가열된 동축류내 층류 디메틸 에테르의 열분해 정도에 따른 부상화염에 특성에 관한 수치해석적 연구

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Pyrolysis effect on the stabilization characteristics of autoignited dimethyl ether jet flames in hot coflow air

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ABSTRACT

The stabilization characteristics of autoignited laminar dimethyl ether (DME) jet flames in heated coflow air is numerically investigated with laminarSMOKE code, which is an openFOAM-based laminar reacting flow solver. According to previous experimental study on autoignited laminar DME jet flame, an unusual liftoff height behavior is observed such that liftoff height of lifted flame increases with decreasing fuel jet velocity. To understand the liftoff and stabilization characteristics of autoignited DME jet flames various numerical studies have been carried out. From additional simulations with modified hydrogen's mass diffusivity, it is revealed that the decreasing liftoff height behavior is mainly attributed to the high diffusive nature of hydrogen molecule, which is generated by DME pyrolysis.

Key Words : Autoignition, Mild combustion, Dimethyl ether (DME), Pyrolysis

From an experimental study of autoignited laminar lifted dimethyl ether (DME) jet flames in heated coflow air, an unusual liftoff height behavior was observed: H_L is inversely proportional to the fuel jet velocity, U_0 [1]. Generally, this decreasing H_L behavior occurs only when two kinds of fuels are mixed in the fuel jet (e.g., methane/hydrogen jet flames) [2], and the differential diffusion effect between the two fuels are significant. Even though DME is a single fuel such that differential diffusion effect of fuel seems to be negligible, DME can be pyrolyzed at high temperatures through fuel nozzles and decomposed into smaller species such as CH_4 and H_2. In this sense, the decreasing H_L behavior of DME would be also related with the differential diffusion effect, but detailed reasons remain unclear [1]. Therefore, the main objective of the present study is to elucidate whether or not high diffusive nature of hydrogen, generated by fuel decomposition, causes the decreasing H_L behavior of the autoignited laminar lifted DME jet flamesa.

The present numerical simulations were performed in a two-dimensional axisymmetric coordinate in the radial, r-, and the axial, z-, directions using laminarSMOKE code [3,4]. The domain size is 6.65 cm × 50 cm in the r- and z- directions, respectively, which is identical to that of experiments [4]. The inner diameter of the fuel jet is 3.76 mm, and the fuel jet nozzle thickness is 0.5 mm. In the r-direction, 100 μm size mesh is uniformly distributed within 1.5 cm, and the stretched mesh is applied to the remaining area while the uniform 100 μm mesh size is used in the z direction. A schematic of the computational configuration for the present simulations is shown at Fig. 1. A skeletal 39-species of dimethyl ether/air kinetic mechanisms [6] is adopted for the present simulations. All the boundary conditions for the present simulations are summarized in Table 1.

Figure 2 shows the variation of liftoff height, H_L, as a function of U_0 together with the

Table1. Boundary conditions

Fuel jet velocity, U_0 [m/s]	1.5 ~ 8
Coflow velocity, U_{co} [m/s]	1.1
Temperature, T_0 [K]	980
Fuel mole fraction (X_F)	0.08
Residence length (L_{res}) [cm]	75

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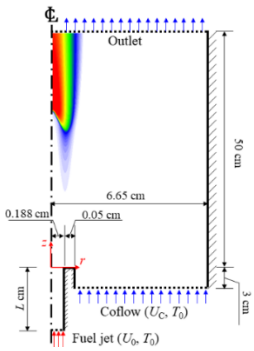

Figure 1. Schematic of the computational configuration for the present simulation.

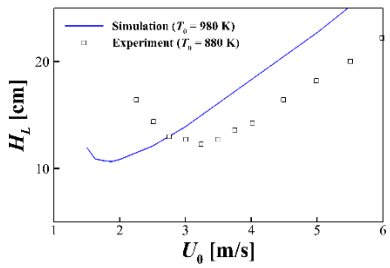

Figure 2. H_L for various U_0 about experimental and simulation results

experimental result. It is readily observed form Fig. 2 that H_L of the lifted flame exhibits a "U" shaped behavior with increasing U_0, which is qualitatively similar to the experimental result.

To identify the differential diffusion effect on H_L, additional numerical simulations are performed by changing the mass diffusivity of hydrogen and methane. Figure 3 shows the results of additional simulations. Note that the red line in Fig. 3 denotes the H_L variation for which the mass diffusivity of H_2, D_{H_2}, is equal to that of DME, D_{DME}; the blue line the H_L variation for which the mass diffusivity of both H_2 and CH_4, D_{CH_4}, are set to be equal to that of DME, respectively. Several points are to be noted from Fig. 3. First, H_L of two modified diffusivity results are nearly identical, which implies that the differential diffusion effect of methane is not significant to that of hydrogen. Second, it is readily observed from the figure that the modified D_{H_2} cases exhibit the monotonous increasing H_L behavior, which demonstrates that high D_{H_2} causes the U-shaped behavior. Therefore, it can be summarized that due to pyrolysis process through the fuel nozzle, relatively-large amount of H_2 is generated at relatively-lower U_0 condition, which ultimately affects unusual flame behavior

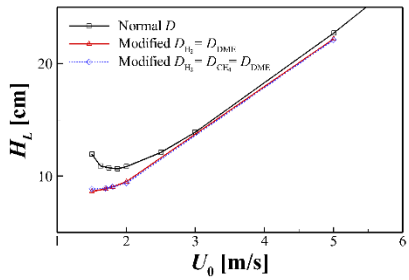

Figure 3. Variation of H_L for various U_0 with normal and modified H_2 diffusivity

Conclusion

In this study, the liftoff characteristics of a laminar dimethyl ether flame are elucidated using 2-D numerical simulations by systematically varying the fuel jet velocity. It is found from the simulation that the decreasing liftoff height region with increasing jet velocity exits, similar to the experimental results. 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. In order to better understand the effect of pyrolysis on the flame, the more detailed numerical simulations will be carried out as a future work.

Reference

[1] S.M. Al-Noman, S.H. Chung, Combust. Flame, 195 (2018) 75-83.
[2] K.S. Jung, S.O. Kim, T. Lu, S.H. Chung, B.J. Lee, C.S. Yoo, Combust. Flame 198 (2018) 305-319.
[3] A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi, Combust. Flame 160 (2013) 870-886.
[4] A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi, Energy. Fuel 27 (2013) 7730-7753.
[5] B.C. Choi, S.H. Chung, Combust. Flame 157 (2010) 2348-2356.
[6] A. Bhagatwala, Z. Luo, T.F. Lu, H. Shen, J.A. Sutton, J.H. Chen, Proc. Combsut. Inst. 35 (2015) 1157-1166.