Radiation Effects of Water Vapor on the Flame Structure of Counterflow Methane Partially-Premixed Flames

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1 Introduction

Water-based fire extinguishing system has a low-toxic pollutant emission characteristics as well as excellent fire suppression performance. One of the most widely used water-based fire extinguishing systems is a water-mist. The major effects for the extinction mechanism of water-mist are the reduction effect of local oxygen concentration, the heat extraction effect lowering flame temperature due to the latent heat of vaporization and higher heat capacity, and attenuation effect of thermal radiation from a flame to ambience. Additionally, the water vapor affects the chemical reactions in the flame directly and indirectly; it also provides the dilution effects for fuel and air.

Lentati et al. [1] developed a water droplet model in one-dimensional (1-D) counterflow configuration for the investigation of the effects of latent heat of vaporization and droplet diameter on the flame extinction. However, the study mainly focused on the development of a water droplet model and the effect of droplet diameter, and the amount of water diluted in the air stream was restricted up to 3% by volume. Pitts et al. [2] numerically investigated the extinction concentration of water vapor in the air stream of counterflow nonpremixed flame at normal temperatures. In the study, however, the latent heat of vaporization, which plays an important role in extinguishing a flame, was not discussed because a water droplet model was not adopted in the simulation. Furthermore, since it was assumed that water vapor can exist as supersaturated state even at the normal ambient temperature and pressure, a more realistic condition for the state of water vapor is required for the investigation of the extinction limit of water vapor that causes flame extinction.

Fires conventionally show features of nonpremixed flame, and they can also show features of partially-premixed flame (PPF), especially at its initial stage because the combustible gas is mixed with ambient air and forms rich premixed mixture before ignition [3]. However, many studies of flame extinction by water mist or vapor mainly conducted for nonpremixed flames. Thus, investigation of the flame extinction of PPF by addition of water vapor (H₂O) is meaningful for the understanding of the suppression mechanism of water for various types of fires. The main objective of this study was to investigate the radiation effects on the structure and extinction limit of PPFs diluted with H_2O numerically.

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2 Numerical Method and Condition

In order to investigate radiation effects of methane partially-premixed flame diluted with H_2O in air stream, we introduced a simple counterflow configuration. One-dimensional OPPDIF, which was widely used for the simulation of counterflow flames, was used in this study. The governing equations and detailed numerical methods of the OPPDIF code can be found elsewhere. The thermodynamic and transport properties were calculated from the Chemkin-II and Transport package, respectively To obtain the flame stretch rate of the counterflow PPF, we defined the global strain rate (a_g) as the following

$$a_g = \frac{2V_U}{L} \left(1 + \frac{V_L}{V_U} \frac{\sqrt{\rho_L}}{\sqrt{\rho_U}} \right), \tag{1}$$

where V is the axial velocity; ρ is the fluid density, and L is the separation distance between the upper and lower nozzles. The subscripts, L and U indicate the lower and upper nozzle, respectively. The separation distance was fixed to 18 mm for all simulations. Ambient pressure was set to 1 atm, and the temperature of fuel stream (methane-air mixture) was set to 300 K. However, the air stream temperature was set to 450 K, which is high enough for water to be vaporized sufficiently. The equivalence ratio (Φ) of methane-air mixture in lower nozzle was chosen to 1.5 and 2.5 to establish rich PPFs.

3 Radiation Models

 H_2O is one of the species that significantly affects the radiation heat transfer from a flame. Thus, to investigate the radiation effect on the flame structure of a counterflow-methane PPF diluted with H_2O in the air stream, we used three different radiation models. The results obtained from the simulations with the three radiation models were compared with experimental results. The first radiation model considered was an adiabatic model (ADIA). The second radiation model adopted in this study was the optically-thin model (OTM) [4], which considers only the radiation heat loss from the flame; reabsorption of the lost heat cannot be considered. The third radiation model is the weighted sum of gray gases model (WSGGM) [5], which considers the radiation heat loss from the flame, as well as reabsorption of the lost heat.

4 Results and Discussion

In order to validate the prediction performance of radiation models adopted in this study, we compared the numerical simulation result with those obtained from a previous experiment for counterflow methane PPF [6].

Fig. 1 shows the comparison of the present simulation results with different radiation models for Φ =1.5 and Φ =2.5 without H₂O addition. In the figure, the zero in horizontal axis indicates the location of the stagnation plane, and distributions of the flame temperature and major species concentration are plotted with respect to the location of stagnation plane. The symbols denote the experimental results and the lines indicate numerical simulation results. The flame temperature profile showed a double-flame structure, that is, the high temperature region distributed widely and flame width was thick. However, the premixed flames of Φ =2.5 showed a single, thin flame structure and the high temperature region was narrow as shown in Fig. 1(b). In terms of radiation model, ADIA, which neglected the radiation heat loss from the flame, over-predicted the maximum flame temperature profile and major species concentration obtained by experiment well. From the comparison of simulations and experiment for flame structure shown in Fig. 1, it can be seen that simulations with GRI-v3.0 and radiation model, WSGGM or OTM showed reasonable results for the flame structure of counterflow methane PPF.



Figure 1. Comparison of the results of the simulation with the GRI-v3.0 mechanism and experiment (Li and Williams, 1999) for a fixed dilution ratio of $X_{H2O} = 0.0$ with different radiation models; (a) $\Phi = 1.5$ and $\Phi = 2.5$.

The maximum flame temperature (T_{max}) and spatially integrated heat-release rate (IHRR) are presented in Fig. 2 to investigate the H₂O addition and radiation effects on the extinction limit and global response with increasing the amount of H₂O addition (X_{H2O}). In Fig. 2, the strain rate, a_g , was fixed to 50 s⁻¹, which was known as a proper strain rate for the investigation of extinction limit of extinguishing gas agents for counterflow flame [7]. The T_{max} and IHRR for Φ =1.5 and Φ =2.5 decreased with increasing the amount of H₂O addition regardless of radiation model. This is because the flame intensity became weak due to the physical and chemical effects of H₂O on the flame as already known from the previous studies [8]. The T_{max} simulated with the ADIA for Φ =1.5 and Φ =2.5 was much higher than those with other radiation models. In addition, the T_{max} with WSGGM was slightly higher than that with OTM because the WSGGM can consider reabsorption of radiative heat while the OTM can consider only heat loss from a flame. It was seen that the magnitudes of T_{max} and IHRR were, from highest to lowest, as ADIA > WSGGM > OTM at the fixed amount of H₂O.

The magnitude of the extinction limits for Φ =1.5 and Φ =2.5 was, from largest to smallest, as ADIA > WSGGM > OTM, which was exactly the same as the trend of T_{max} or IHRR. Furthermore, it was found that the extinction limit for Φ =1.5 was large compared to that for Φ =2.5 because the flame temperature and intensity for Φ =1.5 was higher than Φ =2.5.



Figure 2. Global Flame Reponses predicted by the different radiation models for $a_g=50 \text{ s}^{-1}$ with increasing the amount of H₂O in the air stream; (a) Maximum Temperature and (b) Integrated Heat Release Rate.

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Figure 3. The effects of radiation on the flame temperature and major species for the $\Phi = 1.5$ of partially premixed methane flame diluted with water vapor in the air stream for $a_g=50 \text{ s}^{-1}$; (a) $X_{H2O}=0.30$, (b) $X_{H2O}=0.50$.

In order to investigate the radiation effects of H₂O on counterflow methane PPF in more detail, we plotted the flame structures with the addition of H₂O for Φ =1.5 in Figs. 3. The mole fraction of H₂O added to the air stream was X_{H2O}=0.3 and X_{H2O} =0.5, respectively. It can be seen from the profiles of temperature and species concentration that the PPF of Φ =1.5 had a wide double flame structure. The location of T_{max} moved from nonpremixed zone to rich premixed zone with increasing the amount of H₂O because the nonpremixed flame intensity became weak compared to the rich premixed flame. For X_{H2O} < 0.3, the ADIA predicted T_{max} higher and flame thickness wider than the WSGGM and OTM. However, no significant difference in the flame structure was identified between the results of the WSGGM and OTM. For X_{H2O} = 0.5, it was seen that the profiles of temperature and major species concentration were much differently predicted according to the radiation models. It should be noted that flame structure in the rich premixed zone was much affected by the radiation models compared to the radiation effect, and the effect become significant with increasing the amount of H₂O.

On the contrary to Φ =1.5, narrow flame structure, which is similar to nonpremixed flame, were identified for Φ =2.5 as shown in Fig. 4(a)-(b). No significant difference in the predictions performance of radiation model for the flame temperature and major species concentration for Φ =2.5 was identified even near the partially-premixed zone. Furthermore, the radiation effect for Φ =2.5 was insignificant even when a larger amount of H₂O was added than Φ =1.5 due to the lower flame temperature and narrower flame width.



Figure 4. The effects of radiation on the flame temperature and major species for the $\Phi = 2.5$ of partially premixed methane flame diluted with water vapor in the air stream for $a_g=50 \text{ s}^{-1}$; (a) $X_{H2O}=0.30$, (b) $X_{H2O}=0.35$.

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Figure 5. Radiative heat loss fraction as a function of dilution ratio of water vapor in air stream for two different radiation treatment at the fixed global strain rate, $a_g=50 \text{ s}^{-1}$; (a) $\Phi = 1.5$ and (b) $\Phi = 2.5$.

Fig. 5 shows the radiative heat loss fraction (f_r) [9] with increasing the amount of H₂O in the air stream for Φ =1.5 and Φ =2.5 when the WSGGM and OTM were used for the simulations. The radiative heat loss fraction means the ratio of total heat generated in the flame (I_{React}) to the total heat lost by radiation (I_{Rad}). For both equivalence ratios, the radiative heat loss fraction of WSGGM ($f_{r,WSGGM}$) decreased with increasing the amount of H₂O addition while the radiation heat loss fraction of OTM ($f_{r,OTM}$) increased except for near the extinction limit for Φ =2.5. These are because the OTM can consider only radiation heat loss from a flame while the WSGGM can consider both the radiation heat loss and reabsorption of lost heat. It should be noted that the magnitude of $f_{r,OTM}$ was large by a factor two compared to that of $f_{r,WSGGM}$ near the extinction limit. This means that the OTM overestimated the radiation heat loss by ~ 100%.

To examine the relationship between the amount of added H₂O and the reabsorption rate of radiation, we introduce the reabsorption parameter (f_{Reabs}), which means the ratio of the amount of reabsorbed heat from heat lost by radiation to pure radiation heat loss from the OTM. Fig. 6 shows the trend of f_{Reabs} with the amount of H₂O addition in air stream. For both the equivalence ratios, f_{Reabs} increased continuously with H₂O addition except for near the extinction limit. f_{Reabs} for Φ =2.5 was slightly higher than that for Φ =1.5. As depicted in Fig. 5, the radiative heat loss fraction was larger for Φ =1.5 than for Φ =2.5, but f_{Reabs} showed lower value for Φ =1.5 than for Φ =2.5 as shown in Fig. 6. This means that the radiation heat loss by the OTM for Φ =1.5 was more over-estimated compared with that for Φ =2.5. f_{Reabs} approached around 0.5, and this indicates that ~ 50% of the heat lost by radiation can be reabsorbed.



Figure 6. Reabsorption parameter versus dilution ratio of water vapor in air stream for both equivalence ratios, at the fixed global strain rate, $a_g = 50 \text{ s}^{-1}$.

5 Conclusion

The radiation effect of H_2O on the flame structure of counterflow methane partially-premixed flames was investigated numerically. In order to investigate the effects of radiation heat loss from a flame and reabsorption of the heat lost, three different radiation models were adopted in the numerical simulations. The amount of H_2O in air stream was increased up to a critical concentration which causes methane partially-premixed flame to extinguish.

The ADIA over-estimated T_{max} and flame width, compared with the predictions provided by the WSGGM and OTM. However, the difference in the prediction performance of the WSGGM and OTM was not large for the flame structure except for the extinction limit even H₂O was added in air stream.

 T_{max} and the spatially IHRR decreased for $\Phi=1.5$ and $\Phi=2.5$ with increasing H₂O addition, due to the weakness in the flame intensity. The radiation heat loss for $\Phi=2.5$ was small compared to $\Phi=1.5$.

The flame structures predicted by the OTM and WSGGM were similar when a small amount of H_2O was added regardless of the equivalence ratio. However, the flame structure, especially the flame width, was considerably affected by the radiation models for a large H_2O addition. The difference in the prediction performance of the OTM and WSGGM for a large amount of H_2O addition was attributed from the fact that the radiation reabsorption by H_2O .

The reabsorption parameter was larger for Φ =2.5 than for Φ =1.5 for the same amount of H₂O added. Thus, the reason that the radiation effect for Φ =2.5 was small compared to Φ =1.5 was partly attributed to the increase in heat reabsorption for Φ =2.5

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