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A Numerical Study of the Autoignited Laminar DME Lifted Jet Flames in Heated Coflow Air

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Abstract

The liftoff characteristics of autoignited laminar dimethyl ether (DME) jet flames in heated coflow air is numerically investigated with openFOAM-based laminar reacting flow solver, laminarSMOKE. According to a previous experimental study on autoignited laminar DME jet flame, decreasing liftoff height trend of the lifted jet flames is observed with the increase of fuel jet velocity at relatively-low jet velocities. To understand the unusual liftoff characteristics of the autoignited Lifted DME jet flames, various numerical simulations have been carried out. From additional simulations with modified mass diffusivity of hydrogen, it is found that the decreasing liftoff height behavior is mainly attributed to the high diffusive nature of hydrogen molecule, which is generated by the DME pyrolysis. The temperature profile along the streamline passing through the flamebase shows that actual autoignition delay time deviates from the 0-D ignition delay time trend due to the preferential diffusion effect of hydrogen molecule, leading to the decreasing H_L behavior.

1 Introduction

In the previous experimental study of autoignited laminar lifted dimethyl ether (DME) jet flames in heated coflow air, an unusual liftoff height behavior was observed: liftoff height, H_L, is inversely proportional to the fuel jet velocity, U_0 [1]. In general, the decreasing H_L behavior occurs only when two fuels are mixed in the fuel jet (e.g., CH_4/H_2 [2,3] or CO/H_2 [4] jet), and thus, the differential diffusion effect of the two fuels are significant. In this sense, the existence of hydrogen molecule in the fuel jet, which has a higher mass diffusivity than other molecules, typically leads to the decreasing H_L behavior.

DME is a single fuel such that its differential diffusion effect on the liftoff height may not be that important. However, DME can be pyrolyzed at high temperatures and decomposed into smaller species such as hydrogen and methane. Figure 1 shows the species mole fractions generated by the DME pyrolysis as a function of the residence time from 0-D simulations of DME/nitrogen mixture under initial temperature, T_0 = 980 K, and initial fuel mole fraction, $X_{F,0}$ = 0.08. It is readily observed from Fig. 1 that DME is converted into smaller species (e.g. H_2, CH_4, and CH_2O) as the residence time increases. Therefore, the decreasing H_L behavior of DME jet flames would be also related with the differential diffusion effect, but detailed reasons remain unclear. The main objective of the present study is to elucidate whether or not high diffusive nature of smaller species generated by fuel decomposition can cause the decreasing H_L behavior of the autoignited laminar lifted DME jet flames.

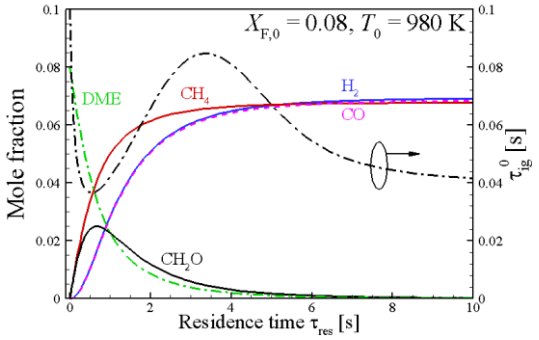

Figure 1. 0-D thermal decomposition of DME/nitrogen mixture under T_0 = 980 K and $X_{F,0}$ = 0.08.

2 Numerical Methods

The present numerical simulations are performed in a two-dimensional axisymmetric coordinate in the radial, *r*-, and the axial, *z*-, directions. We solve the steady compressible Navier-Stokes, species transport, and energy equations with laminarSMOKE code, which is an openFOAM based multi-dimensional laminar reacting flow solver with detailed kinetic mechanisms. For more information on laminarSMOKE, readers are referred to Refs. [5,6].

Figure 2 shows the schematic drawing of the computation domain for the present study. Note that the geometry and boundary conditions applied in the present simulation are identical to the experimental conditions [1]. The main domain size is 6.65 cm × 50 cm in *r* and *z* directions, respectively. To consider the pyrolysis process of DME in the fuel nozzle, 75 cm of fuel nozzle is added to the main domain. Inner diameter of fuel nozzle is 3.76 mm, with the 0.5 mm of nozzle thickness. In the *r*-direction, a uniform grid space of 50 μm is distributed for $0 \leq r \leq 1.5$ cm, and stretched grids spaces are applied for the remaining *r*-direction. In the z-direction, a uniform grid of 50 μm is arranged in the domain.

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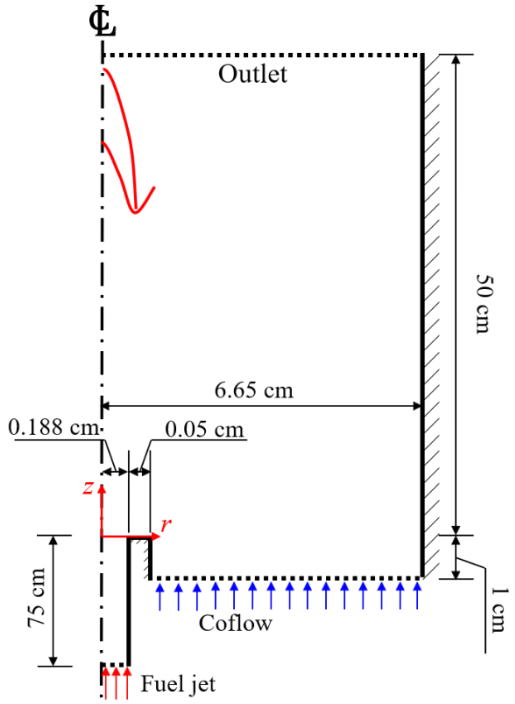

Figure 2. Schematic of the computational domain for simulations of autoignited laminar lifted DME jet flames in heated coflow air.

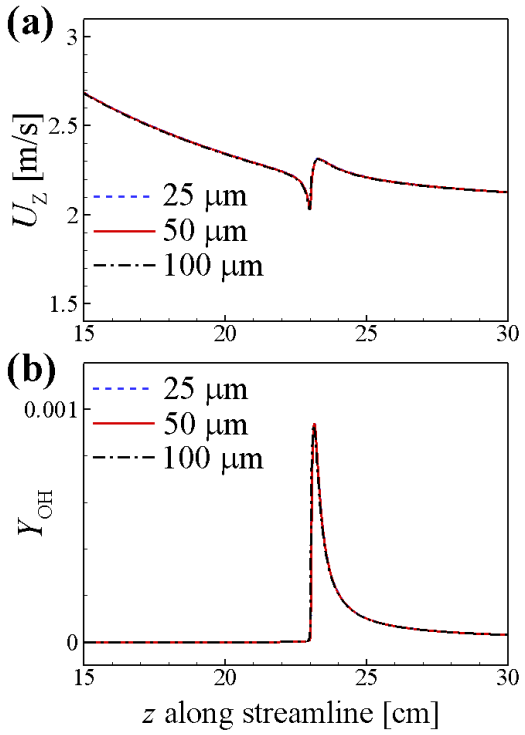

Figure 3. Profiles of (a) axial velocity and (b) mass fraction of OH of the autoignited laminar DME jet flames along the streamline passing through flamebase by varying the grid size from 100 μm (coarser) to 25 μm (finer).

From the fuel nozzle, highly diluted DME is injected from the fuel jet with $X_{F,0} = 0.08$, initial fuel temperature, $T_F = 300$ K, and various fuel jet inlet velocities. The flow velocity in the fuel jet increases as the flow is heated up from the fuel nozzle wall, where the wall temperature, T_w, is specified as 980 K. Fuel jet exit velocity, U_0, then becomes 1.4 ~ 6 m/s as a fully development flow. Air is provided from the coflow inlet with T_0 = 980 K. Pressure outlet boundary condition is atmospheric, and all the other boundary conditions are zero-gradient. Note that T_0 in the present simulation is 100 K higher than that of previous experiment to obtain the comparable H_L behavior. This temperature difference between experiment and numerical simulation has been also reported by previous numerical simulations [3,4,7], and they pointed out that the difference might come from the inaccuracy of the chemical kinetic mechanism, especially at low pressure conditions.

A grid convergence test is carried out for $U_0 = 5$ m/s case. Figure 3 shows profiles of axial velocity and mass fraction of OH of the autoignited laminar DME jet flames along the streamline passing through the flamebase by varying the grid size from 100 μm (coarser) to 25 μm (finer). As shown in Fig. 3, a grid convergence is achieved for the current grid size of 50 μm, which demonstrates that we can resolve the overall flame structures and stabilization mechanism with the 50 μm of grid size. Detailed kinetic mechanism with 53 species [8] is adopted for the present numerical calculations.

3 Overall characteristics of laminar DME flames under MILD combustion

In this section, we carry out a series of numerical simulations of autoignited laminar lifted DME jet flames under the moderate or intense low-oxygen dilution (MILD) combustion regime to understand the unusual decreasing liftoff height characteristics of the flames. As in the previous numerical simulations [3], we initialize the lifted flame by letting the flame to be autoignited (i.e., without applying ignition source). Then, we change U_0 from 1.4 to 6.0 m/s to effectively obtain the U-shape H_L behavior. To verify whether the lifted flames calculated from another steady solution can represent the autoignited lifted flames, we perform several transient numerical simulations of the DME lifted flame. The H_L of transient cases agree well with the corresponding steady solutions, which demonstrates that lifted flames in the present simulation can represent the autoignited lifted flame.

3.1 U-shaped H_L behavior

Figure 4 shows the isocontours of temperature and mass fraction of OH of the autoignited laminar lifted DME jet flames as a function of fuel jet velocity, U_0, under the MILD combustion regime (i.e., $T_0 = 980$ K and $X_{F,0} = 0.08$). As shown in Fig. 4, the U-shaped H_L behavior of autoignited DME jet flames is well captured in the present study. Although not shown in this paper, 0-D ignition delay time of the stoichiometric mixture based on the fuel and air at the inlet exits, $\tau_{ig,0}$, monotonously increases with the increase of U_0. Therefore, the U-shaped H_L behavior of the lifted flames cannot be explained by the conventional H_L correlation, $H_L \sim U_0\tau_{ig,0}^2$ [2].

In the MILD combustion regime, it is ambiguous to distinguish the flamebase with the conventional definition (i.e. certain percentages of maximum T or other flame marker) due to the low peak temperature, as shown in $U_0 = 1.4$ m/s case in Fig. 4. In this study, therefore, the flamebase is defined by the most upstream point of $\mathrm{Re}(\lambda_{exp}) = 0$ isoline, where λ_{exp} is an eigenvalue of the Jacobian of the chemical source term in the differential equations of a typical reacting flow. $\mathrm{Re}(\lambda_{exp})$ becomes greater/smaller than zero when the mixture is able to

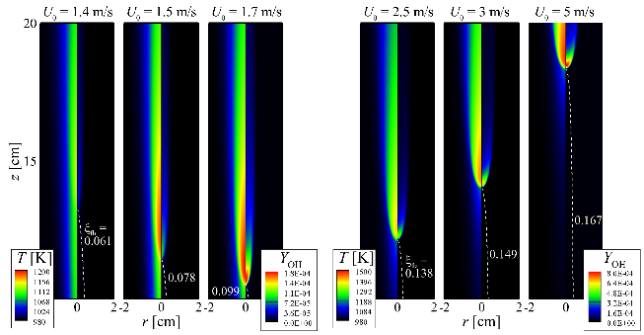

Figure 4. Isocontours of temperature (right) and mass fraction of OH (left) of autoignited lifted DME jet flames with T_0 = 980 K, $X_{F,0}$ = 0.08. White dashed line represents the mixture fraction isoline passing through the flamebase, ξ_{fb}.

ignite/fail to ignite (or already burnt), respectively. Thus, Re(λ_{exp}) = 0 can represent the crossover line between pre-ignition and post-ignition zone in the domain. Readers are referred to [9,10,11] for the more information on the chemical explosive mode analysis (CEMA).

To further analyze the U-shaped H_L behavior of the lifted flames, Fig. 5 shows the variation of H_L for various U_0 under the MILD combustion regime. In contrast to the relatively-high U_0 condition where $H_L \sim U_0$, $H_L \sim 1/U_0$ is observed at the relatively-low U_0 condition (i.e., $U_0 \leq$ 1.7 m/s). As shown in Fig. 5a, the U-shape behavior captured by present simulation is qualitatively similar to that of previous experimental results. Also note that maximum flame temperature decreases with the decrease of U_0 as shown in Fig. 5b, and the autoignited lifted flame is no longer to be observed when U_0 is lower than 1.4 m/s. It is also observed from Fig. 3 that mixture fraction isoline passing through the flamebase, ξ_{fb}, also increases with the increase of U_0, which implies that radial diffusion effect of fuel molecules becomes more significant as U_0 decreases.

3.2 Effect of hydrogen mass diffusivity on the lifted flames

As shown in Fig. 1, the amount of hydrogen molecule generated from pyrolysis of DME increases with the increase of τ_{res} (i.e., decrease of U_0). Therefore, the importance of differential diffusion of H_2 at the radial direction increases with the decrease of U_0, which would affect the decreasing H_L behavior of autoignited DME jet flame. To identify the preferential diffusion effect on H_L, additional numerical simulations are performed in this section by modifying the mass diffusivity of hydrogen, D_{H2}, to be equal to that of DME. Figure 6 shows the results of additional simulations. It is readily observed from Fig. 6 that the modified D_{H2} cases exhibit a monotonously-increasing H_L behavior, which demonstrates that high D_{H2} nature is directly related to the U-shape H_L behavior.

To further understand how high D_{H2} affect H_L, we divide the U-shaped H_L behavior of autoignited DME jet flame into decreasing H_L (i.e., relatively-low U_0) and increasing H_L (i.e., relatively-high U_0) regimes, and temperature profiles along the streamline passing through the flamebase for both regimes are compared in Fig. 7. Note that the temperature profiles are shown as a function of flow residence time, τ_{res}, to understand the two-dimensional autoignition process of lifted DME jet flames. As mentioned earlier, $\tau_{ig,0}$ increases with the increase of U_0, but the actual temperature increasing rate is consistent/inconsistent with the $\tau_{ig,0}$ variations for increasing/decreasing H_L regime: for increasing H_L regime (high U_0), temperature increasing rate becomes slower as U_0 increases, which is consistent with the $\tau_{ig,0}$

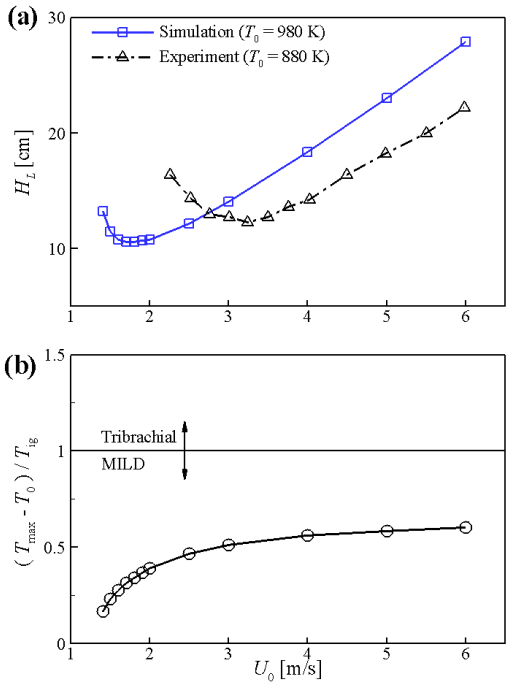

Figure 5. The variations of (a) H_L and (b) (T_{max} - T_0)/T_{ig} for various U_0 for autoignited laminar lifted DME jet flames with T_0 = 980 K, $X_{F,0}$ = 0.08.

variation. Therefore, it implies that the degree of pyrolysis in the fuel jet is relatively-low such that the differential diffusion effect of fuel is not that important on the H_L variation. It is verified by the marginal H_L difference between normal and modified D_{H2} conditions for relatively-high U_0 cases as shown in Fig. 6. For decreasing H_L regime (low U_0), on the other hand, the degree of pyrolysis in the fuel jet is relatively-high such that the differential diffusion effect of large diffusivity of hydrogen and low diffusivity of DME and methane can become significant, which lead to the decrease of actual autoignition process. Thus, the increasing H_L behavior with the decrease of U_0 is mainly attributed to the increase of actual ignition delay time caused by preferential diffusion effect of hydrogen molecule on the radial direction.

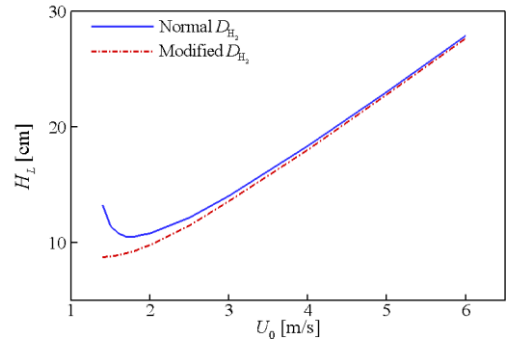

Figure 6. The variations of H_L for various fuel velocities with normal and modified H_2 diffusivity cases.

4 Conclusions

The characteristics of autoignited laminar lifted dimethyl ether jet flames in heated coflow air were numerically investigated

using the laminarSMOKE with a 53-species detailed chemical

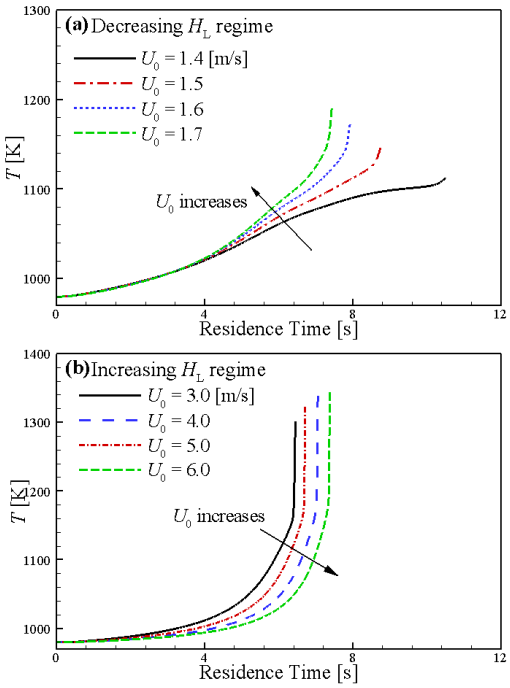

Figure 7. Temperature profile along the streamline passing through the flamebase as a function of residence time with (a) decreasing and (b) increasing H_L regime of autoignited DME jet flame.

mechanism of dimethyl ether oxidation. The detailed numerical simulations were performed for various fuel jet velocities, and the following results were obtained from the simulations.

1. From 0-D simulations, it is verified that CH_4 and H_2 are produced more from the pyrolysis of DME as the residence time increases.

2. The numerical simulations can qualitatively capture the U-shaped liftoff height behavior of the corresponding experiments.

3. To identify the effect of differential diffusion of hydrogen molecule, additional numerical simulations with modified D_{H2} were also carried out for the same conditions. Decreasing H_L regime is no longer to be observed in the modified D_{H2} condition.

4. It was verified that the high diffusive characteristics of the hydrogen is primarily attributed to the decreasing H_L behavior because it differentiates the actual autoignition process from $\tau_{ig,0}$ trend.

To clearly understand the pyrolysis effect on the stabilization mechanisms of the autoignited DME jet flame, further study such as flame speed analysis and transport budget analysis will be carried out.

5 Acknowledgment

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