가열된 동축류내 층류 메탄/수소 부상화염의 특성에 관한 수치해석적 연구

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A numerical study of the characteristics of laminar lifted methane/hydrogen flames in heated coflow

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ABSTRACT

The characteristics of laminar lifted methane/hydrogen jet flames in heated coflow are investigated using 2-D axisymmetric numerical simulations with OpenFOAM. It is found that a highly-diluted laminar methane jet flame with small amount of hydrogen addition exhibits a unique feature that its liftoff height decreases with increasing fuel jet velocity, similar to experimental observation. The Damköhler number and chemical explosive mode (CEM) analyses verify that the decrease of the liftoff height of the methane/hydrogen jet flame is primarily attributed to highly-diffusive hydrogen molecule, which is also confirmed by additional simulations in which the diffusivity of hydrogen molecule is artificially set to that of methane.

Key Words : Lifted flame, Autoignition, MILD combustion, Laminar flame

Recently, hydrogen-enriched natural gas (HCNG or H_2CNG) has drawn a practical interest among researchers because it is able to enhance flame stability and reduce pollutant emission. In a previous study [1], it was reported that unlike conventional jet flames, HCNG jet flame within the low temperature regime has a unique feature that its liftoff height decreases with increasing fuel jet velocity, which was conjectured to be due to the preferential diffusion effect of hydrogen molecule.

The objective of this study is, therefore, to elucidate why this unique feature of the liftoff height behavior using laminarSMOKE code [2, 3] based on an open source code, OpenFOAM. We adopt a skeletal chemical mechanism of methane oxidation composed of 30 species with 184 elementary reactions. The domain size is 6.65 cm × 30 cm in the radial, r, and the axial, z, directions with 124 × 3000 grids. The fuel jet is issued from a circular tube of 1.9 mm radius with 0.5 mm nozzle thickness. In the radial direction, 100 uniform grids are employed within 1 cm from the center ($\triangle r$ = 100 μm) and the remaining grids are stretched toward the outer domain. In axial direction, 3000 grids are uniformly distributed ($\triangle z$ = 100 μm). From a series of grid convergence tests, it was found that the grid resolution of 100 μm is fine enough to resolve the velocity, temperature, and species fields.

In the present simulations, all the boundary conditions are identical to those of the previous experiments [1]. However, the temperatures of the fuel and coflow jets are set to be 100 K greater than those of experiments to obtain similar results. The details of the boundary conditions are listed in Table 1.

The flame base is defined as the OH mass fraction, Y_{OH}, of 0.0002. Steady temperature isocontours for all the cases are shown in Figure 1. Similar to the experimental result, the liftoff height, H_L, decreases as the fuel jet velocity, U_0, increases.

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Fuel jet velocity, U_0 [m/s]	3, 5, 8, 10, 15, 20, 25
Coflow velocity, U_{co} [m/s]	1.1
Temperature [K]	950
Fuel mole fraction (X_F)	0.2
Hydrogen ratio (R_h)	0.3

Table 1. Boundary conditions

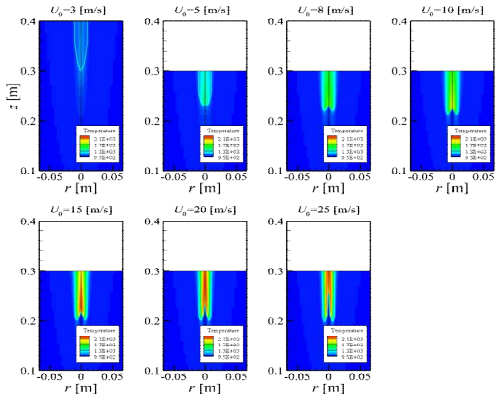


Fig. 1. Temperature profiles with various jet velocities.

For cases with relatively-low fuel jet velocity (U_0 = 3, 5, and 8 m/s), the lifted flames do not exhibit typical tribrachial lifted flame characteristics. Instead, they belong to the moderate or intense-low oxygen dilution (MILD) combustion regime where the conditions of $(T_{MAX}-T_0)/T_{ig}<1$ and $T_0>T_{ig}$ are satisfied.

To understand the stabilization mechanism of the lifted flame, a Damköhler number, *Da*, is evaluated along a streamline which passes through the flame base. For the *Da* anaylsis, *Da* is defined as the ratio of the actual convection time to the ignition delay time at a given point in the streamline. As such, *Da* > 1 indicates that auto-ignition can occur upstream of the flame base and as such, the lifted flame is stabilized by auto-ignition. Otherwise, flame may be stabilized by flame propagation. Figure 2 shows the *Da* profiles along the streamline for the cases with U_0 = 8 and 25m/s. From the figure, it is readily observed that *Da* becomes greater than unity far upstream of the flame base, which verifies that the lifted flame is stabilized by auto-ignition rather than flame propagation. For the other cases, we found a similar trend.

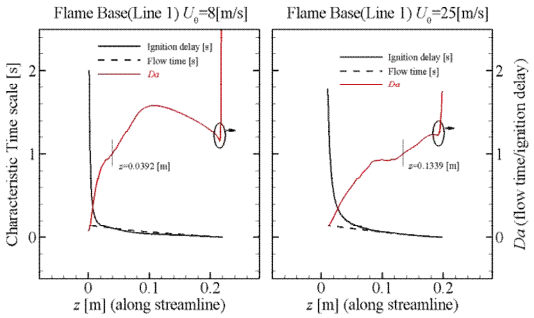


Fig. 2. *Da* analysis for cases U_0 = 8 (left) and 25 m/s (right).

In the previous study [1], it was conjectured that the high diffusivity of hydrogen molecule may cause the decreasing behavior of the liftoff height. To verify the preferential diffusion effect of the hydrogen molecule, we performed additional numerical simulations in which the mass diffusivity of hydrogen molecule is specified to be equal to that of methane.

Fig. 3 show the liftoff height H_L and temperature index $(T_{MAX}-T_0)/T_{ig}$ as a function of the fuel jet velocity for cases with real and modified diffusivities of H_2. As shown in the figure, for the cases with modified diffusivity of H_2, the H_L increases with increasing fuel jet velocity.

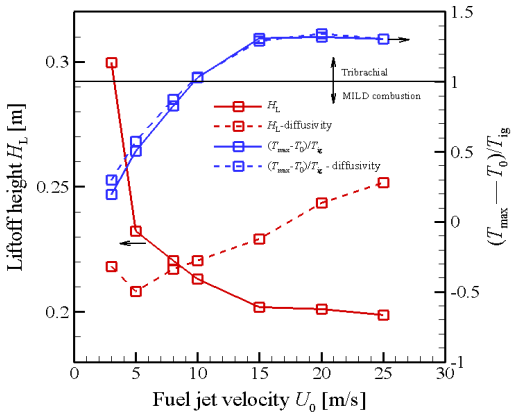


Figure 3. Liftoff height and temperature index for various fuel jet velocities.

These results identify that the decreasing liftoff height with increasing fuel jet velocity for this specific methane/hydrogen jet flame is

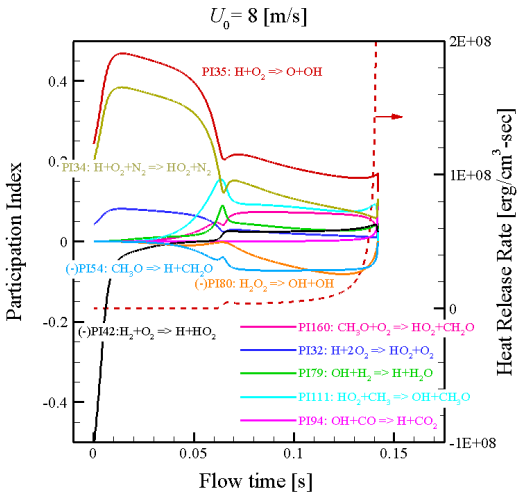
attributed to the highly-diffusive nature of hydrogen molecule.

It is of interest to note that H_L decreases significantly with increasing fuel jet velocity for the relatively-low velocity regime (U_0 = 3 ~ 15 m/s). However, H_L decreases marginally with increasing fuel jet velocity for the relatively-high velocity regime (U_0 = 15 ~ 25 m/s). To elucidate the different behaviors of the liftoff height variation in the two regimes, the chemical explosive mode analysis (CEMA) is carried out. The CEMA is an analysis based on the eigenanalysis of the Jacobian matrix of the chemical source term [5, 6]. In the CEMA, the contribution of a reaction to a chemical explosive mode (CEM) is defined as a participation index **PI**,

$$\mathrm{PI} = \frac{(\mathbf{b}_e \cdot \mathbf{S}) \otimes \mathbf{R}}{\mathrm{sum}\left(\left|(\mathbf{b}_e \cdot \mathbf{S}) \otimes \mathbf{R}\right|\right)}$$

where **S** is the stoichiometric coefficient matrix, **R** is the net reaction rates vector, $\otimes$ is the element-wise multiplication of two vecotrs. Thus, a large value of ith **PI** close to unity indicates that the ith reaction is dominant in the CEM. It is noted that the sign of numerator in PI is omitted, and therefore we can clearly know the direction of ith reaction.

The profiles of important PI's along the streamline passing through the flame base are are shown in Fig. 4 for cases with U_0 = 8, 15, 25 m/s.



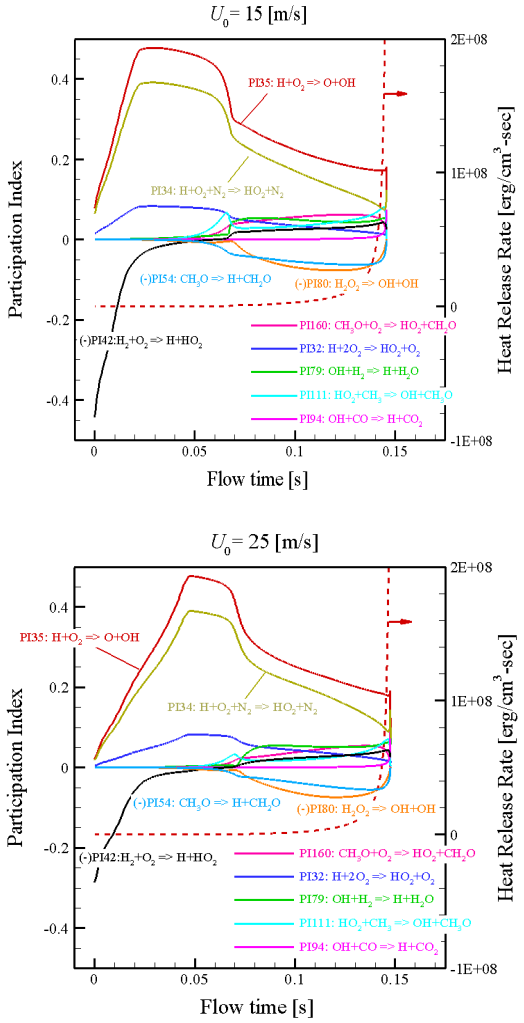


Figure 4. The profiles of important PI's along the streamline passing through the flame base for cases with U_0 = 8, 15, and 25m/s (from top to bottom).

As shown in the figure, three cases exibit similar trend. Hydrogen-involved reactions (e.g. -R42, R35, and R34) occur predominantly upstream of the flame base and intermediate species such as HO_2 or H_2O_2 are produced accordingly. As the ignition progresses, highly exothermic reaction of -R80 (H_2O_2 => OH+OH) and heat release step of hydrogen oxidation of R79 (H_2+OH => H_2O+H) become active, leading to thermal ignition. Near the flame base, the reactions involving species originated from methane (e.g. -R54, R160, and

R111) occur more significantly and finally, the reaction of CO to CO_2 conversion process, R94, takes place.

From the heat release rate profile for the case with U_0 = 8m/s, intermediate thermal ignition process seems to occur approximately at 0.06 s, whereas it is not observed for the cases with U_0 = 15 and 25 m/s. This is because hydrogen-originated reactions occur faster for cases with relatively-low fuel jet velocity which makes more hydrogen to be transported to the fuel lean side, and hence heat release processes such as -R80 and R79 can occur more dominantly far upstream of the flame base. This may lead to the different behavior of H_L in the two different regimes.

Conclusion

In this study, the liftoff characteristics of a laminar methane/hydrogen flame are elucidated using 2-D numerical simulations by systematically varying the fuel jet velocity. It is found that similar to the experimental results, the liftoff height decreases as the fuel jet velocity increases. It is also found that a transition from the tribrachial flame to the MILD combustion occurs at low jet velocities. From the *Da* analysis, it is verified that the lifted flame is stabilized by auto-ignition. Additional simulations with modified hydrogen diffusivity identify that the decrease of the liftoff height with increasing fuel jet velocity is primarily attributed to the high diffusivity of hydrogen molecule. From the CEMA, it is also identified that in the MILD combustion regime, the ignition process is different from that in the tribrachial flame regime.

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