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Effects of CO₂/N₂/Ar addition on liftoff of a laminar CH₄/air diffusion flame

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1. Introduction

Exhaust gas recirculation (EGR) is an effective method to lower peak flame temperatures and reduce pollutant emissions. It has been widely applied in industrial applications, such as high EGR diesel combustion and high temperature air combustion (flameless combustion) [1, 2].

Introduction of exhaust gas into a combustion system may result in variations in some flame properties. One of these variations is that the addition of exhaust gas may cause the transition of a diffusion flame from attached to lifted, i.e. flame liftoff. Understanding the mechanism of the liftoff due to the introduction of exhaust gas is of great help for the further development and improvement of combustion technology employing EGR.

Many studies have been devoted to attached or lifted diffusion flames. Generally the introduction of an additive to the oxidant or fuel stream of a diffusion flame causes variation in flame liftoff and other properties due to the change in combustion intensity. This change in combustion intensity is caused by five possible mechanisms. The first one is the dilution effect resulted from the decrease in the concentration of oxygen or fuel. The second one is the thermal effect caused by the change in specific heat. Thirdly, some components of exhaust gas may participate in chemical reactions and thus cause flame liftoff. This factor is referred to as chemical effect. In addition, some components of exhaust gas may alter flame temperature and cause liftoff by modifying radiation heat transfer rate. This effect is known as radiation effect. The last one is the transport property effect which is due to the difference in transport properties between the exhaust gas and fuel or oxidant.

Carbon dioxide (CO₂) and nitrogen (N₂) are two primary components of exhaust gases. Most previous studies have attributed the impacts of CO₂ and N₂ addition on the extinction or liftoff of a diffusion flame to thermal and dilution effects [3]. While this is true for N₂ addition, it may not be correct for CO₂ addition. Our previous study [4,5] showed that the addition of CO₂ affects some flame properties due to not only thermal and dilution effects, but also chemical effect. Besides, CO₂ addition may also modify a flame through radiation effect. Few studies have been reported on the relative importance of the five possible mechanisms on the liftoff of a diffusion flame, when CO₂ or N₂ is added.

The purpose of this paper is to investigate the relative importance of the five possible effects on the liftoff of a laminar CH₄/air diffusion flame due to the addition of CO₂ and N₂, two primary components of exhaust gases. The study is carried out by numerical simulation, but the results are compared with available experimental data in the literature. To help to understand the mechanism and validate the numerical model, the addition of argon (Ar) is also studied.

2. Flame Configuration and Numerical Model

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The flames investigated are basically those studied experimentally by Min et al. [6]. They were generated in a chamber with section area of $25 \times 25 \text{ cm}^2$ and height of 80 cm. The fuel was injected into the chamber from the center of the chamber bottom by a round stainless tube with inner and outer diameters of 0.60 cm and 1.02 cm, respectively. Air was injected from the area outside the fuel tube at the bottom. Since the section area of the chamber is much bigger than that of the round fuel tube, the formed flames are essentially two dimensional axisymmetric flames. In order to simplify the calculation, numerical simulation was carried out for two dimensional axisymmetric flames.

The simulation domain covers a cylinder with diameter of 18 cm and height of 30 cm. Fuel and air streams enter the domain from the bottom. The base flame is a laminar CH_4/air diffusion flame, with inlet velocities of air and fuel being 10 cm/s and 100 cm/s, respectively, at atmospheric pressure and room temperature. For other flames, the mass flow rates of air and fuel were kept constant as for the base flame, while an additive was added to air. The additives include CO_2 , N_2 , and Ar. The fraction (α) of an additive is defined as the ratio of the volume flow rate of the additive to that of the air.

The numerical model used is basically the same as that used in [5], except for: (1) soot was not included; (2) the reaction scheme used was changed to GRI-Mech 3.0 [7].

3. Results and Discussion

3.1 Critical Fractions of Different Additives

The base flame is an attached laminar diffusion flame. When the fraction (α) of an additive is over a critical value, flame liftoff happens. This was investigated numerically by gradually increasing the fraction of an additive. The increment of the fraction is 0.01 in the calculation. If the liftoff happens between two consecutive additive fractions, we assume that the critical fraction is the mean of the two numbers. For example, Fig. 1 shows the mole fraction distribution of OH radical for the base flame and flames with fractions of 0.11 and 0.12, when CO_2 is added. The calculated flame at the fraction of 0.11 is attached and that at the fraction of 0.12 is lifted. As a result, we assume the critical fraction of CO_2 addition is 0.115. Therefore, the absolute error of the calculated critical fraction of an additive is ± 0.005 .

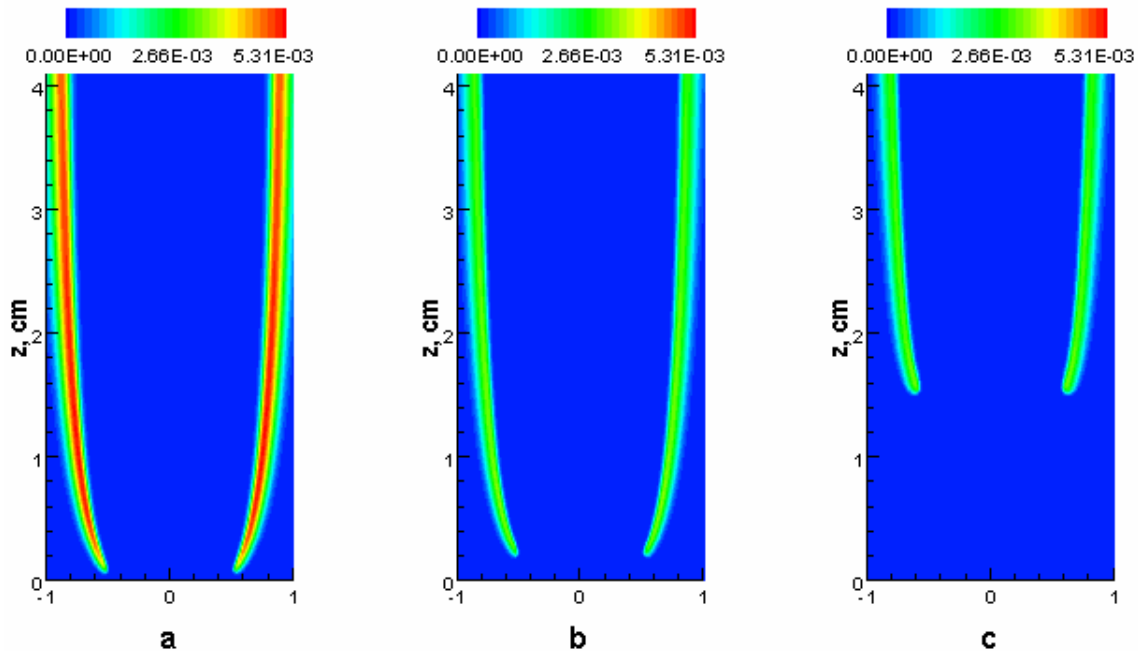


Fig. 1 Mole fraction distribution of OH radical for three flames. a. base flame; b. $\alpha = 0.11$; c. $\alpha = 0.12$.

Figure 2 shows the calculated critical fractions of CO_2 , N_2 , and Ar addition, together with the data measured by Min et al. [6]. It is noted that simulation successfully captured the measured data, confirming that the numerical model is

reasonable. The critical fractions of the three studied additives are in an order of $\alpha_{\text{CO}_2} < \alpha_{\text{N}_2} < \alpha_{\text{Ar}}$, being qualitatively consistent with the previous observation in [3].

As mentioned before, the addition of an additive causes flame liftoff due to five possible effects. Although understanding the relative importance of these effects is of interest for combustion scientists and engineers, little has been reported in the literature. We shall analyze the relative importance below using the flexibility of numerical simulation.

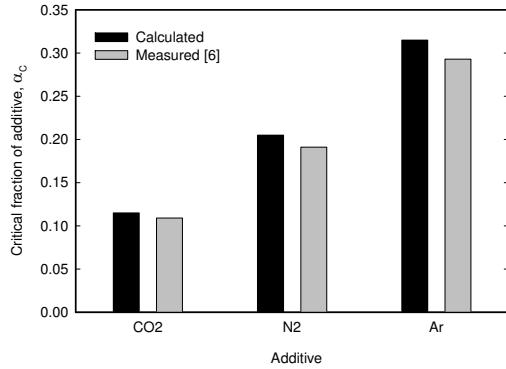


Fig. 2 Critical fractions of CO₂, N₂ and Ar.

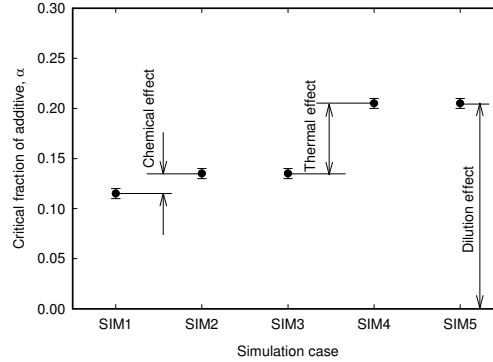


Fig. 3 Critical fractions of five sets of SIMs for CO₂ addition.

3.2 Relative Importance of Different Effects of CO₂ Addition

For all three additives studied in this paper, the addition to air of a diffusion flame may cause flame liftoff due to the dilution, thermal and transport property effects. However, only the addition of CO₂ may do that through chemical and radiation effects. Therefore, we'll first analyze the addition of CO₂.

To identify the relative importance of the five effects when CO₂ is added, five sets of simulations were carried out. The first set (SIM1) is the normal one in which CO₂ was gradually added to the air of the base flame. In the second set (SIM2), the added CO₂ was replaced by an artificial additive that has the same thermal and transport properties as CO₂ but is inert. This artificial additive in SIM2 participates in radiation heat transfer in the same way as CO₂. Therefore, the sole difference between SIM1 and SIM2 is caused by the chemical effect of CO₂ addition. The calculation condition in the third set (SIM3) is basically the same as in SIM2, but the additive does not participate in radiation heat transfer. Consequently, the disparity between SIM2 and SIM3 is because of the radiation effect. In the fourth set (SIM4), the specific heat of the additive was set as the same as air, but other conditions and parameters are the same as in SIM3. Accordingly, the difference between the results from SIM3 and SIM4 is caused by the variation in specific heat, i.e. the thermal effect. Finally, in the fifth set (SIM5), all conditions are the same as in SIM4 except that the transport properties of the additive are the same as air. Consequently, the difference between SIM4 and SIM5 is caused by the transport property effect. Comparing SIM5 and the base flame, the sole difference between them is the concentration of oxygen. Consequently, the base flame and SIM5 differ owing to the dilution effect.

Figure 3 shows the critical fractions from the five sets of simulations. It is observed that the critical fraction in SIM5 is 0.205. This means that the fraction of CO₂ in the oxidant stream should be above 0.205 to cause the base flame to be lifted if CO₂ addition affects the base flame solely due to dilution effect. This critical fraction from SIM5 is close to those of N₂ addition measured in [3] and calculated in this paper, as shown in Fig. 2. It is because the additive in SIM5 is almost the same as N₂. They both are inert and transparent, and have almost same thermal and transport properties (the thermal and transport properties of N₂ are very close to those of air). This similarity in the critical fractions from SIM5 and the N₂ addition confirms that the strategy used above to identify the relative importance is reasonable.

The critical fraction from SIM4 is the same as that from SIM5, implying that the transport property effect on the liftoff of the base CH₄/air diffusion flame is negligible.

Compared to SIM4, the critical fraction in SIM3 drops to 0.135. This is because the higher specific heat of the additive in SIM3 (same as CO₂) than that in SIM4 (same as air) reduces flame temperature. The difference between SIM3 and SIM4 is due to the thermal effect, which has been well understood [3].

Although the additive participates in radiation heat transfer in SIM2 but does not in SIM3, the calculated critical fractions in SIM2 and SIM3 are almost same, suggesting that the radiation effect of the added CO₂ has negligible

effect in terms of flame liftoff. This is because radiation heat loss is not significant in the region near burner rim where stretch rate is high and thus reaction zone is thin. However, we point out that radiation may significantly affect other flame properties in upper flame region, such as pollutant formation that will not be discussed in this paper due to space limit.

The critical fraction reduces to 0.115 in SIM1 compared to the 0.135 in SIM2, meaning that the chemical effect of the added CO₂ reduces the critical fraction by about 0.02. Therefore, the addition of CO₂ affects the liftoff of the CH₄/air diffusion flame due to not only the thermal and dilution effects, but also the chemical effect. This has never been reported in the literature. To identify what causes the chemical effect, we analyze the variation of the heat release rates in SIM1 and SIM2. The simulation indicates that the peak heat release rate in SIM1 is lower than in SIM2, i.e. the chemical effect of CO₂ addition suppresses the heat release. The heat release rate is obtained by $-\sum \omega_K H_K W_K$, where ω_K , H_K and W_K are the formation rate, enthalpy and molecular weight of the kth species.

Figure 4 displays each term inside the summation calculation for the peak heat release rate of the flame with the additive fraction of 0.10. It is found that the primary heat release is due to the formation of H₂O and CO₂. Further, the heat release rate due to the formation of CO₂ in SIM1 is significantly lower than in SIM2, while that due to the formation of H₂O in SIM1 is slightly higher than in SIM2. Therefore, the suppression of heat release due to the chemical effect of CO₂ addition is caused by the reduction in the net formation rate of CO₂ in the flame. A pathway analysis suggests that the reduction of net CO₂ formation rate is because of the reaction OH + CO = H + CO₂. When CO₂ is added, the rate of reverse direction of the reaction is intensified, resulting in the reduction in the net formation rate of CO₂. Therefore, we can conclude that the chemical effect of CO₂ addition on the liftoff of the base flame is caused by the reaction OH + CO = H + CO₂.

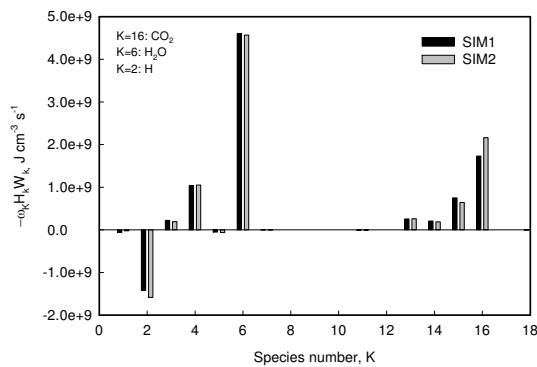


Fig. 4 Distributions of peak heat release rate in SIM1 and SIM2 for the flame with diluent fraction of 0.01.

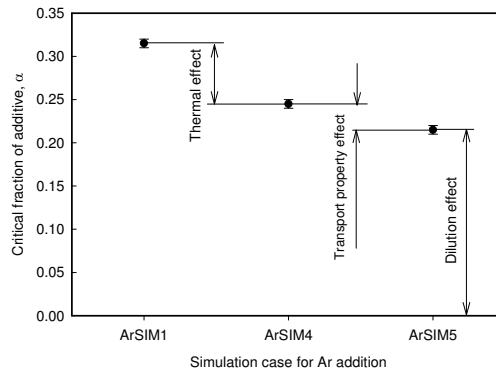


Fig. 5 Critical fractions of three sets of simulations for Ar addition.

The slightly higher formation rate of H₂O in SIM1 than in SIM2 is also analyzed, but will not be discussed in this extended abstract due to the space limit.

Overall, we can conclude that the addition of CO₂ causes the flame liftoff due to not only the effects of dilution and thermal, but also the modification in chemical reactions. The dilution effect is most significant, followed by the thermal effect. Relatively, the chemical effect is small. The radiation and transport property effects on the liftoff of a CH₄/air diffusion flame are negligible.

3.3 Relative Importance of Different Effects of N₂ and Ar Addition

N₂ has similar thermal and transport properties as air, and is inert and transparent. Therefore, its addition to air only modifies the combustion intensity through the modification in the concentration of oxygen, i.e. the dilution effect.

In addition to the dilution effect, the addition of Ar also affects flame due to the thermal and transport property effects. To identify the relative importance of the three effects, similar to CO₂ addition, three sets of simulations (ArSIM1, ArSIM4 and ArSIM5) were conducted. They correspond to SIM1, SIM4 and SIM5, respectively, for CO₂ addition. The corresponded SIM2 and SIM3 in CO₂ addition were not conducted here, since Ar is inert and transparent. The critical fractions from the three sets are shown in Fig. 5. It is observed that the dilution effect is also the most significant one. Being different from CO₂ addition, transport property effect becomes relatively noticeable. Further, both thermal and transport property effects actually increase the critical fraction for Ar addition, relative to that due to dilution effect. The reasons are that Ar has a lower thermal conductivity and smaller specific heat than air. The former results in lower heat loss from the reaction zone, and the latter increases flame temperature. Figure 2 does show that the critical fraction of Ar addition is significantly higher than those of N₂ and

CO₂ addition. Therefore, in addition to dilution effect, Ar addition also affects flame liftoff through thermal and transport property effects, but these two effects counter the dilution effect, i.e. they actually strength the capability of a flame to be attached to the burner.

4. Conclusions

A numerical study on the effects of different additives to air on the liftoff of a laminar CH₄/air diffusion flame has been carried out. Detailed reaction scheme and complex thermal and transport properties have been employed. Three different additives were investigated. Results show that the addition of N₂ affects the flame liftoff due to the sole dilution effect. For CO₂ addition, it causes flame liftoff due to the dilution, thermal and chemical effects, with the dilution effect being the most significant one, followed by the thermal effect. All these three effects tend to reduce combustion intensity and cause flame to be lifted. The radiation and transport property effects are negligible. For Ar, its addition to air causes flame liftoff due to the dilution effect. This dilution effect is countered by the thermal and transport property effects, because of the lower thermal conductivity and specific heat of Ar than those of Air.

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