Numerical study of influence of surface reaction and heat-loss on flame intensity of methane–air flames

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Abstract. This paper reports a numerical study of influence of radical quenching and heat loss on bulk flame characteristics in narrow parallel channels. Flame-wall interaction is an important phenomenon on combustors. Especially, the wall effects on the flame characteristics in a small scale combustor become larger than those on normal scale one. The wall effects are caused by heat loss and surface reaction. The surface reaction on many common non-catalytic materials may weaken or quench the flames, although those for a catalytic wall can strengthen the flames. Authors have investigated the influence of the surface reaction and the heat loss on a non-catalytic wall using numerical simulation. In this study, a two-dimensional slit burner between two parallel plates with or without surface reaction is modelled. The wall temperature is 500 and 1200 K. The flame behavior and heat release rate distributions are examined when the distance between two plates is changed.

1. Introduction

In recent years, minimization of micro electronic and mechanical devices has resulted in demands for smaller and higher power generators. One of the candidates for such generators is an ultra-micro gas turbine (UMGT), which is expected to have several times the energy density of a lithium ion battery [1]. Thus, meso- or micro-scale combustors have been investigated [2]. To further develop the UMGTs, it is important to understand the fundamental phenomena that occur in their small-scale combustors. Many researchers have studied UMGTs and related phenomena [3, 4].

One of the important features of micro-scale combustors is their large surface-to-volume ratio. This large ratio leads to enhanced heat loss and radical quenching by surface reactions on the wall. However, these phenomena are complex due to the effects of many factors, such as temperature, material, and surface texture. Heat-loss effects have been investigated by many researchers [5, 6]. Egolfopoulos et al. [6] have investigated the interaction between a chemically inert wall and a premixed flame using numerical and experimental results. Recently some researchers have made attention to chemical effects of surface [7-9]. The measurements are very difficult since reaction rates of surface reaction for radical quenching is much smaller than that for catalytic reaction and thus the S/N ratio is often small.

For numerical simulation, reaction kinetics models for the surface reaction are proposed by Aghalayam for hydrogen mixture [10] and Raimondeau for methane mixture [11]. These models are not specified for real materials, but they include important species for ignition or quenching. Thus, although

results using these models may be different for real materials, it is useful to understand the radical quenching.

In the present study, a two-dimensional slit burner between two parallel plates is modeled for investigation of chemical effects. This paper reports influence of radical quenching and heat loss on bulk flame characteristics. The flame behavior and heat release rate (HRR) distributions are examined as the flame characteristics when the distance between two plates is changed.

2. Analytical model and numerical calculation method

A two-dimensional slit burner between two parallel plates was modeled using two-dimensional planer coordinates (x, y), as shown in figure 1. Stoichiometric methane-air premixed gas flows into a narrow channel from a slit nozzle of left-hand side. A symmetric condition was adopted at the center of channel of the upper boundary, and a free outflow condition was adopted at the outlet of the right boundary. The inlet velocity in the x direction, u, was assumed to be a Hagen-Poiseuille flow distribution. Here, the average velocity is 0.8 m/s and the pressure is atmospheric. The inlet temperature is 300 K. The bottom boundary (wall A) is a non-slip wall with or without surface reactions. The wall temperature, T_w, is 500 K and 1200 K, because the influence of surface reaction on flame characteristics becomes significant when wall temperature is around 900 K. The position of the wall, y_w, was varied from 3.2 mm to 1.0 mm. For each y_w condition, after ignition by high temperature region located around $x = 0$, the calculation is done until the flame becomes stable or extinct. The rim of the nozzle (wall B) is non-slip inert wall with T_w, and the inside wall of the nozzle (wall C) is non-slip adiabatic wall. The maximum size of the computational domain is 8.0 mm x 3.2 mm, and the corresponding number of grid points is 200 x 160. They are equally spaced in the y direction, and unequally spaced in the x direction. The minimum grid size is 0.02 mm.

For active wall conditions, Langmuir's adsorption model was used, and the desorption reaction rates were expressed in the Arrhenius form. The Raimondeau's surface reaction mechanism was used [11]. In this mechanism, CH_3, H, O, and OH radicals are adsorbed, and recombined to form stable species such as H_2, H_2O, O_2, CH_4 and C_2H_6. This mechanism is not considered particular material, but important radicals for flame ignition and extinction are depicted. The gas phase reaction used in this study does not contain C_2H_6, and for the C_2H_6 desorbed reaction, two CH_3 radicals are desorbed instead of C_2H_6.

The thermodynamic properties for the species were obtained from the CHEMKIN database [12, 13]. The transport properties were calculated according to Smooke's simplified transport model [14]. For the gas phase reaction, the chemical kinetics model is the Smooke's skeletal mechanism [14], consisting of 16 species and 25 elementary reactions. Details of the numerical calculation method are not shown here, but can be found in [15, 16]. Here, the gravity in the x direction was considered.

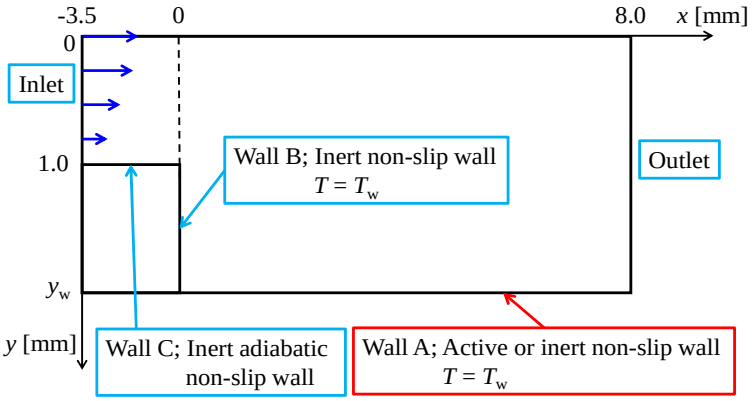


Figure 1. Analytical model and boundary conditions

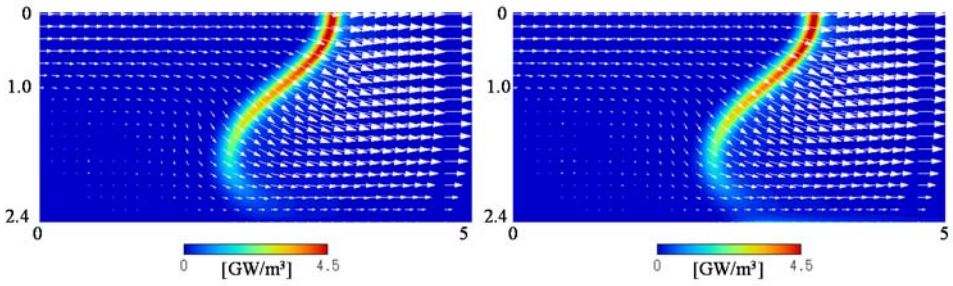
3. Results and discussion

3.1. Flame Behaviors

Table 1 shows the change in flame configuration with y_w. Figure 2 shows the heat release rate distributions and velocity vectors. The attached flames (wall A) are formed in this figure. For large y_w, the flame edge forms near wall B ("Attached (Wall B)" in Table 1). When the y_w becomes smaller, the flame edge moves to near wall A (Attached (Wall A)). Unsteady flames are observed between these conditions, and they swing upstream and downstream [17]. When the y_w decreases further, blow-off occurs. This blow-off is considered as "flame quenching" in the experiments [7, 8] using the burners similar to the present study. Quenching was observed only when T_w = 500 K and y_w = 1.0 mm, which corresponds to the position of slit burner lim.

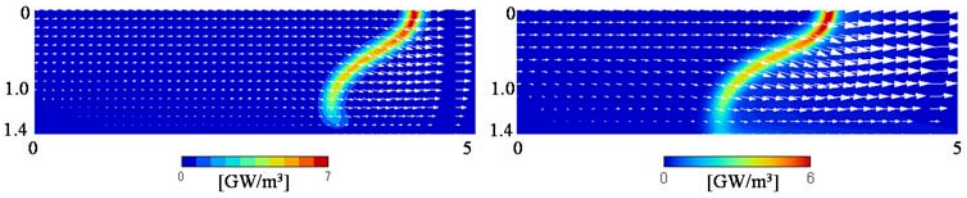
Table 1. Flame behavior

y_w [mm]	T_w = 500 K		T_w = 1200 K	
	Inert	Active	Inert	Active
3.2～2.8	Attached (Wall B)	Attached (Wall B)	Attached (Wall B)	Attached (Wall B)
2.6	Unsteady	Unsteady		
2.4	Attached (Wall A)	Attached (Wall A)		
2.2	Blow off	Blow off		
1.8～1.6			Unsteady	Unsteady
1.4			Attached (Wall A)	Attached (Wall A)
1.3				Blow off
1.2				
1.1			Blow off	
1.0	Quenching	Quenching		



Active wall Inert wall

(a) T_w = 500 K, y_w =2.4 mm



Active wall Inert wall

(b) T_w = 1200 K, y_w =1.4 mm

Figure 2. Distributions of HRR and velocity vectors

For low temperature wall, the blow-off occurs in the same y_w conditions for active and inert wall. For high temperature wall, the blow-off condition for the active wall is larger than that for the inert wall, but the difference is only 0.2 mm, and thus the influence of surface reaction on the blow-off is limited.

Figure 2 (a) shows the distribution of HRR and velocity vectors for the low temperature wall condition. The flame shapes and positions show no difference for active or inert wall conditions. This implies that the influence of heat loss is relatively large, and the influence of surface reaction is limited. The HRR distributions in figure 2 (b) show difference for active or inert wall conditions. First, the flame position for the inert wall is located in the upper stream than that for active wall. The velocity distributions in x direction at center of channel are shown in figure 3. The velocity increases with the decrease in y_w for constant inlet velocity. This tendency for the inert wall condition is more remarkable than that for the active wall condition. There is the high HRR region near the inert wall, whereas HRR is small near the active wall. In the following section, the characteristics of HRR distributions are discussed further.

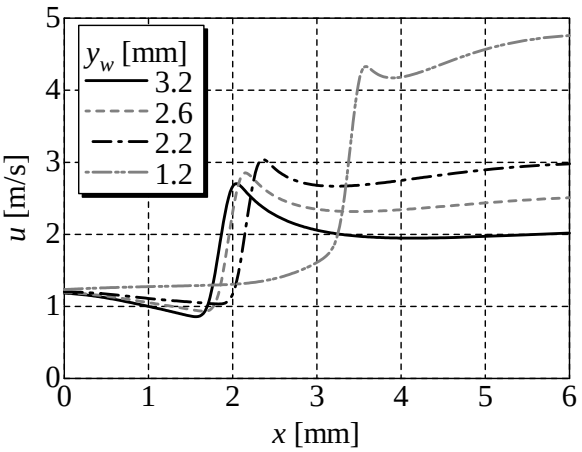


Figure 3. Distribution of velocity in x direction at center of channel;
T_w = 1200 K, Inert wall

3.2. *Influence of surface reaction on HRR*

The variation of summation of HRR, $Q_{\mathrm{sum},y=0}$, in the center line of channel is shown in figure 4. The $Q_{\mathrm{sum},y=0}$ shows no difference for active or inert wall conditions. Therefore, the influence of surface reaction on HRR is limited in center of channel, and the normal premixed flame reaction occurs around here [17].

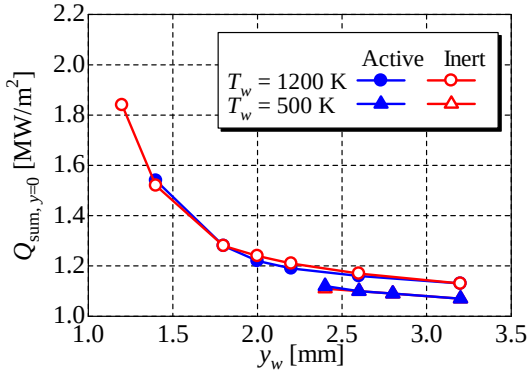


Figure 4. Relation between $Q_{\mathrm{sum},y=0}$ and y_w

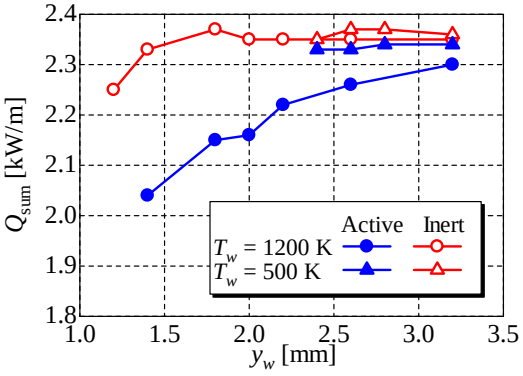


Figure 5. Relation between Q_{sum} and y_w

Figure 5 also shows the total of HRR, Q_{sum}, which is integrated over the whole calculation domain. This figure shows clear difference for active or inert wall conditions and temperature conditions. For the high temperature inert wall, Q_{sum} is almost constant except for $y_w < 1.5$ mm. The Q_{sum} for the inert wall is larger than that for the active wall in the case of high temperature wall. The difference increases with the decrease in y_w. These results clearly show the influence of surface reaction. Even when the flame forms far from wall A, the Q_{sum} is different between the active and inert wall. This is because the reaction which occurs in burned gas, such as $CO + OH = CO_2 + H$, is inhibited by the radical quenching due to the surface reaction. For both active and inert wall with low temperature, the Q_{sum} is constant for y_w and almost the same as that for the high temperature inert wall.

4. Conclusions

The numerical simulation of a two-dimensional slit burner between two parallel plates is conducted to understand the influences of surface reaction and heat-loss to the wall on quenching distance for methane-air mixture. The surface reaction causes radical quenching for active wall condition. The following conclusions are drawn.

1. With the decrease in the distance between the walls, the flame shape changes.
2. In the case of high temperature wall, the total of HRR, Q_{sum}, for the inert wall is larger than that for active wall. The difference increases with the decrease in y_w, and these results clearly show the influence of surface reactions. For low temperature wall, Q_{sum} is constant for y_w and almost the same as that for high temperature inert wall.

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