Numerical Modeling of Turbulent Nonpremixed Lifted Flames

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The present study has focused on numerical investigation on the flame structure, flame lift-off and stabilization in the partially premixed turbulent lifted jet flames. Since the lifted jet flames have the partially premixed nature in the flow region between nozzle exit and flame base, level set approach is applied to simulate the partially premixed turbulent lifted jet flames for various fuel jet velocities and co-flow velocities. The flame stabilization mechanism and the flame structure near flame base are presented in detail. The predicted lift-off heights are compared with the measured ones.

Key Words : Lift-off, Partial Premix, Level-set Approach, Statilization

Nomenclature

G : The scalar representing the flame front in Level-set approach
P : Probability density function
s : Burning velocity
u : Velocity
Y_k : Mass fraction of species k
Z : Mixture fraction

Greek Symbols

χ : Scalar dissipation rate
κ : The curvature of the mean flame front
δ : Mass density

Subscripts

b, u : Burned and Unburned gas, respectiveey
st : Stoichiometry

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1. Introduction

The flame lift-off characteristics considerably influence the flame stabilization and pollutant formation in practical combustion devices and largely depends on flow configurations, fuel type, heat losses and mixing conditions, etc. The lifted nonpremixed turbulent jet flames involve many fundamental mechanisms, which contain flame ignition, local extinction, re-ignition, and flame propagation. Since these physical phenomena are strongly coupled and highly nonlinear, explanations of the stabilization mechanism have been quite controversial. Theories for the flame stabilization mechanism may be divided into three categories. The first one is premixed flame propagation theory (Vanquickenborne and van Tiggelen, 1966) for which the underlying assumptions are that fuel and oxidizer are fully premixed at the base of a lifted diffusion flame and that stabilization occurs at the position where the mean flow velocity at the contour of mean stoichiometric mixture is equal to the burning velocity of a stoichiometric premixed turbulent flame. The second

one is flamelet quenching theory proposed by Peters and Williams (1983). They argued that there is insufficient residence time below the flame base for premixing at molecular level based on time and length scale. They neglected any effects of premixing and proposed where lift-off totally controlled by quenching of laminar diffusion flamelet and extinction of the flame will occur if the probability of quenched flamelets exceeds a critical value and the heat release from chemical reactions cannot balance the heat losses due to diffusion. Finally, Broadwell et al.(1984) proposed that large scale turbulent structures control flame stabilization. Hot combustion products are carried by large-scale turbulent structures to the edge of the jet, where they reenter the jet and ignite the combustible mixture. In their view, both lift-off and blowout occur when the reentered products are mixed so rapidly with unburned jet fluid that there is insufficient time to initiate the reaction before temperature and radical concentration drop below some critical value. Pitts (1988) conducted measurements of concentration along a line at radial location where flame stabilization takes place and found the facts that the premixed mixture within the flammability limits is observed for a certain period, but also during a large fraction of time there is only air or only fuel at the position of stabilization. This means that for a long period it is impossible for a turbulent premixed flame element to propagate against the upstream jet velocity and premixed flame base model could not appropriately explain the experimental observation. The flamelet quenching theory, which excludes molecular premixing at the flame base is not in line with the experiments either, because measurements show that a considerable amount of premixing may be found upstream of the flame base. Pitts (1988) concluded that none of these theories could satisfactorily predict lift-off and blowout behavior. Intensive research has been conducted, but still today the mechanisms controlling flame stabilization are not fully understood. So, flame stabilization is still an open question. For modeling turbulent flame propagation in partially premixed systems, Chen et al.(2000) used model so called Level-Set approach based on the two scalar fields, $G(x, t)$ which determines the location of the premixed flame front and $Z(x, t)$ which express the state of mixing to predict the lift-off heights for methane/air and propane/air lifted flames.

In this study, in order to realistically represent the complex turbulence-chemistry interaction, level set approach has been implemented for the partially premixed turbulent lifted jet flames. Special emphasis is given to modeling the lifted turbulent flames frequently encountered in the practical combustors. Level set approach is applied to simulate the turbulent partially premixed lifted jet flames for various fuel jet velocities and co-flow velocities. Based on numerical results obtained in this study, the detailed discussions have been made for the precise flame structure and the flame stabilization mechanism in the partially premixed lift-off flames.

2. Numerical and Physical Modeling

2.1 Governing equations and numerical modeling

The density-weighted Navier-Stokes equation, k-ε turbulent model equation, energy equation, and mean and variance of mixture fraction equations are employed to predict the turbulent reacting flows in cylindrical coordinate and represented in the following form.

$$\frac{\partial}{\partial t}(\bar{\rho}\phi)+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}\phi)=\frac{\partial}{\partial x_j}\left(\Gamma_\phi\frac{\partial\phi}{\partial x_j}\right)+S_\phi \quad (1)$$

where ϕ includes mean axial and radial velocity, mean enthalpy, turbulent kinetic energy and dissipation rate, mean and variance of mixture fraction and Γ_ϕ and S_ϕ represent the diffusion coefficient and source term of its equation, respectively. The diffusion coefficients and source terms are well described in Ref (Kim, 2000).

The governing equations are solved using a control-volume based finite difference method in an unsteady fashion. The present formulation is based on a curvilinear general coordinate with a non-staggered grid. Second order accurate central differencing scheme is used for the diffusion

terms. To reduce numerical diffusion, second order TVD upwind scheme (Chakravarthy and Osher, 1985) for convection terms is implemented. The pressure-velocity coupling is handled by the improved PISO algorithm (Kim et al., 1994).

2.2 Level set approach

At the base of the lifted turbulent diffusion flame, fuel and oxidizer are partially premixed. The instantaneous surface of stoichiometric mixture separates lean and rich regions. When a flame propagates through the inhomogeneous fluctuating mixture of fuel and oxidizer, an instantaneous flame front separates burned and unburned gases. Thus, a formulation for both premixed and non-premixed combustion has to be used. For this purpose, the flamelet model of non-premixed combustion is combined with the flamelet model for premixed combustion. The mixing of fuel and oxidizer in the turbulent flow field is described by transport equation of mean mixture fraction and its variance.

In order to describe premixed combustion, the level set approach based on the G-equation (Peters, 2000) is introduced. The scalar G is equal to the constant G_0 at the location of the instantaneous premixed flame front. Thus, the surface $G(x, t)=G_0$ divides the flow field into the regions of burned gas where $G(x, t)>G_0$, and unburned gas where $G(x, t)<G_0$. Since G is the non-reacting scalar, it avoids complications associated with counter-gradient diffusion and there is no need for a source term closure. An equation for G can be derived by considering an iso-scalar surface, $G(x, t)=G_0$ and the equation for the mean location of the turbulent flame front is written as

$$\frac{\partial(\bar{\rho}\tilde{G})}{\partial t}+\nabla\cdot(\bar{\rho}\tilde{v}\tilde{G}) =\bar{\rho}s_{T,p}|\nabla\tilde{G}|-\bar{\rho}D_t\bar{\kappa}|\nabla\tilde{G}| \tag{2}$$

where $\bar{\kappa}$ is the curvature of the mean flame front and D_t is the turbulent diffusivity, which can be determined from the integral length scale, l, and the fluctuation velocity, v', (Peters, 2000)

$$D_t=a_4lv', \quad a_4=0.78 \tag{3}$$

The equation for the variance of G is

$$\frac{\partial(\bar{\rho}\tilde{G}''^2)}{\partial t}+\nabla\cdot(\bar{\rho}\tilde{v}\tilde{G}''^2) =\nabla_{\|}\cdot(\bar{\rho}D_t\nabla_{\|}\tilde{G}''^2)+2\bar{\rho}D_t(\nabla\tilde{G})^2-c_s\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{G}''^2 \tag{4}$$

where $\nabla_{\|}$ denotes differentiation only tangential to the mean flame front.

What remains is the determination of the turbulent partially premixed burning velocity, $s_{T,p}$ in equation for the mean location of the turbulent flame front. In order to model this quantity, it is assumed that fuel and oxidizer are locally premixed, so the partially premixed flame propagates through a stratified, but locally premixed environment. For premixed turbulent combustion, the turbulent burning velocity, s_T, can be determined from Ref. (Peters, 2000).

$$\frac{s_T-s_L}{v'}=\frac{a_4b_3^2}{2b_1}Da+\left[\left(\frac{a_4b_3^2}{2b_1}Da\right)^2+a_4b_3^2Da\right]^{1/2} \tag{5}$$

where s_L is the laminar burning velocity of a plane flame, $Da=s_Ll/(v'l_F)$ is the Damkohler number, l and l_F are the integral length scale and the laminar flame thickness, v' is the turbulent intensity, and $a_4=0.78$, $b_1=2.0$ and $b_3=1.0$ are constants derived from turbulence modeling (Peters, 2000). A conditional turbulent Damkohler number, $Da(Z)$, is introduced to determine the conditional burning velocity, $s_T(Z)$, as

$$s_T(Z)=s_L(Z)+v'f\{Da(Z)\} \tag{6}$$

where $f\{\ \}$ represents the right-hand side of equation (5), and $Da(Z)$ is defined as

$$Da(Z)=\frac{s_L(Z)l}{v'l_F(Z)}=\frac{s_L^2(Z)l}{v'D} \tag{7}$$

In the second part of above equation, the laminar flame thickness, $l_F(Z)$, has been replaced by $l_F(Z)=D/s_L(Z)$, where D is the laminar diffusivity. Using presumed probability density function approach, the mean turbulent burning velocity of a partially premixed flame can then be determined from

$$(\bar{\rho}s_{T,p})=\int_0^1\rho(Z)s_T(Z)P(Z)dZ \tag{8}$$

where $P(Z)$ is chosen to be a beta PDF. If

$s_T(Z)$ is defined with respect to the unburned mixture, $\rho(Z)$ is to be evaluated there.

To avoid numerical difficulties, the scalar function $\tilde{G}$ is calculated as a distance function, meaning that a re-initialization procedure of the $\tilde{G}$ field using $|\nabla\tilde{G}|=1$ has to be performed away from the mean flame front. A method proposed by Sussman et al.(1994) solves after each time step in the entire flow field the equation

$$\frac{\partial g}{\partial t}=sign(\tilde{G}(x,\ t)-G_0)\,(1-|\nabla g|) \qquad (9)$$

which has characteristics that originate at the flame surface and propagate the unity gradient information from there into the surrounding field. Starting from the initial condition $g(x,\ t=t_0)=\tilde{G}(x,\ t)$, the g-field is calculated until the stationary solution $g_\infty(x)$ is reached for large times. Then $\tilde{G}(x,\ t)$ is set equal to $g_\infty(x)$ for $\tilde{G}\neq G_0$ at that time step, while the surface $\tilde{G}(x,\ t)=G_0$ remains unchanged.

There are two possible states for the diffusion flamelet, either burning ($G>G_0$) or non-burning ($G<G_0$). For the burning flamelets, the mass fractions of the chemical species are determined by using a steady-state flamelet library with the conditional scalar dissipation rate χ_{st} as a parameter. In the burned gas, the mean mass fractions are calculated using a presumed PDF approach

$$\tilde{Y}_{i,b}(\tilde{Z},\ \tilde{Z}''^2,\ \tilde{\chi}_{st})=\int_0^1 Y_i(Z,\ \chi_{st})\,P(Z)\,dZ \qquad (10)$$

Here, $Y_i(Z,\ \chi_{st})$ is determined from a library of burning diffusion flamelets, setting the conditional scalar dissipation rate, χ_{st}, of the flamelets equal to the conditional mean scalar dissipation rate, χ_{st}, both defined at stoichiometric mixture. The latter can be calculated from

$$\tilde{\chi}_{st}=\frac{\tilde{\chi}f(Z_{st})}{\int_0^1 f(Z)\,p(Z)\,dZ},\quad f(Z)=Z^2\ln Z \qquad (11)$$

$$\tilde{\chi}=c_\chi\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Z}''^2 \quad c_\chi=2.0 \qquad (12)$$

A beta function PDF is used. In the unburned gas, all mass fractions are zero except those of fuel and oxidizer. These mass fractions, being linear in mixture fraction, are evaluated from

$$\tilde{Y}_{F,u}=Y_{F,1}\tilde{Z}\quad \tilde{Y}_{ox,u}=Y_{ox,2}(1-\tilde{Z}) \qquad (13)$$

Within the turbulent flame brush, the average mass fractions are determined from the weighted sum

$$\tilde{Y}_i=p_b\tilde{Y}_{i,b}+(1-p_b)\,\tilde{Y}_{i,u} \qquad (14)$$

Here, p_b denotes the probability of finding burned gas

$$p_b=p_b(G>G_0)=\int_{G=G_0}^{\infty}\frac{1}{\sqrt{2\pi\tilde{G}''^2}}\exp\left(\frac{(G-\tilde{G})^2}{2\tilde{G}''^2}\right)dG \qquad (15)$$

where a Gaussian distribution is assumed for the PDF of G.

3. Results and Discussions

We would try to numerically analyze the detailed flame structure and stabilization mechanism in the lifted partially premixed turbulent jet flames. The present numerical study adopts the Level set approach, which uses two parameters such as mixture fraction and distance function, in order to get closure of turbulence-chemistry interaction. As mentioned earlier, flamelet model have been very useful in combining turbulence and non-equilibrium chemistry since it allows the decoupling of the chemistry calculation from the calculation of the turbulent flow field. In Level set approach, the laminar diffusion flamelet libraries are required and the scalar profiles in mixture fraction space are calculated using one dimensional flamelet equations with chemical kinetics of GRI-Mech 2.11.

The validation case includes the measurement of Muniz and Mungal (1997), which has the detailed experimental data of lift-off height and velocity fields near flame base about various co-flow air conditions. In this experiment, the fuel of methane (99.0% purity) is injected through the nozzle of 4.8 mm diameter and the co-flow velocity ranges from 0 to 1.85 m/s through the nozzle of 300 mm outer diameter.

For the pure methane/air flame, the stoichiometric mixture fraction, Z_{st} is 0.05. In order to initialize the simulation, the cold flow was calculated at first for the different fuel exit velocities

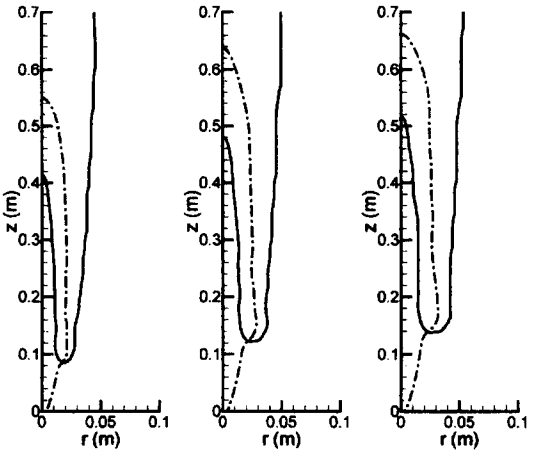

Fig. 1 The mean shape of the turbulent flame front (solid line) for methane/air jet flames at fuel nozzle exit velocities of (a) 16 m/s, (b) 26 m/s and (c) 32 m/s and co-flow air velocity of 0.34 m/s using Level-Set approach. The dashdot lines denote the mean stoichiometric lines

and co-flow air velocities. Then, the mixture was ignited at a downstream location by initialization of G-field in such a way that $\tilde{G}=G_0\pm|\vec{x}-\vec{x}_0|$. After ignition, the flame front propagated until it finally reached a steady state, stabilizing at the lift-off height.

Figure 1 shows the mean flame fronts, $\tilde{G}=G_0$, and the stoichiometric mixture fraction lines for different fuel exit velocities with the co-flow air velocity of 0.34 m/s after stabilization has been reached. The stabilization points are located the slightly lean side and is increasing the distance from the nozzle exit and centerline by increasing the fuel jet velocity.

Figure 2 represents the iso-lines of mean mixture fraction, temperature field, turbulent flame speed, and distribution of OH mass fraction for different fuel exit velocity with a co-flow air velocity of 0.34 m/s. The expansion at the flame front deflects the streamlines and mixture fraction iso-lines. The turbulent flame speed has high value near flame stabilization point. Since the net convective flux of G is equal to the production of G due to the turbulent flame speed near the

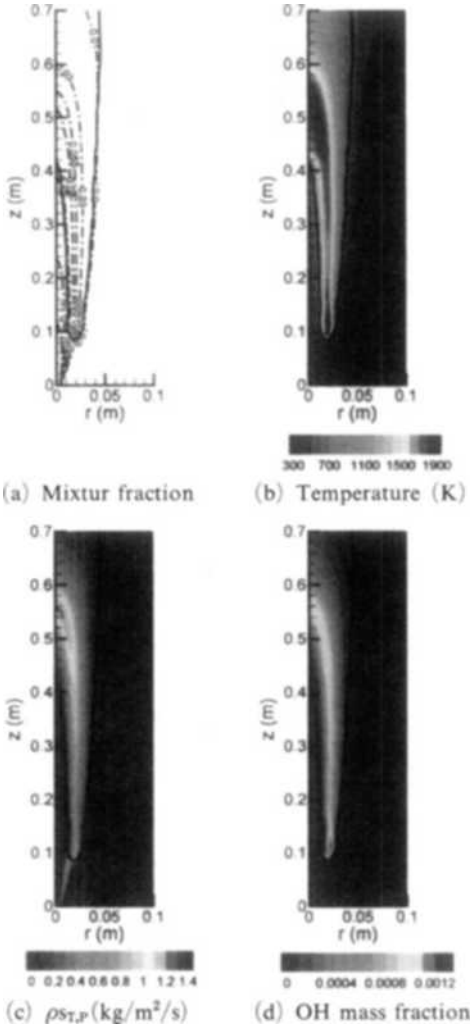

Fig. 2 Results of Level-Set approach for the methane/air jet flame with a fuel nozzle exit velocity of 16 m/s and co-flow air velocity of 0.34 m/s; (a) iso-lines of mean mixture fraction, (b) mean temperature, (c) turbulent flame speed, and (d) OH mass fraction. Solid lines denote the flame fronts

flame base, the stabilization of lifted flame is accomplished. The location of the maximum OH concentration indicates the location of the trailing mean diffusion flame between two premixed flame fronts expressed by G_0 surface.

In Fig. 3, the lift-off heights predicted by the present level set approach are compared with experimental data for three different jet exit

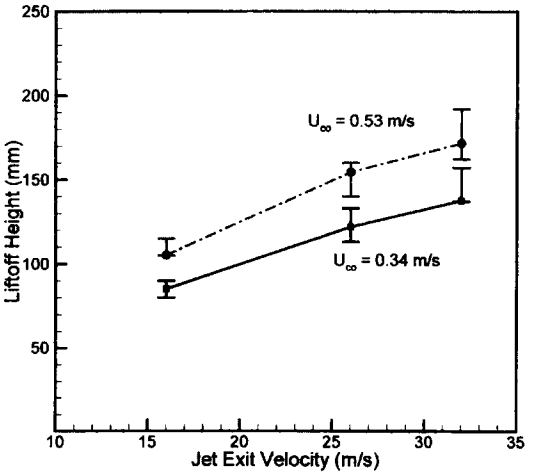

Fig. 3 The comparison of lift-off height as a function of jet exit velocity (Error bars represent the experimental data, solid line denotes cases for co-flow velocity of 0.34 m/s)

velocities and two co-flow conditions. The predicted lift-off heights are defined as the distance between nozzle exit and the lowest axial location of G_0. The lift-off heights predicted by the level set approach are favorably agreed with experimental data for all cases.

4. Conclusions

Numerical and physical models developed in the present study have been applied to numerically investigate the flame structure, flame lift-off and stabilization in the partially premixed flames. Based on the numerical results for stabilization mechanism of lifted partially premixed turbulent jet flames, the following conclusions can be drawn.

(1) The predicted lift-off heights well agree with the experimental data and the lift-off height increases and the stabilization point is progressively apart from centerline by increasing co-flow and jet exit velocity.

(2) The thermal expansion near the flame front deflects the flow streamline and the mixture fraction iso-lines near the flame base and considerable amount of pre-mixture of fuel and oxidizer exist in the zone between jet exit and flame base.

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