH+OH=HNO+H$	R251	$CH_2+NO=H+HCNO$
R194	$NH+O_2=HNO+O$	R252	$CH_2(S)+NO=H+HNCO$
R195	$NH+O_2=NO+OH$	R253	$CH_2(S)+NO=OH+HCN$
R197	$NH+H_2O=HNO+H_2$	R254	$CH_2(S)+NO=H+HCNO$

CH₂(S): singlet state of methylene

Fig.11 Sensitivity coefficients with respect to NO concentration

Fig.12 Profiles of total production rate of NO with different CO additions at $\varphi=0.70$

reactions (R178, R179, R180, R186, R189, R249) with different CO additions at $\varphi=0.70$. The results demonstrate that (1) as CO addition rises from 0.2 to 0.6, the peak values of the four positive reactions reduce a lot, especially R179 ($\text{N}+\text{O}_2=\text{NO}+\text{O}$), whose peak value changes from 9.0×10^{-9} to 1.5×10^{-9} , about 80%; (2) with an increase in the CO mole fraction, the valley values vary greatly at the flame height and the changes of R249 and R186 are remarkable; (3) the positions of the R179, R180, R189 peak

Fig.13 Profiles of NO production rate of the main reactions with various CO additions at $\varphi=0.70$

Fig.14 Temperature variation with strain rate with different CO additions at $\varphi=0.70$

values are consistent with that of the total production rate peak value in Fig.12. But R178 is somewhat different, and the primary reason is that the temperature of R178 $\text{N}+\text{NO}=\text{N}_2+\text{O}$ reaction must be higher than 1500 K, which is in keeping with the temperature profiles in Fig.8.

2.3 Extinction strain rate

From the above analysis, the lean combustion can cause a decrease in the flame temperature and make the NO_x emissions under the effective control, but in the theory, the lean combustible gas has a weak stability, the flame stretch may possibly cause flameout. By CO addition, we hope that at low temperatures, it can maintain the high combustion intensity. Hence, it is important to investigate the changes of the strain rate and define the extinction strain rate. Egolfopoulos *et al.*^[31] studied the effects of the flame stretch experimentally and numerically. They focused on the flame structures and the extinction strain rates of the opposed jet and the single jet wall configuration. Ren *et al.*^[5] mainly aimed at the lean condition and got the extinction strain rate of the CH_4/air flame by using the opposed jet, symmetric, twin-flame configuration. In this present study, we also adopt the opposed jet, symmetric, twin-flame configuration to get the effects of the strain rate on the CO enhanced lean CH_4/air flame. The preheat temperatures of the two nozzles are set to 400 K and the pressure is 1.0×10^5 Pa. And in this section, we study the radial strain rate S_{rad} , which is defined as $S_{\text{rad}} = \frac{1}{r} \frac{\partial(vr)}{\partial r}$, where r is the flame radius and v is radial velocity. Fig.14 demonstrates that at three test cases, as the strain rates increase, the flame temperatures decline monotonously. And when the flame temperature is below 1580 K, the flame will become unstable, so the strain rate at 1580 K just is the extinction strain rate. From Fig.14, we can observe that, at the equivalence ratio $\varphi=0.70$, the extinction strain rate is 1387 s^{-1} ($\alpha=0.2$), 1426 s^{-1} ($\alpha=0.4$), 1465 s^{-1} ($\alpha=0.6$) respectively, i.e., with CO content increases, the extinction strain rate rises, which indicates that adding CO is able to strengthen the stability of the lean combustion.

3 Conclusions

Numerical computations of the effects of CO addition on the

fundamental characteristics, such as the laminar burning velocity, the NO_x emissions, the extinction strain rate, are carried out with detailed chemistry and transport properties.

(1) The laminar burning velocity decreases with CO mole fraction from 0.2 to 0.7 in the lean conditions of $\varphi=0.65, 0.70, 0.75$. And the velocity depends on the peak value of H+OH mole fraction, moreover more CO mole fraction in the fuel can cause the decrease of the maximum OH+H mole fraction.

(2) Under lean condition, the flame temperature declined and the formation of NO is restrained much with CO addition, which can infer from the NO mole fraction profiles macroscopically and the production rate of the important reactions microscopically. Besides, the important reactions about NO production got from sensitivity analysis can help obtain the effective methods to reduce NO_x emissions.

(3) With CO enrichment, the extinction strain rate is increased in a certain extent, that is, the CO addition can enhance the stability of the CH₄/air flame under the equivalence ratio $\varphi=0.70$.

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