A numerical study of the pyrolysis effect on autoignited laminar lifted dimethyl ether jet flames in heated coflow air

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Abstract

The liftoff, autoignition, and stabilization characteristics of autoignited laminar lifted dimethyl ether (DME) jet flames in heated coflow air are numerically investigated by varying the fuel jet velocity, U_0 . The detailed numerical simulations are performed using the laminarSMOKE code with a 55-species detailed kinetic mechanism of DME oxidation. An unusual U-shaped liftoff height, H_L , behavior under MILD combustion condition is observed from the simulations, which is qualitatively consistent with previous experimental results. From additional numerical simulations with modified mass diffusivity of hydrogen, it is verified that the decreasing H_L trend of the lifted flames under relatively-low U_0 conditions is mainly attributed to the fast diffusion of hydrogen generated from the DME pyrolysis. The species transport and displacement speed analyses verify that the differential diffusion effect renders the lifted flames to be leaner at the center of the jet, ultimately leading to the change of their stabilization mechanism from the autoignition to the autoignition-assisted flame propagation mode with increasing U_0 . The chemical explosive mode analysis (CEMA) identifies important variables and reactions contributing to the autoignition of the DME jet flames, through which the fast diffusion rates of small species are found to cause the deviation of 2-D autoignition characteristics from that of 0-D homogeneous ignition. The effects of DME pyrolysis on the characteristics of the autoignited laminar DME jet flames are further investigated by varying the fuel tube length, L_{res} . H_L shows a non-monotonic behavior with increasing L_{res} because the flame structure changes from a MILD combustion to a tribrachial edge flame and to an

attached flame while the stabilization mechanism also changes from the autoignition to the autoignition-assisted flame propagation mode as the degree of the DME pyrolysis increases.

Keywords: Dimethyl ether (DME), autoignited laminar lifted jet flame, flame stabilization, MILD combustion, CEMA

1. Introduction

Nonpremixed jet flames have received great attention during the past decades because they have been utilized in many practical combustors such as diesel engines, gas turbines, and boilers. When the fuel jet velocity is high enough at a relatively low temperature condition, nonpremixed jet flames are detached from the burner rim and stabilized in the form of lifted flames. However, real combustion devices generally operate under high pressures and temperatures at which autoignition inevitably affects the stabilization of lifted flames. Many studies have been performed to elucidate their stabilization and flame structure characteristics under autoignitive conditions for turbulent flames with various fuels [1–5].

Laminar lifted flames under autoignitive conditions have also been recently investigated because they can play a fundamental role in elucidating the liftoff and stabilization characteristics of corresponding turbulent lifted flames [6–15]. Under non-autoignitive conditions, a laminar lifted flame usually exhibits a tribrachial structure which consists of two rich/lean premixed flame branches and a trailing diffusion flame branch [16]. The intersection point of these three branches is called a tribrachial (or triple) point at which the lifted flame comes to be stabilized by the dynamic balance between the incoming flow speed and flame propagation speed [17]. However, the autoignited laminar lifted flames can be stabilized not only by flame propagation but also by autoignition. Chung and coworkers [6–9] investigated the characteristics of autoignited laminar lifted flames for various fuels, and they found that autoignited lifted jet flames can be stabilized without an external ignition source when the coflow temperature is above a critical value. In addition, they suggested that the

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liftoff height, H_L , of autoignited laminar lifted jet flames with tribrachial structure can be correlated to the fuel jet velocity, U_0 , and the 0-D homogenous ignition delay time of the stoichiometric fuel/air mixture based on the fuel tube exit condition, $\tau_{\text{ig,st}}$: i.e., $H_L \sim U_0 \tau_{\text{ig,st}}^2$. This relation is originally derived from thermal balance between heat release from autoignition and heat loss by diffusion in a jet mixing layer [6], which can be interpreted based on the balance between the autoignition time scale, $\tau_{\text{ig,st}}$, and the diffusion time scale of $\sqrt{H_L/U_0}$. Such correlation can predict the experimental H_L variations satisfactorily for single-component fuels, implying that 0-D homogeneous ignition delay plays a critical role in determining the liftoff height and stabilization of autoignited laminar lifted jet flames.

Among many fuels utilized for compression ignition engines, dimethyl ether (DME) has been highlighted as a clean high-efficiency fuel due to its low particulate/ NO_x emissions and high cetane number [18, 19]. DME can also be used as a fuel additive for enhancing engine performance as an ignition improver because of its low autoignition temperature compared to those of other hydrocarbon fuels [20]. To understand the fundamental characteristics of DME combustion, many experimental and numerical studies have been carried out [10, 12, 14, 15]. For instance, Krisman et al. [12] performed high-fidelity numerical simulations of laminar lifted DME jet flames in heated air. They found that autoignition can affect the flame structure varying from a tribrachial to a pentabrachial edge flame with increasing temperature. They also found that the lifted DME jet flames can be stabilized by either flame propagation, autoignition, or autoignition-assisted flame propagation mode. Deng et al. [14, 15] numerically investigated the characteristics of laminar DME jet flames under highly-autoignitive conditions. Based on the numerical results, they delineated stabilization mechanisms of the autoignited DME jet flames as functions of the fuel jet temperature and velocity.

Recently, Al-Noman et al. [10] experimentally investigated the liftoff characteristics of laminar jet flames of DME in heated coflow air. They found that autoignited lifted flames exhibit either tribrachial edge structure, or moderate or intense low-oxygen dilution (MILD) combustion with faint blue color depending on the degree of nitrogen dilution in the fuel stream. Unlike previous experimental results on liftoff height increasing monotonically with

the increase in U_0 for single component fuels [6–8], they observed an unusual ‘U’-shaped liftoff height behavior within the MILD combustion regime: H_L decreases with increasing U_0 for relatively-low U_0 conditions while H_L increases with increasing U_0 for relatively-high U_0 conditions. In fact, the decreasing H_L behavior with increasing U_0 has been observed for autoignited laminar lifted jet flames of binary mixture fuels such as methane/hydrogen [8, 11] and carbon monoxide/hydrogen fuels [21]. The differential diffusion effect of two fuel components is found to lead the decreasing H_L behavior [11]. Since DME can be easily pyrolyzed into small species such as methane, hydrogen, and formaldehyde at high temperature condition [22, 23], we may partially explain the U-shaped H_L behavior of the autoignited lifted DME jet flames by the differential diffusion effect of fuel components decomposed from DME. However, the detailed mechanism behind the U-shaped H_L behavior for the single component DME fuel has not been fully explored.

The objective of the present study is, therefore, to elucidate the liftoff characteristics of autoignited laminar lifted DME jet flames, especially the pyrolysis effect of DME on the unusual U-shaped H_L behavior. For this purpose, we perform two-dimensional numerical simulations with a detailed chemical kinetic mechanism of DME oxidation which includes its unimolecular thermal decomposition reactions. Note that the characteristic DME pyrolysis time is much shorter than those for typical hydrocarbon fuels [10]. Thus, DME in the fuel jet can be pyrolyzed into small species along the fuel tube before issuing from the fuel tube exit, and hence, the fuel composition at the fuel tube exit is not pure DME but includes many small species of which mole fractions vary depending on U_0 and the fuel tube length, L_{res} . Also note that in the present study, the DME fuel jet is highly diluted with nitrogen under autoignitive temperature condition such that its overall flame characteristics are quite different from those of typical non-autoignited lifted flames of which flamebase lies at the stoichiometric mixture fraction isoline. To better understand the liftoff height variation, the stabilization mechanisms of the autoignited laminar lifted DME jet flames are delineated by adopting the species transport budget and displacement speed analyses. The chemical explosive mode analysis (CEMA) is also conducted to figure out the effects of pyrolysis on the autoignition characteristics of the lifted flames. Finally, the effects of DME pyrolysis on

the liftoff and flame structure characteristics are further investigated by varying the degree of DME pyrolysis with extended fuel tube length.

2. Numerical methods

Detailed numerical simulations of laminar lifted DME jet flames in heated coflow air are performed on 2-D axisymmetric coordinates of the radial, r -, and the axial, z -, directions. The steady conservation equations of mass, momentum, species, and energy are solved using the laminarSMOKE code [24, 25], which is an open-source code based on OpenFOAM [26] for simulations of multi-dimensional compressible laminar reacting flows with skeletal/detailed chemical mechanisms. Details can be found in [24, 25]. To consider the Soret effect, thermal diffusion is included in the species transport equations. Figure 1 shows a schematic of the computational domain. The main domain size is $R_0 \times L_z = 6.65 \text{ cm} \times 50 \text{ cm}$ in the r - and z - directions, respectively. The inner radius of the fuel tube is 0.188 cm and its thickness is 0.05 cm. A 75 cm long fuel tube is attached to the domain, which protrudes 1 cm above the coflow air inlet. Note that the configuration of the present computational domain is identical to those of previous experimental studies [6–8, 10].

The DME jet diluted by nitrogen enters from the bottom of the fuel tube with the initial fuel mole fraction, $X_{F,0}$, of 0.08, the initial fuel temperature, T_F , of 300 K, and the uniform fuel inlet velocity, U_F . Since the temperature boundary condition for the fuel tube wall is set to $T_0 = 980 \text{ K}$, the fuel jet is heated to T_0 while passing through it and the mean velocity at the fuel tube exit, U_0 , attains the speed of $1.4 \sim 6 \text{ m/s}$. Normalized velocity profiles at the fuel tube exit for different U_0 are shown in the supplementary material, which demonstrates that the effect of DME pyrolysis on U_0 is minimal. The coflow air inlet velocity, U_C , is fixed to 1.1 m/s in accordance with the previous experiment [10], and the coflow air temperature is set to T_0 . Pressure outlet boundary condition is atmospheric, and zero-gradient boundary condition is applied for all the remaining boundaries. In the r - direction, $50 \mu\text{m}$ mesh size is uniformly distributed within 1.5 cm, and a stretched mesh is applied to the remaining area. A uniform $50 \mu\text{m}$ mesh size is used for the z - direction.

Figure 1: Schematic of the computational domain for simulations of autoignited laminar lifted DME jet flames in heated coflow air.

Figure 2: Profiles of (a) axial velocity, (b) temperature, mass fractions of (c) CH_2O and (d) OH for an autoignited laminar lifted DME jet flame along the streamline passing through the flamebase for three different grid resolutions for $X_{\text{F},0} = 0.08$, $T_0 = 980$ K, and $U_0 = 5$ m/s.

Figure 2 shows the profiles of axial velocity, temperature, mass fractions of CH_2O and OH for an autoignited laminar DME jet flame along the streamline passing through the flamebase for three different grid resolutions, which confirms that the grid resolution of 50 μm can reasonably resolve the profiles when compared to the fine grid resolution of 25 μm . Note that the thinnest flame thickness in the present study, defined by $\delta_f \equiv (T_{\text{max}} - T_{\text{min}})/\max(dT/dz)$, along the streamline passing through the flamebase is approximately 1.6 mm. Therefore, the present grid space of 50 μm can resolve the flame thickness with approximately 30 grids, which is fine enough to capture the flame structure and liftoff characteristics of the autoignited laminar lifted DME jet flames. We performed another grid convergence test for a tribrachial edge flame in Sec. 5, which verified that 50 μm grid space is also fine enough to resolve the structure of the tribrachial edge flame.

A detailed chemical kinetic mechanism of the DME oxidation with 55 species and 290 reactions is adopted for the present study [18]. Figure 3 shows the progress of 0-D DME

Figure 3: Variations of mole fractions of DME, CH_4 , H_2 , CH_2O , and CO as a function of the residence time, τ_{res} , from the 0-D pyrolysis of DME/nitrogen mixture with $T_0 = 980$ K and $X_{\text{F},0} = 0.08$. Dash-dot line represents the corresponding 0-D homogeneous ignition delay of the stoichiometric mixture, $\tau_{\text{ig,st}}$, at given τ_{res} .

pyrolysis in terms of the variations of important species mole fractions as a function of the residence time, τ_{res} . The initial conditions of the DME/nitrogen mixture are $T_0 = 980$ K and $X_{\text{F},0} = 0.08$, which are the same as those of the fuel jet at the fuel tube exit. The variation of the homogenous ignition delay of the stoichiometric mixture, $\tau_{\text{ig,st}}$, is also shown in the figure, where $\tau_{\text{ig,st}}$ is evaluated using the temporal mixture composition at given residence time and the initial temperature of 980 K. For 2-D cases, the fuel jet is readily heated to 980 K within $5 \sim 20$ cm from the tube inlet for $U_0 = 1.4 \sim 6$ m/s. Therefore, τ_{res} represents approximately the residence time of the fuel jet within the fuel tube, L_{res}/U_0 , while $\tau_{\text{ig,st}}$ denotes the influence of DME pyrolysis on the autoignition of the mixture. As shown in the figure, DME is readily decomposed into other small species as τ_{res} increases. It is also found that especially for small τ_{res} , $\tau_{\text{ig,st}}$ varies significantly and non-monotonically with increasing τ_{res} , which is primarily attributed to the amount of CH_2O generated from the DME pyrolysis. CH_2O has been found as an ignition improver at high temperatures [27, 28], and as such, we can expect that $\tau_{\text{ig,st}}$ is decreased with increasing CH_2O . Note that CH_2O varies non-monotonically with τ_{res} due to the formation of CO and H_2 [10]. This result implies that DME pyrolysis can significantly alter the ignition characteristics of the DME fuel jet flames, potentially leading to H_L variation. Note that the residence time for

the fuel jet passing through the fuel tube is $0.125 \sim 0.536$ s for $U_0 = 1.4 \sim 6$ m/s.

Identical to our previous numerical study of autoignited lifted methane/hydrogen jet flames [11], we first obtain a stationary autoignited laminar lifted DME jet flame of $X_{F,0} = 0.08$, $T_0 = 980$ K, and $U_0 = 5$ m/s without applying any external ignition source (i.e., literally autoignition). Then, we obtain steady solutions for other lifted flames at different U_0 by systematically adjusting U_0 from the first steady solution. To validate our procedure to obtain steady solutions for different autoignited lifted flames, we carried out several transient numerical simulations without applying external sources (now shown here). The results show that the liftoff and flame characteristics of stationary lifted flames obtained by transient simulations are identical to those of the corresponding steady solutions, which demonstrates that the lifted flames in the present simulations are indeed autoignited lifted flames.

3. Overall characteristics of autoignited flames

In this section, the unusual U-shaped H_L behavior [10] of autoignited laminar lifted DME jet flames in the MILD combustion regime is numerically investigated. Prior to examining the details of numerical results, we need to clarify several definitions, which will be used through the following sections. First, we determine that autoignition occurs within the computational domain if the homogeneous ignition delay of the stoichiometric mixture evaluated from the fuel mixture at the fuel jet exit is less than one-jet flow-through time of the coflow air, L_z/U_{co} , as in our previous study [11]. Thus, the autoignition temperature, T_{ig} , can be defined as the minimum temperature of which $\tau_{ig,st}$ is less than L_z/U_{co} . Since the components of the fuel mixture at the fuel tube exit can vary with U_0 by the change in the residence time along the fuel tube as shown in Fig. 3 due to the pyrolysis of DME, T_{ig} also changes for different U_0 .

Second, combustion process can be defined as MILD combustion when two conditions are satisfied [29, 30]; (1) the inlet temperature of a reactant mixture is greater than its autoignition temperature, $T_0 > T_{ig}$, and (2) the maximum allowable temperature increase with respect to the inlet temperature, $T_{max} - T_0$, is smaller than its autoignition temperature,

or $(T_{\max} - T_0) < T_{\text{ig}}$. In the present study, T_0 of 980 K is well above T_{ig} , and hence, $(T_{\max} - T_0)/T_{\text{ig}} \geq 1$ can be used as a criterion to determine whether an autoignited lifted DME jet flame exhibits the characteristics of the conventional tribrachial edge flame or the MILD combustion [6, 11, 29]: a lifted flame with tribrachial edge occurs when $(T_{\max} - T_0)/T_{\text{ig}} > 1$ while a lifted flame with MILD combustion appears when $(T_{\max} - T_0)/T_{\text{ig}} < 1$ is satisfied. Note that for the present simulations, we adopt T_0 of 980 K which is 100 K larger than that of the experiments [10]. This is because we can only capture the lifted flames within the computational domain by raising T_0 and make the numerical H_L comparable to that of experiments. This issue has been discussed from previous numerical studies of autoignited laminar lifted flames [9, 11, 21] and is presumably attributed to the inherent inaccuracy of chemical kinetic mechanisms at the atmospheric pressure and transport data. Note that chemical kinetic mechanisms are usually validated against laminar burning velocities at atmospheric and somewhat elevated pressures of $O(1)$ atm, and against ignition delays in shock tube experiments at high pressures of $O(10)$ atm. Therefore, we believe that the discrepancy is partly because of the limitation of ignition delay time that can be measured in shock tube experiments ($\sim O(10)$ ms). In addition, it can be aggravated by the inaccuracy of DME pyrolysis mechanisms reported in previous experimental studies [31, 32]. To figure out if this issue is related to a specific chemical kinetic mechanism, we compared several different mechanisms [18, 23, 33] by calculating the 0-D pyrolysis, ignition delay times, and extinction residence times of highly diluted DME mixtures (see the supplementary material). The results show that their overall pyrolysis process and ignition/extinction behaviors are qualitatively similar to each other, indicating that the discrepancy in the inlet temperature between the experiment and numerical simulations would still exist with different chemical kinetic mechanisms.

Third, for the lifted flames with MILD combustion, temperature and species mass fractions gradually change across the flame zone such that it may be ambiguous to precisely determine the flamebase location with conventional flame markers such as a certain value of temperature or OH mass fraction [3, 4]. For the present study, the flamebase is defined as the most upstream point of $\text{Re}(\lambda_{\text{exp}}) = 0$ isoline, where λ_{exp} is an eigenvalue of the Jacobian

of the chemical source term in the discretized governing equations for the CEMA [11, 34–37]. When a mixture exhibits positive $\text{Re}(\lambda_{\text{exp}})$, it is more likely to autoignite if there are no heat and radical losses. However, when a mixture shows negative $\text{Re}(\lambda_{\text{exp}})$, it is already burned or fails to autoignite. Therefore, $\text{Re}(\lambda_{\text{exp}}) = 0$ isoline represents the transition from the unburned to the burned mixture, and hence, it can be used as a marker for the flamebase [38].

3.1. *U-shaped H_L behavior*

Figure 4 shows the isocontours of temperature, T , and mass fractions of OH, H_2O_2 , CH_2O , CO, and H_2 of autoignited laminar lifted DME jet flames with MILD combustion for various fuel jet velocities with $T_0 = 980$ K and $X_{\text{F},0} = 0.08$. Note that the mixture fraction, ξ , is evaluated using the Bilger’s formula [39]. As in the previous experiments [10], the U-shaped H_L behavior of autoignited laminar lifted DME jet flames is successfully captured from the present simulations. Moreover, the autoignition process featured by the increase of temperature and the build-up of intermediate species such as H_2O_2 upstream of the flamebase is readily observed, which implies that autoignition may play an important role in stabilizing the lifted jet flames. It is of interest to note that the mass fractions of the major species generated from the DME pyrolysis (e.g., CH_2O , CO, and H_2) increase at the fuel tube exit with decreasing U_0 , which indicates the increase of the degree of DME pyrolysis within the fuel tube.

It is also readily observed that for high U_0 , the mass fraction of CH_2O first decreases immediately after issuing from the fuel tube exit and then, it starts to increase again, exhibiting its maximum value near the flamebase [10]. Meanwhile, the mass fractions of CO and H_2 increase rapidly right after the CH_2O increase. This is because CH_2O is an intermediate product of DME pyrolysis, while CH_4 , CO, and H_2 are its final products as shown in Fig. 3. These characteristics also indicate that the DME jet is continuously decomposed into the small species even within the burner, especially right upstream of the flamebase where the thermal ignition process occurs. However, the mass fraction of H_2 near the flamebase rapidly decreases with decreasing U_0 although the initial amount of H_2 at the fuel tube exit

Figure 4: Isocontours of (a) T (left half) and Y_{OH} (right half), (b) $Y_{H_2O_2}$ (left half) and Y_{CH_2O} (right half), and (c) Y_{CO} (left half) and Y_{H_2} (right half) for autoignited laminar lifted DME jet flames for various U_0 with $T_0 = 980$ K and $X_{F,0} = 0.08$. The dashed and dash-dot lines in (a) represent the mixture fraction isoline passing through the flamebase, ξ_{fb} , and the stoichiometric mixture fraction isoline, $\xi_{st} = 0.472$, respectively.

is much higher at low U_0 than that at high U_0 . This implies that small species generated by DME pyrolysis are more likely to diffuse out radially-outward with decreasing U_0 due to their fast diffusion rate.

To compare the numerical results with those of experiments from [10], Fig. 5 shows both H_L variations as a function of U_0 together with $(T_{\max} - T_0)/T_{\text{ig}}$ and $\tau_{\text{ig,st}}$. Here, H_L is defined as the axial length from the fuel tube exit to the flamebase. Several points are noted from the figure. First, although the present numerical simulations adopt T_0 larger than that of the experiments, they qualitatively reproduce the U-shaped H_L trend of the experiments: H_L increases with increasing U_0 under relatively-high U_0 conditions (i.e., $U_0 > 1.7$ m/s), H_L decreases with increasing U_0 under relatively-low U_0 conditions (i.e., $U_0 \leq 1.7$ m/s). As U_0 decreases further (i.e., $U_0 < 1.4$ m/s), the DME fuel jet fails to autoignite due to the increase of fuel and temperature diffusion toward the coflow air. Second, $(T_{\max} - T_0)/T_{\text{ig}}$ is found to be much lower than unity, which confirms that all the lifted flames satisfy the criteria selected to identify MILD combustion. Third, $\tau_{\text{ig,st}}$, which is evaluated from the fuel mixture at the fuel jet exit, increases with increasing U_0 such that the conventional H_L ($\sim Y_{\text{F},0} U_0 \tau_{\text{ig,st}}^2$) correlation [7] for autoignited laminar lifted flames can predict only a monotonic increase in H_L with increasing U_0 . Therefore, the decreasing H_L behavior under relatively-low U_0 conditions cannot be solely explained by the conventional H_L correlation even though the DME pyrolysis effect is already incorporated in $\tau_{\text{ig,st}}$.

3.2. Differential diffusion effect

Instead of the effect of DME pyrolysis, we conjecture that the fast diffusion rate of small species generated from the pyrolysis of DME may induce the U-shaped H_L behavior as demonstrated in our previous study on the binary fuel mixture of CH_4/H_2 [11]. This is because the slower the fuel jet is, the more small species such as H_2 is produced from the DME pyrolysis (see Fig. 3). Moreover, the differential diffusion effect becomes more prominent for relatively-low U_0 because the small species can have longer time to diffuse out from the fuel jet. Since the mass diffusivity of hydrogen, D_{H_2} , exhibits the largest value among the major species generated from the DME pyrolysis, additional simulations

Figure 5: Variations of (a) H_L and (b) $(T_{\max} - T_0)/T_{\text{ig}}$ and $\tau_{\text{ig,st}}$ as a function of U_0 for the autoignited laminar lifted DME jet with $T_0 = 980$ and $X_{F,0} = 0.08$.

are performed by setting D_{H_2} to that of DME, D_{DME} , to test the differential diffusion effect on H_L .

Figure 6 shows the isocontours of temperature and mass fractions of OH, H_2 , and H_2O_2 of autoignited laminar lifted DME jet flames with modified D_{H_2} under the same conditions as in Fig. 4: i.e., $T_0 = 980$ K and $X_{F,0} = 0.08$. It is readily observed from OH and H_2 isocontours that H_L increases monotonically with U_0 . Thus, the lifted flames do not exhibit the U-shaped H_L behavior any more, which verifies that the U-shaped H_L behavior of the DME jet flames is primarily attributed to the differential diffusion effect between the species generated from the DME pyrolysis through the fuel tube, especially to the fast diffusion rate of hydrogen.

To further identify the liftoff characteristics of both cases, Fig. 7 shows the variations of H_L and $(T_{\max} - T_0)/T_{\text{ig}}$ as a function of U_0 for the normal and modified D_{H_2} cases. Two points are noted from Fig. 7. First, it is readily observed that the difference of H_L between the two

Figure 6: Isocontours of (a) T (left half) and Y_{OH} (right half) and (b) $Y_{\text{H}_2\text{O}_2}$ (left half) and Y_{H_2} (right half) for autoignited laminar lifted DME jet flames with modified D_{H_2} for various U_0 with $T_0 = 980$ K and $X_{\text{F},0} = 0.08$. The dashed and dash-dot lines in (a) represent the mixture fraction isline passing through the flamebase, ξ_{fb} , and the stoichiometric mixture fraction isline, $\xi_{\text{st}} = 0.472$, respectively.

Figure 7: Variations of (a) H_L and (b) $(T_{\max} - T_0)/T_{ig}$ as a function of U_0 for the normal and modified D_{H_2} cases with $T_0 = 980$ K and $X_{F,0} = 0.08$.

cases becomes significant for relatively-small U_0 , while it becomes negligible for relatively-large U_0 . As mentioned above, the degree of DME pyrolysis and the resultant differential diffusion effect become significant for relatively-small U_0 , and hence, H_L show such large difference for relatively-small U_0 . Second, for relatively-small U_0 , $(T_{\max} - T_0)/T_{ig}$ also shows a large disparity, which becomes negligible for relatively-large U_0 . For the modified D_{H_2} case, the radially-outward diffusion of H_2 from the center of the fuel jet, which is originally generated from the DME pyrolysis, is significantly suppressed due to small modified D_{H_2} (see Fig. 6b), and consequently, the mixture fraction at the flamebase, ξ_{fb} , exhibits slightly larger value than that of the corresponding normal D_{H_2} case (see Figs. 4 and 7), which leads to the increase of $T_{\max}$ for the modified D_{H_2} case.

It is also of importance to note that even if other high-hydrocarbon fuels such as *n*-heptane and *iso*-octane can be decomposed under high temperature conditions, they would not exhibit a U-shaped H_L behavior under MILD combustion condition as in [40, 41]. We

performed 0-D simulation of n -heptane pyrolysis at T_0 and $X_{F,0}$ (not shown here), which revealed that the overall pyrolysis process of DME is much faster than that of n -heptane. Furthermore, the main products of DME pyrolysis are small species such as CH_4 , CO , and H_2 , while n -heptane pyrolysis produces relatively-large species such as C_2H_4 . This result implies that much higher T_0 is required to amplify the pyrolysis effect of n -heptane; however, autoignited laminar lifted n -heptane jet flames would not exhibit under such high temperature because they might be attached to the jet nozzle. We believe that the differential diffusion effect induced by DME pyrolysis is the primary reason for the U-shaped H_L behavior which is, therefore, a unique feature of autoignited lifted DME jet flames under MILD combustion condition.

4. Flame stabilization and autoignition characteristics

In the previous section, we investigated the U-shaped H_L behavior of autoignited DME lifted jet flames and found that the fast diffusion rate of hydrogen generated from the DME pyrolysis mainly attributes to such H_L behavior. In this section, we elucidate the flame stabilization mechanisms of autoignited laminar lifted jet flames for the decreasing/increasing H_L regimes by adopting the species transport budget, flame speed, and chemical explosive mode analyses.

4.1. Stabilization mechanisms

The species transport budget analysis has been widely adopted to elucidate the stabilization mechanisms of autoignited lifted jet flames [11, 12, 42, 43]. In a steady state, the convection ($\mathbf{C}$), diffusion ($\mathbf{D}$), and reaction ($\mathbf{R}$) terms of a species equation balance one another. Instead of $\mathbf{D}$ itself, we use its decomposed components such as parallel $\mathbf{D}_s$ and perpendicular $\mathbf{D}_t$ to the streamline to identify flame back diffusion by $\mathbf{D}_s$ and transverse stratification by $\mathbf{D}_t$. Note that in the reaction zone of a typical premixed flame, $\mathbf{D}_s$ and $\mathbf{R}$ terms balance each other while $\mathbf{C}$ is negligibly small. In an inhomogeneous autoignition process, however, $\mathbf{C}$ and $\mathbf{R}$ terms balance each other with negligible $\mathbf{D}_s$ [12]. In some cases including autoignited jet flames stabilized by “autoignition-assisted flame propagation”, $\mathbf{C}$,

Figure 8: Profiles of convection (**C**), flame back diffusion (**D_s**), and chemical reaction (**R**) terms along the streamline passing through the flamebase for (a) the decreasing H_L , and (b) the increasing H_L regimes.

D_s, and **R** terms can balance one another. For such an autoignited lifted jet flame, its lift-off height is determined by the balance between the flame propagation speed and the local flow velocity at the flamebase while the flame propagation speed is enhanced by thermal ignition process upstream of the flamebase [11–13, 44, 45].

Figure 8 shows the profiles of **C**, **D_s**, and **R** along the streamline passing through the flamebase for the decreasing and increasing H_L regimes. In the present study, we adopt hydroxyl radical (OH) for the transport budget analysis because it is one of the representative flame markers in hydrocarbon fuel jet flames. In addition, we normalize the budget terms by the maximum absolute value of **R** for each U_0 case to qualitatively compare the flame characteristics with U_0 .

For the increasing H_L regime ($3 \leq U_0 \leq 6$ m/s) in Fig. 8b, **C-D_s-R** balance is achieved at the flamebase, which implies that the autoignited lifted jet flames within this regime are stabilized by the autoignition-assisted flame propagation mode. Although **C/D_s** slightly

increases/decreases with increasing U_0 , the overall flame structure such as the flame thickness and the contribution of each term to the species equation is nearly identical to each other regardless of U_0 .

For the decreasing H_L regime ($1.4 \leq U_0 \leq 1.7$ m/s) in Fig. 8a, however, the species transport budgets exhibit distinct features compared to those of the increasing H_L regime. First, the relative importance of $\mathbf{D}_s$ in the species equation significantly decreases with decreasing U_0 , and ultimately $\mathbf{D}_s$ nearly vanishes for $U_0 = 1.4$ m/s case. Therefore, **C-R** balance becomes predominant for the decreasing H_L regime. Second, the flame thickness significantly increases with decreasing U_0 . These results demonstrate that the stabilization mechanism for the decreasing H_L regime gradually changes to the autoignition mode as U_0 decreases. It is of interest to note that in our previous study [11], the decreasing H_L behavior of autoignited laminar lifted methane/hydrogen jet flames occurs due to the flame mode change from the MILD combustion to the tribrachial edge flame by the fast diffusion rate of hydrogen. In the present study, however, the decreasing H_L behavior occurs for autoignited lifted jet flames with MILD combustion only, of which stabilization mechanism seems to change from autoignition to autoignition-assisted flame propagation mode with increasing U_0 .

To further identify the stabilization mechanisms of the lifted jet flames, we perform the displacement speed analysis by evaluating the ratio of the propagation speed of autoignited lifted DME jet flames, S_e , to the corresponding reference flame speed, S_R [13]. Since S_R is the flame propagation speed of a 1-D unstrained laminar premixed flame, S_e would be comparable to the corresponding S_R when the lifted flames are stabilized by the flame propagation mode. On the other hand, S_e would be much faster than S_R if the lifted flames are mainly stabilized by autoignition [11, 46]. To estimate S_e and S_R , we adopt the density-weight displacement speed, S_d^* , which is defined by [47–49],

$$S_d^* = \frac{1}{\rho_u |\nabla Y_k|} (\omega_k - \frac{\partial}{\partial x_j} (\rho Y_k V_{k,j})), \quad (1)$$

where Y_k is the mass fraction, $V_{k,j}$ the diffusion velocity in the j -direction, ω_k the net production rate of species k , and ρ_u is the density of the unburnt mixture. S_d^* has been widely used to estimate the propagation speeds of reaction fronts [3, 4, 42, 50–52]. Here, we adopt OH for the evaluation of S_d^* . Note that S_d^* represents the relative displacement speed of the isocontours such that we can estimate S_e by evaluating S_d^* at the flamebase of the lifted flames.

In the present study, S_R upstream of the flamebase is estimated from 1-D transient reactive simulations as in [11, 42, 51, 53]. Since the autoignition process is underway upstream of the flamebase, it is not straightforward to determine the initial mixture conditions for the 1-D S_R calculations. By observing that the flamebase for each case usually lies in the middle of the flame thickness, we specified them as the mixture conditions at a half flame thickness, $\delta_f/2$, upstream of the flamebase along the streamline passing through the flamebase. The simulations started with a high-temperature ignition source in the middle of the 1-D domain, and consequently, two combustion waves developed from the ignition source propagate into the initial reactive mixture ahead of them. The mixture upstream of the combustion waves is reactive but it would not autoignite till τ_{ig}^0 . Therefore, the propagation speed of the combustion wave, S_d^* , can be regarded as the laminar burning velocity, S_R , similar to that in the diffusive limit in previous studies [42, 51, 53]. The obtained S_R is then compared to the S_e of the corresponding lifted flames. Note that only major species upstream of the flamebase such as DME, CH₄, H₂O, etc. are taken into account in the initial mixture conditions of S_R calculations to prevent any occurrence of autoignition during the early stage of the simulations. We also examine how much S_R varies within the flame thickness by varying its evaluation location from $(\delta_f/2) \times 0.8$ to $(\delta_f/2) \times 1.2$ upstream of the flamebase (see supplementary material). The result demonstrates that S_R does not change much with the location for its evaluation.

Figure 9 shows the variations of S_R and S_e/S_R for the decreasing and increasing H_L regimes. It is readily observed from the figure that S_e/S_R exhibits nearly unity for the increasing H_L regime, demonstrating that the autoignited lifted flames within this regime are stabilized by the flame propagation mode. However, it is of importance to note that

Figure 9: Variations of S_e/S_R (blue) and S_R (red) at $\delta_f/2$ upstream of the flamebase along the streamline passing through the flamebase for various U_0 cases.

autoignition also plays a major role in stabilizing the flames even for these cases because the thermal ignition of the DME jet is in progress upstream of the flamebase, leading to temperature increase upstream of the flamebase. Figure 10 shows the temperature profiles at the upstream of the flamebase along the streamline passing through the flamebase, which shows that temperature increases from T_0 ($=980$ K) at the upstream of the flamebase. Consequently, S_e is considerably enhanced by the temperature increase compared to that of the non-autoignited flames, and the lifted flames can be stabilized by the kinematic balance between the local flow velocity and the propagation speed of the flamebase, which is called by “autoignition-assisted flame propagation” [13, 54].

For the decreasing H_L regime with U_0 , however, S_e/S_R is above unity and decreases with increasing U_0 , which indicates that the effect of autoignition on the flame stabilization becomes more significant for lower U_0 . In this regime, relatively-small species such as H_2 generated from the DME pyrolysis have more time to radially diffuse out from the flame region with decreasing U_0 , which renders the mixture at the flamebase to be leaner with decreasing U_0 . As a result, local temperature upstream of the flamebase decreases with decreasing U_0 as shown in Fig. 10a. Consequently, S_R also decreases significantly with decreasing U_0 as shown in Fig. 9. To overcome the upcoming local flow velocity, the autoignited lifted flames become more dependent on the ignition front speed, $S_{ig} \sim 1/|\nabla\tau_{ig}|$, which is much faster

Figure 10: The profiles of temperature along the streamline passing through the flamebase for (a) the decreasing H_L regime and (b) the increasing H_L regime.

than S_R near the ignition kernels [46]. These results demonstrate that the stabilization mechanism of the autoignited lifted DME jet flames changes from the autoignition to the autoignition-assisted flame propagation mode for the decreasing H_L regime due to the fast diffusion of hydrogen produced from the DME pyrolysis, which is consistent with the result of the transport budget analysis.

As mentioned previously, the decreasing H_L behavior for CH_4/H_2 mixture flames occurs by the stabilization mechanism changes from the autoignition to the autoignition-assisted flame propagation mode, along with the flame regime change from the MILD combustion to the tribrachial edge flame regime [11]. In the present DME flames, the decreasing H_L behavior can be explained by the stabilization mechanism change from autoignition to autoignition-assisted flame propagation mode in only the MILD combustion regime. These results imply that the decreasing H_L behavior can occur by the transition of the stabilization mechanism from the autoignition to the autoignition-assisted flame propagation mode regardless of the flame regime change.

Figure 11: Schematic for the stabilization of autoignited laminar DME lifted flames with (a) decreasing H_L and (b) increasing H_L regimes.

To illustrate how the autoignited lifted flames are stabilized with U_0 and H_L is accordingly determined, a schematic of the H_L variation depending on the flow regimes is shown in Fig. 11. The axial velocity, U , increases with increasing U_0 , while the overall profile along the streamline passing through the flamebase is found to be different depending on the decreasing/increasing H_L regimes. Since the autoignited laminar lifted flames are mainly stabilized by either the autoignition-assisted flame propagation or the autoignition mode, the propagation speed of the leading edge of the lifted flame, S_e , features the reference laminar flame speed enhanced by ongoing temperature increase (S_R) for the former, or the spontaneous ignition front speed (S_{ig}) for the latter [46]. Therefore, the lifted flame can be stabilized where S_e balances U as illustrated in Fig. 11.

For the increasing H_L regime where the DME pyrolysis and resultant differential diffusion

effects are negligible, the overall autoignition characteristics do not change much with U_0 , and hence, the local temperature, T , and resultant S_e are just spatially elongated with increasing U_0 as shown in Figs. 10b and 11b. As such, once U_0 increases, the lifted flame is stabilized further downstream than that with low U_0 as illustrated in Fig. 11b. In addition, the stabilization mechanism for the increasing H_L regime, or the conventional autoignited lifted flames with single fuel component, slowly changes from the autoignition-assisted flame propagation to the autoignition mode with the increase in U_0 as illustrated in Fig. 8b.

For the decreasing H_L regime where the pyrolysis of DME and resultant differential diffusion effect are significant, the overall temperature profile and resultant S_e of relatively-high U_0 move towards upstream compared to those of low U_0 due to spatially-enhanced ignition process as shown in Fig. 10a. This is because the radial diffusion of small species is more suppressed for high U_0 , leading to the increase in ξ and T at the flamebase. As such, the lifted flame with high U_0 is stabilized further upstream than that with low U_0 as described in Fig. 11a. It is also interest to note that the flame temperature, T_f , notably increases with increasing U_0 , and thus, the corresponding S_R profile also dramatically changes. In this sense, the stabilization mechanism of the lifted flames with large differential diffusion effect is more sensitive to the U_0 variations as shown in Fig. 8a.

4.2. Ignition characteristics based on CEMA

To further understand how the fast diffusion rates of small species control the ignition characteristics of the autoignited lifted DME jet flames, we carry out the CEMA that has been widely adopted for many combustion problems including laminar/turbulent jet flames [4, 11, 14, 15, 34, 35, 55, 56] and various types of homogenous charge compression ignition (HCCI) combustion [36, 37, 57–61]. The CEMA is based on the Jacobian of the local chemical source term, $\mathbf{J}_\omega$, in the discretized conservation equations for a reacting flow. As mentioned earlier, the eigenvalue, λ_e , can be defined by the eigenmode of the Jacobian as $\lambda_e = \mathbf{b}_e \cdot \mathbf{J}_\omega \cdot \mathbf{a}_e$, where $\mathbf{a}_e$ and $\mathbf{b}_e$ are the pair of the left and right eigenvectors, respectively. A chemical explosive mode (CEM) is a chemical mode for which the real part of λ_e is positive, and hence, the local mixture is expected to autoignite unless there exist thermal and radical

losses.

The normalized contributions of each variable and each reaction to a CEM are measured by evaluating the explosive index, **EI**, and the participation index, **PI**, which are defined by [35–37]:

$$\mathbf{EI} = \frac{|\mathbf{a}_e \otimes \mathbf{b}_e^T|}{\sum |\mathbf{a}_e \otimes \mathbf{b}_e^T|}, \quad (2)$$

$$\mathbf{PI} = \frac{|(\mathbf{b}_e \cdot \mathbf{S}) \otimes \mathbf{R}|}{\sum |(\mathbf{b}_e \cdot \mathbf{S}) \otimes \mathbf{R}|}, \quad (3)$$

where **S** and **R** represent the stoichiometric coefficient matrix and the net reaction rate vector, respectively. The symbol $\otimes$ denotes the element-wise multiplication of two vectors. Thus, the key variables and reactions contributing to the ignition can be identified by evaluating **EI** and **PI**. We perform the CEMA for cases with $U_0 = 1.5$ and 5.0 m/s where the differential diffusion effect is significant and marginal to the autoignition, respectively. For comparison purposes, we also carry out the CEMA of the 0-D homogeneous ignition of the fuel/air mixture at the fuel jet exit for both cases, and as such, we can identify different ignition characteristics of the 0-D homogeneous reactor and the 2-D axisymmetric flame; the former does not include any mass transport while the latter takes into account different mass diffusion rates for each species.

Figure 12 shows the EI of important variables including temperature for the 0-D ignition of DME/air mixtures and 2-D cases along the streamline passing through the flamebase. For 2-D simulation cases, we estimate τ_{res} by numerically integrating $\Delta s/U$ along the streamline passing through the flamebase. Note that we separate the ignition process into two stage: the “preheated stage” and the “thermal ignition stage”. The former/latter represents a stage when the EI of temperature is smaller/larger than those of species.

Several points are noted from Figs. 12a and b. For the 0-D case with $U_0 = 1.5$ m/s where the initial DME is highly decomposed into other species, the duration of the preheated stage is approximately two times shorter than that for the 0-D case with $U_0 = 5$ m/s where the

decomposition of the initial DME is negligible. However, the durations of the thermal ignition stage for two cases are nearly identical. This trend remains the same for different equivalence ratios (see the supplementary material). This implies that the main role of the degree of initial DME pyrolysis on the ignition is to reduce the preheated stage and advance the start of thermal ignition stage. Also note that the contribution of H_2O_2 to the CEM is the greatest among the species during the preheated stage, indicating that H_2O_2 plays a key role in this stage [62].

As shown in Figs. 12c and d, the duration of the preheated stage for the 2-D case with $U_0 = 1.5$ m/s is approximately two times shorter than that for $U_0 = 5.0$ m/s case, which is consistent with the 0-D results. However, the duration of the thermal ignition stage for the 2-D case with $U_0 = 1.5$ m/s is much longer than that for 2-D case with $U_0 = 5.0$ m/s as well as that for 0-D case with $U_0 = 1.5$ m/s, implying that the differential diffusion effect extends the duration of the thermal ignition stage of the 2-D case with $U_0 = 1.5$ m/s. Moreover, the overall ϕ profile along the streamline for $U_0 = 1.5$ m/s case is much lower than that for $U_0 = 5.0$ m/s case in the thermal ignition stage. This result substantiates that for 2-D case with $U_0 = 1.5$ m/s, the increasing differential diffusion effect renders the mixture to be leaner, which eventually retards the autoignition process in the 2-D jet flames.

To further elucidate the contribution of each elementary reaction to the CEM of autoignited DME jet flames, the participation index (PI) of important reactions for the autoignition of DME flames for the same 0-D and 2-D cases are shown in Fig. 13. From the 0-D ignition cases in Figs. 13a and b, we can identify the fundamental reaction pathways of the DME flames: the thermal decomposition of DME (R239–247) (R is the reaction number in [18]), the conversion of CH_2O to H_2O_2 through $\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{HCO} + \text{H}_2\text{O}_2$ (R46), the conversion of CH_3 to CH_3O to CH_2O (R48–51, R71, R73–77), the chain branching of H_2O_2 through $\text{H}_2\text{O}_2 \rightarrow \text{OH} + \text{OH}$ (R20), the chain branching of H_2 through $\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$ (R1), and the HO_2 formation through $\text{H} + \text{O}_2 \rightarrow \text{HO}_2$ (R13), and the final CO to CO_2 conversion step (R29; not shown here) are sequentially and/or simultaneously observed

Figure 12: EI of important species and temperature for (top) 0-D homogeneous ignition of DME flames, and (bottom) autoignited laminar lifted DME jet flames along the streamline passing through the flame base. U_0 = (left) 1.5 and (right) 5.0 m/s cases are selected to the analysis.

[23, 63, 64].

During the preheated stage, the relative contributions of R46 and R20 to CEM increase as DME is more decomposed (i.e., $U_0 = 1.5$ m/s case). Therefore, the amount of CH_2O produced by the initial DME pyrolysis plays an important role in generating H_2O_2 through R46, consequently leading to the thermal ignition by activating R20 that is one of the intermediate radical growth reactions in hydrocarbon oxidation. Since the mass diffusivities of CH_2O and H_2O_2 are relatively small, the overall ignition behavior for 2-D cases at the preheated stage does not change much, thereby following the 0-D homogeneous ignition trend during the preheated stage.

During the thermal ignition stage, T increases through R20 up to approximately 1050 K for 0-D cases (red vertical line in Figs. 13a and b), and then, the relative importance of R20 becomes decreasing, while the chain branching step of hydrogen (R1) start to contribute the most to the CEM [65] regardless of the initial ϕ (see supplementary materials). In addition, the contribution of HO_2 formation step (R13) on the autoignition of DME is marginal for

Figure 13: PI of various reactions for (top) 0-D homogeneous ignition of DME flames, and (bottom) autoignited laminar lifted DME jet flames along the streamline passing through the flame base. $U_0 =$ (left) 1.5 and (right) 5.0 m/s cases are selected to the analysis. Red vertical line represents the time when T reaches to 1050 K.

the relatively-high ϕ , but R13 becomes important to the CEM when ϕ is 0.2 or lower as shown in the supplementary materials. This is because the rate of temperature increase is relatively low at lean conditions such that R1, an endothermic reaction, is not favored while R13, an exothermic step competitive to R1, starts to participate in the autoignition [66].

During the thermal-ignition stage for 2-D cases in Figs. 13c and d, it is readily observed that the autoignition process after $T > 1050$ K is significantly delayed for case with $U_0 = 1.5$ m/s, compared to the 0-D cases as well as the 2-D case with $U_0 = 5.0$ m/s. It is of interest to note that the contribution of R13 to the CEM for case with $U_0 = 1.5$ m/s is much larger than that for case with $U_0 = 5$ m/s. As mentioned above, this is attributed to the differential diffusion effect for case with $U_0 = 1.5$ m/s; the small species generated from the pyrolysis can diffuse out more from the flame zone for the low U_0 case than the high U_0 case. Then, the overall ϕ profile along the streamline decreases more significantly for the low U_0 case, and consequently, the autoignition process driven by high temperature chemistry such as R1 is not that explosive, which significantly delays the thermal ignition process compared to that for high U_0 case. These results demonstrate that the variation of ϕ and resultant autoignition characteristics are very sensitive to U_0 for the decreasing H_L regime. For the increasing H_L regime, however, the differential diffusion effect on the overall ignition characteristics is not significant, and thus, they do not change much with U_0 . Therefore, H_L increases with increasing U_0 .

5. Flame regime change by pyrolysis

In the previous sections, we investigated the effects of the DME pyrolysis on the autoignited lifted flames. However, the degree of DME pyrolysis in the fuel tube is limited by the fuel tube length, L_{res} , of 0.75 m. As shown in Fig. 3, the 0-D pyrolysis of the DME/nitrogen mixture does not reach its equilibrium even after 6 s. Therefore, to figure out how much the degree of DME pyrolysis affects the liftoff characteristics of autoignited DME jet flames, we first simulate numerically three additional cases with different L_{res} of 0, 3.0 m, and ∞ by varying the fuel jet velocity. $L_{\text{res}} = 0$ case represents a DME jet without pyrolysis such that mixture composition at the fuel tube exit is set to pure DME diluted

with nitrogen. In addition, the fully developed flow boundary condition is applied at the fuel tube exit and the temperature of fuel tube exit is specified to T_0 of 980 K. $L_{\text{res}} = \infty$ case denotes a fully-pyrolyzed DME fuel jet of which composition is obtained from the 0-D numerical simulation of DME pyrolysis as in Fig. 3. Note that the computational domain and boundary conditions of $L_{\text{res}} = \infty$ case are identical to those of $L_{\text{res}} = 0$ case except for the fuel composition at the fuel tube exit.

Figure 14 shows the H_L variations of autoignited DME jet flames as a function of the fuel jet velocity at the inlet of the fuel tube, U_F , for various L_{res} . Since U_0 increases with L_{res} due to the decrease of fuel mixture density by the DME pyrolysis, H_L variations are shown as a function of U_F for fair comparison. Several points are noted. First, for case with $L_{\text{res}} = 0$, H_L increases monotonically with increasing U_F . Even if a certain degree of pyrolysis of the DME jet occurs along the jet within the burner, it is not high enough to induce a U-shaped H_L behavior. Second, for case with $L_{\text{res}} = 3.0$ m, the degree of DME pyrolysis and the resultant differential diffusion effect become more significant than those of the cases with $L_{\text{res}} = 0$ and 0.75 m, thereby leading to a more distinct U-shaped H_L behavior.

It is of interest to note that any attached flames are not observed for the cases with $L_{\text{res}} = 0$, 0.75, and 3.0 m. This is opposite to the behavior of conventional non-autoignited jet flames [16, 17] or 1-D premixed flames [13] that become attached to the fuel jet nozzle at low jet velocities. Since lifted flames with MILD combustion are located further downstream of the stoichiometric mixture fraction isoline, the overall diffusion timescale of fuel in the radial direction can be longer than that of conventional non-autoignited lifted flames for which the flamebase lies at the stoichiometric mixture fraction isoline. Therefore, as the fuel jet velocity decreases, small species can have longer time to diffuse out from the reaction zone of the lifted flame, which makes it weaker and even fail to autoignite.

Third, for the case with $L_{\text{res}} = \infty$ where the degree of DME pyrolysis is maximized, a lifted flame becomes attached to the fuel tube exit when U_F becomes larger than approximately 0.6 m/s. As shown in Fig. 3, we can expect that the overall characteristics of autoignited DME jet flames change from those of DME jet to those of $\text{CH}_4/\text{H}_2/\text{CO}$ jet as the degree of DME pyrolysis increases with increasing τ_{res} or L_{res} . This fuel transition may

Figure 14: Variations of H_L as a function of U_F for the $L_{res} = 0, 0.75, 3$, and ∞ m cases with $T_0 = 980$ K and $X_{F,0} = 0.08$.

significantly change its flame structure and liftoff characteristics. Note that the attached flame for $L_{res} = \infty$ is not lifted off by high U_F as far as the fuel jet is laminar.

To further identify the pyrolysis effect on the flame structure and liftoff characteristics, we vary L_{res} from 0 to 23 m for $U_F = 1.53$ m/s this time. Figure 15 shows the isocontours of temperature and mass fractions of OH, HO₂, and H₂O₂ of autoignited laminar lifted DME jet flames for various fuel tube lengths at $T_0 = 980$ K, $X_{F,0} = 0.08$, and $U_F = 1.53$ m/s. For these cases, the mean fuel jet velocity at the fuel tube exit, U_0 , is found to vary from 5 to 6.3 m/s with increasing L_{res} , which is inevitable due to the DME pyrolysis (see supplementary material). Nonetheless, we believe that the characteristics of autoignited jet flames with different L_{res} are mainly affected by the fuel composition variation due to the DME pyrolysis rather than by U_0 change. This is because the liftoff height of the lifted flame keeps decreasing with increasing L_{res} when $L_{res} > 8$ m and then, it becomes even attached to the burner in spite of relatively-large U_0 at large L_{res} due to the DME pyrolysis.

It is readily observed from Fig. 15 that H_L shows a non-monotonic behavior with increasing L_{res} while the flame structure changes from the lifted flame with MILD combustion to the lifted flame with tribrachial edge to the attached flame [11]. The degree of DME pyrolysis is increased with increasing L_{res} while passing through the fuel tube, and consequently, approximately 16% and 93% amounts of the initial DME are decomposed into small species for cases with $L_{res} = 0.75$ and 14 m, respectively. In addition, the amount

of CH_2O generated from the pyrolysis is found to be maximized at $L_{\text{res}} = 5$ m as can be expected from Fig. 3. Since the conversion of CH_2O to H_2O_2 through $\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{HCO} + \text{H}_2\text{O}_2$ (R46) occurs right after CH_2O generation, we can observe more H_2O_2 upstream of the flamebase for small L_{res} cases while the amounts of CH_2O and H_2O_2 are marginal for large L_{res} cases. All of these results imply that the flame structure change can be highly related to the change of fuel type from DME to $\text{CH}_4/\text{H}_2/\text{CO}$ at the fuel tube exit.

To further identify the characteristics of the autoignited lifted jet flames with different L_{res} , the variations of H_L and $(T_{\text{max}} - T_0)/T_{\text{ig}}$ are shown in Fig. 16. The conventional H_L correlation for the autoignited laminar lifted jet flames (i.e. $H_L \sim U_0 \tau_{\text{ig,st}}^2$ [6]) is also shown in Fig. 16 to compare with the actual H_L . Note that the fitting coefficients for $H_L = \alpha U_0 \tau_{\text{ig,st}}^2 + \beta$ are obtained from the data between $L_{\text{res}} = 0$ and 8 m. Based on the radial location of the flamebase and $(T_{\text{max}} - T_0)/T_{\text{ig}}$ [11], we categorize the DME jet flames into four different regimes: Regime I or the MILD combustion regime – the lifted flame with MILD combustion with $(T_{\text{max}} - T_0)/T_{\text{ig}} < 1$ and the flamebase being located at the centerline; Regime III or the tribrachial edge flame regime – the lifted flame with tribrachial edge with $(T_{\text{max}} - T_0)/T_{\text{ig}} > 1$ and the flamebase being located radially outside the centerline; Regime II or the transition regime – the transition regime between Regimes I and III with $(T_{\text{max}} - T_0)/T_{\text{ig}} < 1$ and the flamebase being located radially outside the centerline; Regime IV or the attached flame regime – the attached flame to the fuel tube exit with $(T_{\text{max}} - T_0)/T_{\text{ig}} > 1$.

In Regime I or the MILD combustion regime ($0 \leq L_{\text{res}} \leq 8$ m), the lifted flames exhibit MILD combustion structure with being $(T_{\text{max}} - T_0)/T_{\text{ig}} < 1$ as shown in Fig. 16b. In this regime, H_L exhibits a U-shaped behavior and is well correlated with $U_0 \tau_{\text{ig,st}}^2$, indicating that the U-shaped behavior in this regime is primarily attributed to $\tau_{\text{ig,st}}$ induced by the DME pyrolysis or the 0-D ignition characteristics of the DME/air mixture. The differential diffusion effect induced by DME pyrolysis is not significant for this regime.

In Regime III or the tribrachial edge flame regime ($13.5 \leq L_{\text{res}} < 17$ m), the lifted flames

Figure 15: Isocontours of (a) T (left half) and Y_{OH} (right half) and (b) $Y_{\text{H}_2\text{O}_2}$ (left half) and $Y_{\text{CH}_2\text{O}}$ (right half) for autoignited laminar DME jet flames for various L_{res} with $T_0 = 980$ K and $X_{\text{F},0} = 0.08$ at a fixed $U_{\text{F}} = 1.53$ m/s. The dashed and dash-dot lines in (a) represent the mixture fraction isoline passing through the flamebase, ξ_{fb} , and the stoichiometric mixture fraction isoline, $\xi_{\text{st}} = 0.472$, respectively.

Figure 16: Variations of (a) H_L and its fitting curve (b) $(T_{\text{max}} - T_0)/T_{\text{ig}}$ and $\tau_{\text{ig,st}}^2$ as a function of L_{res} for the DME jet flames with $T_0 = 980$ K, $X_{\text{F},0} = 0.08$, and $U_{\text{F}} = 1.53$ m/s.

exhibit the tribrachial edge structure with $(T_{\text{max}} - T_0)/T_{\text{ig}}$ being above unity while H_L keeps decreasing with increasing L_{res} . In this regime, more than 90% of the initial DME is decomposed into small species such as CH_4 , H_2 , and CO at the fuel tube exit, and hence, the characteristics of the jet flames changes to those of $\text{CH}_4/\text{H}_2/\text{CO}$ flames rather than those of DME flames. To further understand the characteristics of H_L behavior in this regime, we carried out transient numerical simulations of cases with $L_{\text{res}} = 1.5$ and 14 m, which represents MILD combustion and tribrachial edge flame regimes, respectively (see supplementary material). For case with $L_{\text{res}} = 1.5$ m in the MILD combustion regime, an ignition kernel develops at the centerline, while for case with $L_{\text{res}} = 14$ m in the tribrachial edge flame regime, it does radially outside the centerline. This indicates that the amount of small species that diffuse out from the fuel jet becomes high enough to form the ignition kernel outside the centerline. Therefore, the fast diffusion rates of small species serve to decrease H_L of the tribrachial edge flames for which the flamebase lies outside the centerline. This result shows the different role of the differential diffusion effect on H_L behavior depending

on the location of the flamebase: in the MILD combustion regime, the differential diffusion effect increases H_L since the flamebase locates at the centerline; in the tribrachial edge flame regime, it decreases H_L since the flamebase locates radially outside the centerline, which is consistent with our previous study [11].

In Regime II or the transition regime ($8 < L_{\text{res}} < 13.5$ m), the flamebase locates radially outside the centerline although $(T_{\text{max}} - T_0)/T_{\text{ig}}$ is still below unity. This regime represents the transition of the lifted DME jet flame from the MILD combustion to the tribrachial edge flame. H_L decreases with increasing L_{res} and starts to deviate from the prediction of $U_0 \tau_{\text{ig,st}}^2$, which indicates that the degree of DME pyrolysis and the resultant differential diffusion effect become large enough to move the flamebase radially outside, consequently decreasing H_L .

In Regime IV or the attached flame regime ($L_{\text{res}} \geq 17$ m), the DME jet flame is attached to the nozzle with $(T_{\text{max}} - T_0)/T_{\text{ig}}$ being greater than unity. The more DME is decomposed with increasing L_{res} , the more amount of small species is transferred to the flamebase located at the outside the centerline. As a result, the propagation speed of the lifted flames continuously increases with increasing L_{res} , consequently leading to the attachment of the flames.

In summary, the pyrolysis of the DME jet and/or the resultant differential diffusion effect can change the flame structure and the stabilization mechanism of the autoignited lifted DME jet flames, which leads to the non-monotonic H_L behavior with increasing L_{res} . Note that it is of importance to identify a thermodynamic regime where the DME pyrolysis effect becomes significant to the stabilization of autoignited laminar lifted DME jet flames. However, their liftoff characteristics are highly affected not only by the degree of DME pyrolysis at different pressures, temperatures, and fuel dilutions, but also by the degree of differential diffusion induced by the pyrolysis and the fuel jet velocity. Thus, more extensive experimental and numerical studies are required to generalize the effects of DME pyrolysis, which will be left for future research.

6. Conclusions

The characteristics of autoignited laminar lifted DME jet flames in heated coflow air were numerically investigated with a 55-species detailed chemical kinetic mechanism of the DME oxidation. The detailed numerical simulations were performed for various fuel jet velocities and fuel tube lengths using the laminarSMOKE code. The present numerical simulations successfully captured the unusual U-shaped liftoff height behavior of the highly-diluted DME fuel jet flame with increasing fuel jet velocity under autoignitive temperature condition, which is qualitatively similar to that observed in experiments. Additional simulations with the modified mass diffusivity of hydrogen were also performed to understand the unusual U-shaped H_L behavior, which was not fully explained by previous experiment. The species transport, displacement speed, and chemical explosive mode analyses elucidated the detailed stabilization and ignition characteristics of the lifted flames. To further investigate the pyrolysis effect on the autoignited lifted flame, additional numerical simulations were performed by changing the fuel tube length L_{res} from 0 to 23 m. The numerical results showed the non-monotonic H_L behavior with L_{res} . The following results are obtained from the present study.

1. From the simulations with normal and modified D_{H_2} , it is verified that the U-shaped H_L behavior is primary attributed to the fast diffusion rate of H_2 . Since the DME jet is readily decomposed into small species such as CH_4 , H_2 , and CO in the heated fuel tube, the different mass diffusivities of the species generated from the pyrolysis of DME cause the unusual U-shaped H_L behavior.
2. The species transport budget and displacement speed analyses revealed that the lifted flames in the increasing H_L regime are stabilized by autoignition-assisted flame propagation mode. Furthermore, the stabilization characteristics of these flames do not depend on U_0 because the differential diffusion effect is marginal. For the decreasing H_L regime where the differential diffusion effect becomes significant, the flame stabilization mechanism readily changes from the autoignition-assisted flame propagation to the autoignition mode with decreasing U_0 . The flame becomes leaner as the differ-

ential diffusion effect increases, and consequently the stabilization of lifted flames are more dependent on the autoignition mode.

3. CEMA identified the important variables and reactions contributing to the autoignition of the DME jet. For the increasing H_L regime, the overall autoignition characteristics are not much affected by U_0 . For the decreasing H_L regime, on the other hand, the autoignition characteristics are highly affected by the differential diffusion effect, and thus, the ignition delay and resultant H_L change with U_0 . The results indicate that 0-D homogeneous ignition delay time, $\tau_{ig,st}$, does not always represent the autoignition characteristics of 2-D jet flames, especially for the highly diffusive fuels.
4. Based on the characteristics of the DME jet flames with different L_{res} , we categorized them into four different regimes: (I) the MILD combustion regime, (II) the transition regime, (III) the tribrachial edge flame regime, and (IV) the attached flame regime. In the MILD combustion regime, the pyrolysis of the DME jet is negligible for the relatively low L_{res} . The differential diffusion effect of small species generated by the DME pyrolysis starts to affect the lifted flame as L_{res} increases. From the transition to the tribrachial edge flame and to the attached flame regime, H_L keeps decreasing, which is primarily attributed to the increasing differential diffusion effect induced by the pyrolysis of the DME jet.

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