The Chemical Structures of Laminar Opposed-Jet Diffusion flames of CH₄/CO Versus Air

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1 Introduction

In the present study, the flame characteristics of laminar diffusion opposed-jet flames of CH₄/CO versus air were studied. The combustion characteristics of carbon monoxide, which is a major intermediate product in hydrocarbon flames, are different from those of most alkanes. Its oxidation can be characterized by dry oxidation, i.e. $CO + O_2 \rightarrow CO_2 + O$. However, it is very difficult to ignite and sustain the dry oxidation process in practical combustion. Generally, the oxidation of CO can be significantly accelerated by the reaction $CO + OH \leftrightarrow CO_2 + H$ when there is a small amount of hydrogen-containing species in the fuel or oxidizer stream [1]. The burning velocity of CO with hydrogen containing species liberated from hydrogen, alkanes, or even water vapor is several orders higher than that of dry oxidation [2]. Moreover, the effect of hydrogen and hydrocarbon addition on the CO flames has been further experimentally and numerically studied [2][6][7]. In our previous study [6] [7], the effect of CO addition on the characteristics of methane/air premixed flames was examined systematically. It has been concluded that the effect of CO addition on the laminar burning velocity of the stoichiometric CH₄/CO/air flames is due mostly to the transition of the dominant chemical kinetic steps.

It has been well know that a diffustion flame consists of fuel-rich zone, fule-lean zone and reaction zone. The radicl pool in reaction zone provide enough H, O and OH atom by diffusion to ignite fuel and to decompose oxygen. Moreover, since carbon monoxide is a major intermediate of hydrocarbon flames, the intrinsic interaction between the original CO in the blended fuel and that produced from oxidization of hydrocarbons is worthy to be deeply investigated. Based on the similar methodologies of the previous study, a laminar diffusion opposed-jet flame of CH_4/CO versus air was numerically studied. Calculated chemical kinetic structures for selected flames are compared and the key reactions that affect the flame structure and are also discussed.

2 Methodology

The flame conditions, adiabatic flame temperatures of the premixed stoichiometric CH4/CO/air opposed-jet flames are listed in Table 1. The flame structures of counterflow diffusion flames are simulated using the OPPDIF package with the GRI-Mech3.0 chemical kinetic mechanisms [8] and detailed transport properties. For the flame calculations, the computation domain and input parameters for each flame condition are in accordance with experiments. The temperature at both jet exits are set as 300 K. In flowfield computation, the flow is reduced mathematically to one dimension by assuming that the radial velocity varies linearly in the radial direction, which leads to a simplified form in which the flowfield properties are functions of the axial distance only. The adaptive regridding method is applied to solve the flame structure, and the grid independence of the solutions is achieved by tuning the GRAD and CURV parameters in the package. The number of grid lines is set to more than 400 for each case. The minimum grid dimension is approximately $0.1 \ \mu m$, which is sufficient to resolve the flame thickness and the steep temperature gradient.

Table 1	Conditions	of laminar	counterflow	diffusion	flames of	CH4/CO	Versus Air
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# —	fue	fuel		train rate		La	Le
	CH_4	СО	$a_{\rm o}$	a_{f}	I ad	Le _{CH4}	Le _{CO}
1	100	0	87.9	116.0	2258.3	0.89	N/A
2	90	10	89.2	113.8	2263.8	0.9	1.02
3	80	20	90.4	111.9	2270.2	0.9	1.02
4	70	30	91.6	110.1	2277.6	0.9	1.02
5	60	40	92.8	108.5	2286.2	0.9	1.03
6	50	50	93.9	107.0	2296.5	0.91	1.03
7	40	60	95.0	105.6	2308.8	0.91	1.03
8	30	70	96.1	104.3	2323.8	0.92	1.03
9	20	80	97.1	103.0	2342.6	0.93	1.03
10	10	90	98.2	101.9	2366.8	0.94	1.04
11	6	94	98.6	101.5	2378.6	0.94	1.04
12	2	98	99.0	101.1	2384.8	0.95	1.04

3 Results and Discussion

Photographs of the laminar counterflow diffusion flames of CH₄/CO Versus air are shown in Fig. 1. For different CO volumetric contents in fuel stream, global strain rate of oxidizer and fuel are tabled in Table 1.For fuel sream, CH₄ and CO are metered and mixed in a mixing chamber prior to the opposed-jet burner. The oxidizer (air) is supplied by the compressed air system which coupled with a refrigeration dryer. The flame shielded from ambient air by a nitrogen coaxial flow which is controlled using a rotameter. The dew point of air can be reduced to -20°C. The uniform velocities from the fuel and oxidizer nozzles are 100 cm/s, and the separation distance beteen the nozzles is 2 cm. For photography, a Nikon D80 is used for image recording. The suttle time of images shown in fig. 1 are 1/400 second with F/5.6. Fig. 1(a) shows that for 100%CH4 versus air, a single thin planar flame exist and the flame is blue in color. As the



Figure 1. Photographs of the laminar Counterflow Diffusion flames of CH_4/CO Versus air: (a) flame 1, (b) flame 2, (c) flame 3, (d) flame 4, (e) flame 5, (f) flame 6, (g) flame 7, (h) flame 8 (i) flame 9, (j) flame 10, (k) flame 11, (l) flame 12, (m)

concentration of CO in fuel stream is increased, the flame becomes bright and thick. For the 100%CO case, the flame can not sustained. These results indicates that the existance of CO in fuel stream

Explosions, Detonations, and Reactive Systems



Figure 2. Computed axial distribution of temperature, mixturfraction, species mole fraction for (a)flame 1; (b)flame 4; (c) flame 10; (d)flame 12.



Figure 4. Computed axial distribution of net reaction rate of significant reaction steps for (a)flame 1; (b)flame 4; (c) flame 10; (d)flame 12.



Figure 3. Computed axial distribution of production rate for (a)flame 1; (b)flame 4; (c) flame 10; (d)flame 12.



Figure 5. Computed axial distribution of heat release rate of significant reaction steps and total heat release rate for (a)flame 1; (b)flame 4; (c) flame 10; (d)flame 12.

changes the flame color and visible flame thickness.

On purpose to further understand the effect of the variation of CO volumetric concentraion in fuel stream on flame characteristics, flame structures of four characteristic flames selected are examined. The profile of the temperature, mixtrue fraction, species mole fraction, production rate, net reaction rate, and heat-release rate of the major elementary steps along the jet axis are plotted in Figs. 2, 3, 4, and 5 for flames 1, 4, 10, and 12, respectively. In the figures, the dashed line indicates the axial location of the stoichiometric which defined based on mixture fraction, and the centerline indicates the axial location of the stagnation. Fig. 2(a) shows typical profile for diffusion opposed-jet flame of CH_4 versus air. As the concentraion of CO is increased, the flame characteristic shift toward a different structure. For a large amount of CO composition in fuel stream, more H and O radical are accmulated in flame zone. Fig. 3, 4, 5 show production rate, net reaction rate, heat release rate of four selected flames. The major reaction steps discussed in this paper are summarized in Table 2. Results show that

Oleg G. Penyazkov

flame 4 has similar species production rate with that of flame 1 and can be classified as methane-like diffusion flame. The dominant heat release steps of methane-like flame are R10, R84, and R99. Among these heat release step, R84 provide major heat to sustain R38 which is important step to decompose oxygen and produce O and OH. As the CO concentration is increased to 90%, the consumption of fuel is dominated by CO oxidation

chemistry, and R38 becomes less important. Hence, part of CO is comsumed via R12 and induces thicker reaction zone.

4 Conclusions

In the present study, the effect of CO addition on the chemical structures of laminar opposed-Jet diffusion flames of CH_4/CO versus Air was examined. The flame structures are simulated using the OPPDIF package wiht GRI-Mech 3.0 mechanisms and detailed transport properties. The transition of the dominat chemical kinetic steps casused by addition of CO are discused. The results show that the generation of radicals including H, O, and OH is shifted. Thereby, the variation of radical pool, induces different decomposition of fuel and oxygen.

Table 2 Summary of the major reaction steps				
Reaction step	Reaction number			
$O + CH_3 \leftrightarrow H + CH_2O$	R10			
$O+CO(+M) \leftrightarrow CO_2(+M)$	R12			
$\mathrm{H} + \mathrm{O}_2 \leftrightarrow \mathrm{OH} + \mathrm{O}$	R38			
$\mathrm{HO}_2 + \mathrm{H} \leftrightarrow \mathrm{OH} + \mathrm{OH}$	R46			
$\mathrm{H} + \mathrm{CH}_4 \leftrightarrow \mathrm{H}_2 + \mathrm{CH}_3$	R53			
$\mathrm{H} + \mathrm{CH}_{2}\mathrm{O} \leftrightarrow \mathrm{H}_{2} + \mathrm{HCO}$	R58			
$\mathrm{OH} + \mathrm{H}_2 \leftrightarrow \mathrm{H} + \mathrm{H}_2\mathrm{O}$	R84			
$OH + CH_3 \leftrightarrow CH_2(S) + H_2O$	R97			
$\mathrm{OH} + \mathrm{CH}_4 \leftrightarrow \mathrm{CH}_3 + \mathrm{H}_2\mathrm{O}$	R98			
$OH + CO \leftrightarrow H + CO_2$	R99			
$OH + CH_2O \leftrightarrow HCO + H_2O$	R101			
$HO_2 + CH_3 \leftrightarrow OH + CH_3O$	R119			
$\mathrm{HCO} + \mathrm{H_2O} \leftrightarrow \mathrm{H} + \mathrm{CO} + \mathrm{H_2O}$	R166			
$HCO + M \leftrightarrow H + CO + M$	R167			
$O_2 + HCO \leftrightarrow HO_2 + CO$	R168			
$\mathrm{O} + \mathrm{CH}_3 \longrightarrow \mathrm{H} + \mathrm{H}_2 + \mathrm{CO}$	R284			

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