Study of Liftoff Mechanism of Nonpremixed Jet Flame near Unity Schmidt Number

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Nonpremixed jet flames of dimethyl ether (DME) were studied both experimentally and theoretically to investigate flame liftoff near unity Schmidt number. It was found experimentally that although the DME nonpremixed flames have a Schmidt number larger than unity it cannot be lifted directly by increasing the flow rate. Lifted flames can only be established by igniting the mixture in a narrow region downstream of the jet at low flow rates. The results also show that the liftoff flow rate is less than that of the blowout limit of the attached flame. Theoretically, the self-similar Landau-Squire solution for a round jet is revisited and the combined effects of stretch and flame curvature on triple flame propagation speed were considered. It was found that the critical Schmidt number for liftoff shifts around unity. The critical Schmidt number is less than unity for fuel Le numbers larger than 0.5 and larger than unity for Le numbers less than 0.5.

I. Introduction

Dimethyl ether (DME), CH₃OCH₃, is the simplest aliphatic ether and has no carbon and carbon bonds in its molecule. DME can be synthesized from natural gas, coal or biomass¹. It has low boiling point (-25.1°C), low tendency of soot formation, and high cetane number(55~60), which makes it an attractive alternate fuel and fuel additive to achieve low soot emission for gas turbine and diesel engines²⁻³. Moreover, DME is also expected to be used in power generation and home applicants. The study of combustion characteristic of DME has received extensive attention recently. Fisher et al.⁴ and Curran et al.⁵ developed a detailed chemical mechanism of DME oxidation. Daly et al.⁶ measured the laminar flame speed of DME-air mixtures at room temperature and atmospheric pressure by a constant volume spherical bomb. Zhao et al.⁷ measured the burning velocities of DME by using particle image velocimetry (PIV) method in a stagnation flame configuration. The laminar flame speeds of DME-air at elevated pressures were measured by Qin et al.⁸ Zheng et al.⁹ studied nonpremixed ignition of DME experimentally and computationally.

On the other hand, little work has been conducted on nonpremixed DME flames. Nonpremixed combustion is the dominate process in many industrial applications such as, gas turbine, diesel engine and industrial burners and furnaces. Flames liftoff is a characteristics phenomenon in the stabilization of nonpremixed flames. Extensive experimental and numerical work has been conducted to understand the liftoff mechanism of nonpremixed jet flames¹⁰⁻¹³. A jet flame will be lifted from the burner rip and remains suspended at a certain distance above the burner if the mass flow rate exceeds a critical value. Lifted flames have been observed only for certain fuels and the triple flame (also called edge flame or tribrachial-flame) structure is the mechanism for the stabilization of a lifted flame in the far field of jet.

It is well known that the liftoff process is dominated by the mass transfer of fuel and oxidizer and momentum transport of the jet. As such, the lifted flame is characterized by the Schmidt number (Sc=υ/DF, υ is the kinematic viscosity, DF is the diffusivity of fuel). Chung et al.¹⁰ studied the stabilization mechanism of laminar nonpremixed jet. After assuming the triple flame speed equal to the stoichiometric planar flame speed and using the far field approximation (cold jet theory) for a jet issuing from a point source of momentum, they showed that flames can be lifted if Sc is larger than unity. Ruetzch et al.¹⁴ studies the heat release effect on triple flames propagation and found that heat release increases the triple flame speed by deviation of streamlines in front of the flame. The effects of heat release and mixture fraction gradient on flame speed are coupled. Daou and Linan¹⁵ found that stretch affects the
propagation of triple flames in a similar way as that of the stretched premixed flames. Ghosal et al.\textsuperscript{12} found that the critical Schmidt number for the lifted flame shifts to 0.8 when the effects of the mass fraction gradient and heat release are considered.

Despite of these work, the stretch effect on lifted flames has not been studied yet though Daou and Linan\textsuperscript{15} showed that the triple flame speed is affected by flame stretch. Moreover, there is little work done on the flame liftoff study for fuels with Schmidt number near unity. The Schmidt number of DME is around 1.15. This makes DME a good fuel candidate to validate the previous theory. Therefore, the objective of the present work is to investigate the stabilization mechanism of lifted DME flames experimentally. Theoretically, the self-similar Landau-Squire solution for a round jet will be revisited and the combined effects of stretch and flame curvature on triple flame speed will be considered.

II. Theoretical Analysis

2.1 Self-similarity solution:

Figure 1 shows the schematic of the coordinates system. For an axisymmetric, steady laminar round jet with a uniform velocity profile at the nozzle exit, the corresponding Landau-Squire solution to a point source of momentum at the distances large compared to the nozzle diameter yields

\[ u = \frac{1}{r \sin \theta} \frac{\partial \psi}{\partial \theta} = \frac{\nu}{r \sin \theta} f(\theta) \]

\[ v = -\frac{1}{r} \frac{\partial \psi}{\partial r} = -\frac{\nu}{r \sin \theta} f(\theta) \]

with \( f(\theta) \) defined by

\[ f = \frac{4\theta^2}{\theta^2 + \theta_0^2} \]

Here \( \psi(r, \theta) \) is the stream function. \( \theta_0 \) is related to the jet Reynolds number.

\[ \theta_0 = \frac{16}{3} Re^{-1} \]

The velocity distribution in the far field is

\[ u = \frac{\nu}{r} \frac{8 \theta_0^2}{(\theta^2 + \theta_0^2)^{3/2}} \]

Similarly, the mass distribution at any point in the far field is

\[ Y = \frac{\sqrt{2} (2Sc + 1) d}{6 \theta_0 \nu} \left( \frac{\theta^2}{\theta_0^2} + 1 \right)^{2Sc} \]

\( d \) is the diameter of nozzle.

2.2 Velocity distribution along the stoichiometric contour

If the chemical reaction of fuel and air is

\[ \nu_F F + \nu_{\text{air}} (O_2 + 3.76N_2) \rightarrow aCO_2 + \beta H_2O + 3.76\nu_{\text{air}}N_2 \]

Then, the mass fraction of fuel on stoichiometric condition can be defined as:

\[ Y_{F, st} = \frac{\nu_F M_F}{\nu_F M_F + \nu_{\text{air}} M_{\text{air}}} \]

By substituting the mass fraction \( Y_{F, st} \) into Eq. (6), we can obtain the location of the stoichiometric contour

\[ r_s = \frac{\sqrt{2} (2Sc + 1) d}{6 \theta_0 Y_{F, st}} \left( \frac{\theta^2}{\theta_0^2} + 1 \right)^{2Sc} \]

If we define \( x = \theta/\theta_0 \), and substitute Eq. (8) into Eq. (5). The axis velocity along stoichiometric contour is

\[ u_{st} = \frac{48 Y_{F, st} \nu}{\sqrt{3} (2Sc + 1) d \theta_s d} \left( \theta^2 + 1 \right)^{2Sc-2} = \frac{3U_0 Y_{F, st}}{2Sc + 1} \left( \theta^2 + 1 \right)^{2Sc-2} \]
The velocity distribution along the stoichiometric contour depends on $Y_{F,st}$, the mass fraction of fuel at the stoichiometric condition, and $Sc$ if the exit velocity $U_0$ is fixed. The local velocity along the stoichiometric contour decreases with the downstream locations if $Sc$ is larger than unity and increases if $Sc$ less than unity. The velocity along the stoichiometric contour also depends on the mass fraction of fuel at the stoichiometric condition $Y_{F,st}$. The velocity will decrease with the decreasing of $Y_{F,st}$. For instance, the velocity along the contour for propane is less than DME at the same exit velocity because $Y_{F,st}$ for propane is 0.0602 and $Y_{F,st}$ for DME is 0.10. As such, the stoichiometric contour of propane is extended more to the oxidizer side compared with DME. Therefore, the local velocity distribution along the stoichiometric contour for propane is lower than DME.

2.3 Triple flame speed

To predict the triple flame speed more accurately, the effects of unequal diffusivities of fuel and oxidizer [17], flame curvature effect and heat release are considered.

When the radius of curvature is large compared with the laminar flame thickness, the triple flame speed can be expressed as

$$u_p = 1.4S_e^0\left\{1 + \frac{\sqrt{5}}{\sqrt{\pi}} \varepsilon \left[1 + \frac{L_F - L_o}{2} - \frac{L_F - L_o}{4}\right]\right\}$$

(10)

where $\varepsilon = L_{st}/(L/\beta)$; $L=\beta(L_{st}-1)$ and $L_o=\beta(L_{st}-1)$. $L_{st}$ is the laminar flame thickness. $L/\beta$ represents the expected characteristic value of the radius of curvature of the flame front. Here $L=(2D_F/\alpha)^{1/2}$ is the thickness of the mixture layer and $\beta$ is the Zeldovich number.

The strain rate at the triple flame can be approximated by

$$a = \frac{\partial u}{\partial x}_{x=x_{up}}$$

(11)

Physically, the effects of flame curvature and stretch decrease with the downstream locations because the velocity and mass fraction gradient decreases with the increasing length of mixture layer. As such, the triple flame speed is increasing with downstream locations and reaches an asymptotic value in the far field when the $Le$ number of fuel is larger than unity.

2.4 Stretch and flame curvature effect on the critical Schmidt number

As mentioned in the introduction, it was found that Schmidt number is the controlling parameter in flame liftoff phenomenon, which determines the relative location of isovelocity contour and stoichiometric contour. It is also suggested that flame can be lifted when Schmidt number of fuel is larger than unity [10]. However, this theory is based on constant triple flame velocity.

Using the liftoff condition, $u_{st} = u_{up}$ and combining similar terms, the liftoff solution can be expressed as

$$\left(1 + x^2\right)^{2Sc-2}\left[1 + A\left(1 + x^2\right)^{2Sc-1}\right] = B$$

(12)

where

$$A = 1.4S_e^0\frac{4\sqrt{5}p_{st}^{1/2}Y_{F,st}}{D_F(2Sc + 1)\theta_{th}} \frac{\sqrt{2}}{\sqrt{\pi}} \frac{1 + \frac{L_F - L_o}{2} - \frac{L_F - L_o}{4}}{4}$$

(13)

which represents stretch effect.

$$B = 1.4S_e^0\frac{2Sc + 1}{3U_0Y_{F,st}}$$

Here $B$ is a function of exit velocity, $U_0$, mass fraction at the stoichiometric condition, $Y_{F,st}$ etc. Thus, define

$$f(x) = \left(1 + x^2\right)^{2Sc-2}\left[1 + A\left(1 + x^2\right)^{2Sc-1}\right]$$

(14)

The solution of Eq. (12) is stable when the gradient of $u_{st}$ along the stoichiometric contour is smaller than that of $u_{up}$ which means $f'(x)>0$. The critical Schmidt number is achieved when the maximum of function $f(x)$ becomes a point of inflexion. Mathematically, the critical Schmidt number is achieved when

$$f'(x) = 0, \text{ and } f''(x) = 0$$

(15)
The critical Schmidt number for the liftoff phenomenon shifts with the effects of stretch and flame curvature. Figure 2 shows the relation of the critical Schmidt number and $A$. Factor $A$ represents the combined effects of flame curvature and stretch assuming unity of oxygen $Le$ number. When the $Le$ number of fuel is larger than 0.5, factor $A$ is positive and the critical Schmidt number is less than unity. The critical Schmidt number is larger than unity when the $Le$ number is less than 0.5. This shift of the critical Schmidt number is caused by the combined effects of stretch and flame curvature. The Lewis number effect on the triple flame speed plays a similar role as in premixed flames. For $Le$ larger than unity, triple flame speed decreases with the stretch effect, which has the same tendency as the flame curvature effect. However, when $Le$ is less than unity, triple flame speed increases with strain rate, and has opposite tendency from the flame curvature effect. The stretch and flame curvature effects can cancel with each other. The triple flame speed can increase until $Le$ of fuel is less than 0.5. At this point, the stretch effect is larger than flame curvature effect. Therefore, the critical Schmidt number shifts to the right hand side of unity when $Le$ is less than 0.5.

For lean DME flame, the $Le$ is around 1.6. The corresponding critical Schmidt number is less than unity. Theoretically, lifted DME flame can be obtained because its Schmidt number is larger than this critical Schmidt number. However, because the Schmidt number of DME is near unity, the window for liftoff flame is narrow compared with propane, even though it is enlarged by the stretch and flame curvature effect. Lifted DME flame, if it exists as theoretically predicted, will be more sensitive compared with propane lifted flame and the range of the mass flow rate for lifted DME flame will be limited.

### III. Experiment

The experimental setup is composed of a nozzle, a mass flow controller, and a measurement system. The nozzles are made from a quartz tube with nozzle exit diameters of 0.2 mm and 0.27 mm. The contraction ratio of the nozzle is about 200 to yield nearly a uniform exit velocity at the nozzle exit. The mass flow controller is used to control the exit velocity accurately. An $18\times18$ cm$^2 \times 50$ cm long vinyl enclosure, with a $15\times15$ cm$^2$ mesh near the bottom of each side, was used to shield the nozzle to minimize the disturbances from the ambient air. CP grade (99.5%) methane, propane and DME fuels were used.

### IV. Results and Discussion

#### 4.1 System validation

To validate the present measurement system, liftoff heights of propane jet flames were measured and the results were compared with Chung’s data [10] in Fig. 4. The accuracy and reliability of present system is demonstrated by the good agreement between the experimental data.

#### 4.2 Blow out limit of the attached DME nonpremixed flames

As shown in section 2.4, it is expected that DME jet flames will be lifted as propane. However, experimental results show that attached DME flame blows out directly when mass flow rate exceeds a critical value, which is similar to methane. Figure 5 shows the flame heights for attached methane, DME and propane flames. The propane flame is lifted (denoted L.O.) at certain flow rate, while the methane and DME flame blow out directly from their
attached states. Attempts to reignite were not successful. Therefore, DME lifted flame cannot be obtained by directly increasing flow rate.

The blowout of DME attached flame can be explained from the analysis of local flow velocity distribution along stoichiometric contour at the exit velocity near the blowout conditions. Figure 6 shows triple flame speed and velocity distribution along the stoichiometric contours of DME and propane. The velocity along the stoichiometric contour for DME at the blowout condition is in the range of 1.03–1.26 m/s at \( U_0 = 11.28 \text{ m/s}, Y_{F,st} = 0.10 \) and \( Sc = 1.15 \), which is much bigger than the asymptotic triple flame propagation speed \( u_p = 1.45L_0 \text{ m/s} \). This means velocity along stoichiometric contour is always larger than \( u_p \). There is no solution for local flow velocity to match triple flame speed. However, the velocity along the stoichiometric contour of propane is in the range of 0.44–0.7 m/s with \( U_0 = 10 \text{ m/s}, Y_{F,st} = 0.0602 \) and \( Sc = 1.37 \). As such, there is a position that \( u_p \) matches \( u_{st} \) and the lifted flame can stabilize at the intersection and this point is the liftoff position. Therefore, the attached DME flame is always blow out directly from the burner tip and cannot be lifted as propane.

In the work of Chung et al. [10], they considered methane, ethane, propane and n-butane to validate their model and found that \( Sc > 1 \) when \( Y_{F,st} \) is fixed. They did not discuss the effect of \( Y_{F,st} \) on the local flow velocity distribution. The corresponding \( Y_{F,st} \) for these fuels are 0.055, 0.059, 0.06 and 0.061, respectively, which are close to each other. Therefore, \( Y_{F,st} \) was neglected in their discussion. But DME has an oxygen atom in its molecule, the mass fraction of DME at \( \phi = 1 \) is around 0.1 which is quite larger than the other fuels. This will dramatically affect the location of the stoichiometric contour and thus changes the local velocity distribution along \( Y_{F,st} \). The minimum downstream velocity along \( Y_{F,st} \) at the blowout exit velocity is around 1.03 m/s for DME jet. However, it is still larger than the maximum triple flame propagation speed. The larger \( Y_{F,st} \) of DME leads to directly blow out of the attached flame.

![Figure 4 Liftoff height of nonpremixed propane jet flame as a function of mass flow rate of jet](image1)

![Figure 5 Flow rate versus attached flame height (d=0.27mm) showing the conditions of liftoff (L.O.) and blowout (B.O.)](image2)

![Figure 6 Triple flame speed and velocity along stoichiometric contour of DME and propane](image3)
4.3 Lifted DME flame

As discussed above, the blowout of DME attached flame is caused by the large local velocity along the stoichiometric contour. If decreasing the exit velocity, the local flow velocity can match the triple flame speed and there will be a stable solution. To find lifted DME flames in our experiment, the mixture was ignited by a spark discharge at a location downstream of the jet. The Lifted DME flame has a typical triple flame structure at the bottom.

Figure 7 shows the experimental results of the liftoff heights of DME flame as a function of flow rates. It is found that the lifted DME flame was very sensitive to the perturbations from environment. Lifted flame can only exist in the range of 22.9–23.7 ml/min, which is very narrow compared with that of propane (20–27 ml/min, c.f. Fig. 4). There are two stable solutions for DME flame in this range, one is the attached flame, and the other is the lifted flame in the far field which was observed here. The experimental data in figure 7 is also fitted in the form of $H_1=aQ(2Sc-1)/(Sc-1)=aQ^n$ [10] as shown in solid line, which gives $n=11.50$. This corresponds to the Schmidt number of 1.11 and is in good agreement with the Schmidt number of DME from CHEMKIN. The theoretical prediction of lifted DME flame is observed in the experiment. The measured relation of lifted height and flow rate is consistence with the theoretical analysis [10].

Figure 8 shows the liftoff heights of lifted and flame length of attached flames of DME and propane, respectively. Figure 8 (a) shows the hysteretic phenomenon of propane. There are two stable solutions for propane flame when the mass flow rate is between 18.8 ~ 20.7 ml/min. Whether the flame is attached or lifted is dependent on the flame history. Flame will not be lifted until the mass flow rate is larger than 20.7 ml/min. When the flow rate decreases, the lifted flame will reattach to the burner at 18.8 ml/min. In Fig. 8 (b), the flame regimes of DME are very different from propane. The maximum flow rate (23.7 ml/min) for lifted DME flame is less than the blowout limit (38.7 ml/min) of the attached flame. The liftoff height decreases with decreasing flow rate until it attaches the burner. The narrow regime and earlier blowout of lifted flame for DME is caused by its near unity Schmidt number and larger mass fraction at stoichiometric condition.
V. Conclusions

The stretch effect on the critical Schmidt number of flame liftoff is studied theoretically. The liftoff phenomenon for DME is experimentally investigated to understand liftoff mechanism of nonpremixed jet flame near unity Schmidt number. The following results were observed.

1. Stretch effect can change the critical Schmidt number for lifted flames. The critical Schmidt number is less than unity for fuel $Le$ numbers larger than 0.5 and larger than unity for $Le$ numbers less than 0.5.

2. A DME jet flame cannot be lifted directly by increasing the flow rate although it has a Schmidt number larger than unity. It can only be established in a narrow region by igniting the mixture downstream. The liftoff flow rate is less than the blowout limit of the attached flame.

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References