Numerical Study on Methane Micro-Diffusion Flames

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Abstract

Detailed flame structure of a small methane micro-diffusion flame, established under normal gravity over a vertically oriented 0.3 mm diameter straight tube with a 2.0 m/s methane fuel jet was studied numerically. The predictions of a numerical model consisting of 32 chemical species and 177 reaction steps were compared favorably with the published micro flame experimental results. An iso-CH concentration line matched with the experimentally obtained visible flame shape, and the calculated flame height and width respectively agreed with the corresponding experimental result. Our numerical results suggest that the oxidizer side structure of the micro-diffusion flame is similar to the buoyancy controlled laminar diffusion flame, while the fuel side structure is similar to the zero gravity flame.

Keywords; Flame Base Structure, Laminar Flame, Micro-Diffusion Flame, Numerical Simulation

Introduction

Ban et al [1] employed vertically oriented sub millimeter diameter needles, issued a fuel through that needle and established a very small circular shape diffusion flame, called micro flame, at its exist. Micro flame is a type of momentum-diffusion controlled flame [2] and differs from momentum-controlled (Burke-Shumann type [3]) flame and buoyancy-controlled (Roper type [4]) flame. Ban et al. [1] have demonstrated its buoyancy insensitivity by rotating the flame and reported that the flame shapes were kept in the various orientation angles. The size and buoyancy insensitivity are significant features of the microflame when industrial use is considered; it can be a point heat source with no preference for the orientation angle. The microflame is formed in Re~O(1) and Fr>>1 according to the flame theory by Williams [5], suggesting the flame is in a laminar flame regime. The combination of these two non-dimensional numbers can be done by using small/large characteristics length/velocity; for example a couple hundred micron of burner diameter with a few meter per second fuel exit velocity from the burner.

To understand this newly proposed flame characteristics, the theoretical and experimental studies have been conducted and the flame shape parameters (ex. flame height, thickness) with the various flowing condition and a region of the combustible zone by visualizing CH, OH emission from the flame were investigated [1,6]. However, theoretical analyses need assumptions in thermal properties of the gas (ex. constant properties must be used to make the analyses possible) as well as the chemical reaction (ex. infinitely fast). Also experimental study could show the limited data and visualize itself is very difficult since the flame size is, at most, in order of a few millimeter. Flame stability is the one of most important combustion characteristics and it strongly related with the flow pattern, quenching zone by the burner surface, which they are difficult to access theoretically as well as experimentally. With this respect, we have introduced

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the numerical analyses to understand the thermal and flow dynamic structure by using of the simple kinetics model [7-8]. Although the overall structures were understood by this approach, there still needs further development; for example the radical structures must be resolved to understand the quenching behavior.

In the present study, we have conducted the numerical simulation of the microflame (jet diffusion flame configuration) to access the detail flame structure with full kinetics model (GRI-mech2.11) and have attempted to understand the characteristics on its stability. Firstly the numerical model is verified by using the corresponding experimental data by Ida et al. [6], then the structures at the flame base are investigated with the comparisons of Takahashi et al.'s reaction kernel studies [9-10].

Numerical Model

Fig.1 shows a schematic illustration of the numerical model. Since the all transport/chemical phenomena are symmetric at the burner center axis, axisymmetric 2-D plane is considered as the numerical domain. A burner, whose inner/outer diameters of 0.3mm/0.8mm, is placed in the atmospheric air vertically, and the pure methane is ejected to the upward (against the gravity vector) with 2.0m/s. A micro-diffusion flame is established over the burner steadily with a few millimeter flame height. The burner is kept as the room temperature so that it causes the heat loss in the system and avoids any catalytic effect there. As seen in the figure, the inside of the burner is in the numerical domain and 'back diffusion' of the species into the burner is possible. Numerical origin is set at the center of the burner surface, and two-dimensional coordinate (r, x) is imposed.

Ordinal set of the conservation equations (mass, momentum, energy, species) with the equation of reaction rate and the equation of the state are solved numerically by finite volume method [11]. GRI-mech2.11 [12], which includes 32 chemical species and 177 reactions (NO_X formation reactions are excluded from the original set), is applied to the chemical reaction model. Thermal properties are given by CHEMKIN database, while transport properties are given by Smooke's simplified transport model [13]. Open boundary conditions are imposed at the boundaries except for the center axis (symmetric). Non-slip condition is applied at the burner surface.

Results and Discussion

Verification of the Numerical Model

Fig.2 shows the (a) simulated CH distribution and (b) experimentally observed CH emission [6]. The comparison shows a good agreement between simulated and observed flame shape, height and thickness. The large discrepancy is found, however, at the flame base; simulation predicts wider CH region than experiment. This might be because that experimentally observed CH emission is not perfectly corresponds to CH distribution, rather, the signal sent when CH in the excited level (=CH*) is back to its basic state. CH needs the energy to be

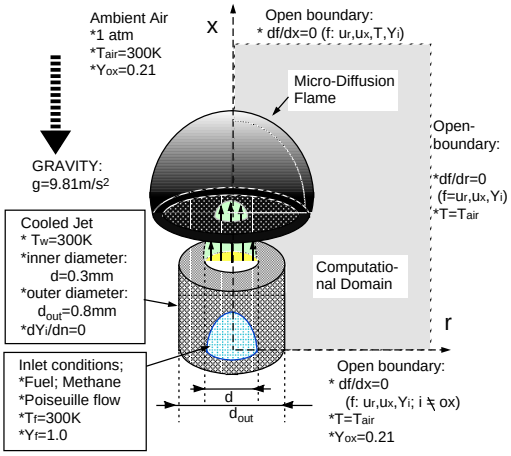

Figure 1 Schematic Illustration of Numerical Model

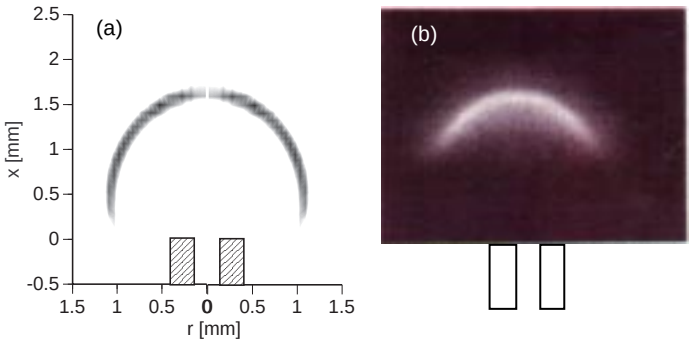

Figure 2 CH image: (a) Present Simulation, (b) Experiment [from ref. 6].

pumped to CH*, however temperature at the flame base is relatively lower [7-8]; thus it is possible that CH is there but no emission from CH* is recognized. According to the results, the numerical model applied here is found to give the precise flame structures in the microflame.

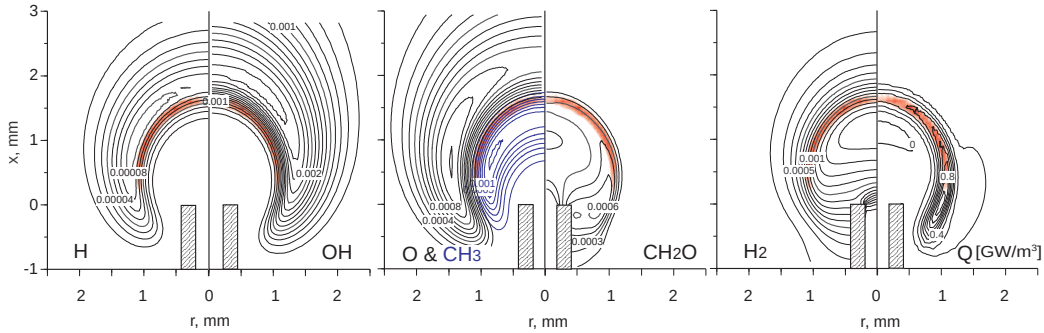

Figure 3 2-D contours of Species (H, OH, O, CH_3, CH_2O,H_2) and Heat Release Rate (Q)

2-D distributions of the Important Quantities

Fig.3 shows that 2-D contours of the important radicals (H, OH, CH_3, CH_2O, O, H_2) and heat release rate. Major quantities, such as temperature, methane oxygen, flow fields, are not shown here since they are quite similar to the previous results [7-8]. CH (red gradation in the figure) is superimposed to the all figures to express the visible flame. From the figure, H, OH, O are formed and distributed mainly in the oxidizer side of the flame, while CH_3, CH_2O, H_2 are in the fuel size. The strong heat release zone is appeared at the flame base. These overall trends are the same as the typical diffusion flame. It is found the negative heat release rate region in the fuel side. Note the interesting trend in hydrogen; since H_2 is strongly diffusive, it diffuses upstream through the quenching region formed along the burner. It could burn if special treatment is applied at the burner surface (e.g. catalytic); this treatment may increase the flame stability because the quenching region is diminished.

Flame Base Structures

One of the important characteristics of the diffusion flame is stability which strongly related with the flame base structure. Since the microflame shows the spherical shape (indicating little buoyancy effect as described in earlier), it is expected the similar structures with no buoyancy flame, i.e. microgravity flame. Takahashi et al. have shown that the flame base structure in 1g jet flame [9] and in microgravity flame [10] with the sophisticated numerical model. These data are quite useful to determine if the microflame has categorized as 1g type or 0g type in terms of the flame base structure.

Fig.4 shows (a) the selected elementally reactions and (b) the selected reactions which provide the large heat release rate. As seen in Fig.4(a), methyl (CH_3) radical is produced by methane reacts with OH or H radicals, and former is a bit larger than the latter. This trend is similar to the 0g flame [10]. CH_3 is then reacts with oxygen atom which gives the most significant heat release in the system and the familiar chain-branching reaction of hydrogen atom ($H+O_2$->$OH+O$) occurs widely at the flame base. These are consistent with 1g as well as 0g results. In Fig.4(b), it is found that the final-product formation reactions ($CO+OH$->CO_2+H, H_2+OH->H_2O+H) contribute the heat release rate in the system rather than O_2+H->HO_2,

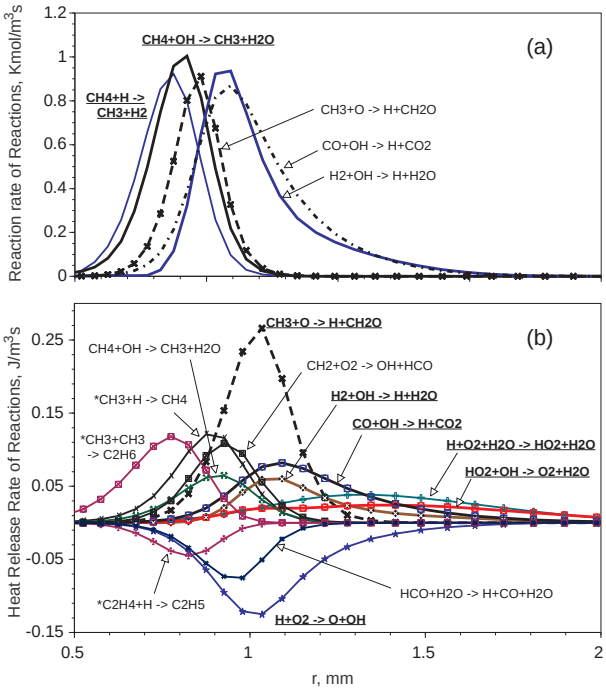

Figure 4 Contribution of Elementally Reactions at Flame Base (x=-0.09mm).

HO_2+OH->H_2O+O_2; this trend is similar to the 1g flame [9]. Therefore, one can conclude that microflame has bimodal feature of its structure at the flame base; the structure is similar to the 0g flame in the fuel side, while 1g flame in the oxidizer side.

Concluding Remarks

The detailed flame structure of the microflame has been investigated with detail chemical kinetics (GRI-mech2.11) in axisymmetric 2-D configuration. Each of the numerically calculated flame shape, flame height, and flame width is favorably compared with the corresponding experimentally measured data. Micro flame has unique flame base structure: its oxidizer side's flame structure is similar to the Roper type flame, while its fuel side is similar to a candle-like microgravity flame.

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