LARGE EDDY SIMULATION OF LIFTED NON-PREMIXED JET FLAMES USING 2-SCALAR FLAMELET MODEL

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ABSTRACT

In this paper we introduce the LES of lifted non-premixed jet flames based on two-scalar flamelet modeling. The flamelet G-equation for premixed combustion and the conserved scalar equation for non-premixed combustion are combined to express partially premixed flame propagation. In order to close filtered G-equation, the subgrid burning velocity model is proposed based on the concept that small triple flamelet are projected into unburnt gas from the flame-base of the lifted non-premixed flame. The calculation results are shown that wrinkling lifted flames are simulated and the difference of the lift-off height and the flame-shape with the variation of the co-flowing velocity is predicted. It is also confirmed that the conditional axial velocity near the flame base is on the order of two - three times of the laminar burning velocity, which agrees well with the experimental data.

INTRODUCTION

Phenomena in turbulent combustion strongly depend on the flow field. In many engineering applications such as a gas-turbine combustor or a furnace, the turbulent mixing plays an important issue. The solution methods, which have a higher accuracy, are essential. In this respect, A Large Eddy Simulation (LES) is useful to describe the turbulent mixing compared with Reynolds Averaged Navier-Stokes equations (RANS), because the LES can capture unsteady dynamics of turbulence in the resolved field.

Recently, combustion modeling for the LES using the flamelet-concept is investigated and the flamelet model using the conserved scalar approach is successfully applied in LES for non-premixed flames [1,2,3]. This approach is suitable for LES because a turbulent flame is modeled as the assembly of the laminar flamelet on the subgrid-scale and the large-scale interaction of vortices and flames can be expressed directly on the grid-scale.

The conserved scalar approach cannot, however, treat a lifted jet flame or partially premixed flame propagation because of the assumption that the mixing surface represents the flame surface. Some extended models are needed to express the unburnt gas and the burnt gas of lifted jet flames. In this problem, Müller (1994) [4] proposed the flamelet modeling for a partially premixed combustion and simulated lifted jet flames using the RANS model. In this model, the flamelet G-equation and the conserved scalar approach are combined to express partially premixed flame propagation.

In the present work, we have formulated a similar approach for the LES, called as "two-scalar flamelet model" [5]. The advantage of this method is that the lift-off height can be predicted if the turbulent burning velocity of the flame base is estimated correctly. The aim of this work is to make a LES-subgrid burning velocity model for the partially premixed combustion and the verification for the LES-two-scalar flamelet model to predict the characteristic of unsteady lifted jet flames.

BASIC EQUATION OF TURBULENT FLOW

In this work, constant-pressure combustion with the low-Mach number approximation is assumed in order to treat a variable density flow with the low speed combustion. Equations for the flow field can be written as:

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i)=0 \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j)=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(2\mu\tilde{S}_{ij}-\frac{1}{3}\delta_{ij}\tilde{S}_{ij}-\tau_{ij}\right) \tag{2}$$

where $\bar{\phi}$ means the spatial filtered value for ϕ, $\tilde{\phi}=\overline{\rho\phi}/\bar{\rho}$ means the Favre filtered value for ϕ, ρ is the density, μ is the viscosity, τ_{ij} is unclosed term generated by filtering operation, which represents the Sub-Grid Scale (SGS) stress and approximated by Smagorinsky model as:

$$\tau_{ij}=\bar{\rho}\left(\widetilde{u_iu_j}-\tilde{u}_i\tilde{u}_j\right)-\frac{2}{3}k_{SGS}\delta_{ij}=-2\mu_{SGS}\left(\tilde{S}_{ij}-\frac{1}{3}\delta_{ij}\tilde{S}_{ij}\right) \tag{3}$$

$$\mu_{SGS}=\bar{\rho}(Cs\Delta)^2\sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}} \tag{4}$$

where μ_{SGS} is the subgrid eddy viscosity, $\tilde{S}_{ij}$ is the mean strain rate , Δ is characteristic grid width. The thermo-dependency of the viscosity is assumed as $\mu_{SGS} = \mu_{cold}\left(\tilde{T}/T_{cold}\right)^{0.76}$, T is the temperature, Cs is the Smagorinsky constant.

Under the assumption of constant-pressure combustion, only the dynamic part of the pressure $p_d(x,t)$ is affected to the momentum in equation (2) because the spatial difference of the static (thermal) pressure P_0 is negligible, written as:

$$\bar{p} = \overline{p_d(x,t)} + p_0 \ , \ \frac{\partial p_0}{\partial x_i} \approx 0 \qquad (5)$$

COMBUSTION MODEL

Flamelet Concept and Flame Propagation model

In practical turbulent flow, the combustion process usually occurs in the very small length and time scale as the smallest turbulent smallest scales. In this case, the combustion state is categorized as fast-chemistry combustion and the turbulent flame can be modeled as the assembly of the laminar flamelet (Peters 1986[6]). In the flamelet model, the position of the premixed flame surface and the flame propagation can be expressed as the iso-surface of a level set scalar G in G-equation (Williams 1985[7]), described as follows:

$$\frac{\partial G}{\partial t} + u_k \frac{\partial}{\partial x_k} G = S_L \left(\frac{\partial G}{\partial x_k} \frac{\partial G}{\partial x_k} \right)^{\frac{1}{2}} \qquad (6)$$

where S_L is the laminar burning velocity

The index of scalar G is assigned the value zero in unburnt region and unit in the burnt region with the thin flame identified by a fixed value of $0 < G < 1$.

"Two-Scalar Flamelet Model" for Partially Premixed Flame

In this work, in order to treat partially premixed combustion such as a lifted non-premixed jet flame, the laminar burning velocity is assumed to be prescribed function of the equivalence ratio or the mixture fraction ξ because the effect of the turbulent mixing of the fuel gas and the oxidizer change the laminar burning velocity S_L in space and time, written as:

$$S_L(x_i,t) = S_L(\xi(x_i,t)) \qquad (7)$$

where ξ is the mixture fraction, in order to know the mixing of the unburnt fuel gas and the oxidizer, the transport equation of the mixture fraction must be solved.

Fig.1 shows a schematic figure of the triple flame, which is typical sample of partially premixed flame. Assumptions of the flamelet model for a partially premixed flame are summarized in table 1.

Table 1 Assumption of 2-scalar flamelet model

I. The flame propagation is expressed by the transport equation of the level set scalar G, which represents the position of the flame surface.
II. The mixing of fuel and air is expressed by transport equation of the mixture fraction ξ.
III. The scalar G is used to distinguish between the burnt and unburnt region. In this work, scalar G is not treated as level set scalar but like as the reaction progress variable.

In the LES formulation, the set of flamelet equations in the current modeling can be derived by applying a spatial, density–weighed (Favre) filter to the mixture fraction transport equation and the flamelet G equation are solved.

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{\xi} + \frac{\partial}{\partial x_k}\bar{\rho}\tilde{u}_k\tilde{\xi} = \frac{\partial}{\partial x_k}\left(\frac{\mu}{Sc}\frac{\partial \tilde{\xi}}{\partial x_k} - \eta_k^{\xi} \right) \qquad (8)$$

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{G} + \frac{\partial}{\partial x_k}\bar{\rho}\tilde{u}_k\tilde{G} = \frac{\partial}{\partial x_k}\left(\frac{\mu}{Sc}\frac{\partial \tilde{G}}{\partial x_k} - \eta_k^{G} \right) + \overline{\rho S_L \left(\frac{\partial G}{\partial x_k}\frac{\partial G}{\partial x_k} \right)^{\frac{1}{2}}} \qquad (9)$$

where Sc is the Schmidt number, η_k^{ϕ} is subgrid flux term for ϕ

There is unclosed two terms is exist in equation (9). The subgrid scalar flux η_k^{ϕ} is usually approximated using a gradient diffusion model as:

$$\eta_j^{\phi} = \bar{\rho}\left(\widetilde{\phi u_j} - \tilde{\phi}\tilde{u}_j \right) = \frac{\mu_{SGS}}{Sc_{SGS}} \frac{\partial \tilde{\phi}}{\partial x_j} \qquad (10)$$

The last terms of right hand of equation (9) is modeled using subgrid burning velocity S_T and the gradient of filtered scalar G written as:

$$\overline{\rho S_L \left(\frac{\partial G}{\partial x_k}\frac{\partial G}{\partial x_k} \right)^{\frac{1}{2}}} = \bar{\rho} S_T \left(\frac{\partial \tilde{G}}{\partial x_k}\frac{\partial \tilde{G}}{\partial x_k} \right)^{\frac{1}{2}} \qquad (11)$$

The interference between the turbulence and the flame surface is modeled in S_T, which should be modeled like the turbulent burning velocity in the ensemble averaging formulation.

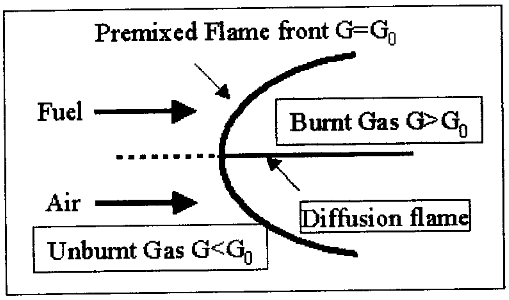

Fig.1 Schematic view of triple flame

Subgrid Burning Velocity For Lifted Jet Flame

In order to formulate a subgrid burning velocity model of G-equation in this work, it is needed to assume the stabilization mechanism of turbulent lifted non-premixed jet flames.

Recent investigations suggest that the triple-flame-like turbulent leading edge flames play an important role on the stabilization problem. (Müller et al 1994 [4], Múniz and Mungal 1997 [8])

In case of a laminar triple flame, Ruetsch et al.(1995)[9] found that the flame speed (the propagation velocity of the flame) of a laminar triple flame is faster than the corresponding premixed flame, which is caused by the divergence of flow ahead of the flame. Chen and Bilger (2000) [10] proposed a general expression of the propagation velocity of a laminar triple flame with the heat loss such as:

$$\frac{U_{partial}}{S_L^0} = \sqrt{\rho_u / \rho_b}\left(1 - \alpha \left(\frac{\chi_{st}}{\chi_q} \right)^m \right) \qquad (12)$$

where $U_{partial}$ is the propagation velocity of a laminar triple flame, S_L^0 is the laminar burning velocity of an un-stretched premixed flame, ρ_u/ρ_b is the density ratio of unburnt and burnt gas, χ_{st} is the scalar dissipation rate of the mixture fraction with stoichiometric mixture and χ_q is the scalar dissipation rate of the mixture fraction with the flamelet quenching of the diffusion flame, α and m are model constants.

In case of a turbulent lifted flame, Múniz and Mungal (1997) [8] found that the conditional axial velocity rarely exceeds three times of S_L^0 on the flame base of methane-air lifted diffusion flame using OH-LIF and PIV measurements. They implied that the stabilization mechanism of turbulent lifted flame is similar to a laminar triple flame. Han et al. (1998) [11] measured the conditional axial velocity on the flame base of a methane-air lifted diffusion flame with Re=7000 and found the conditional axial velocity of the flame surface is mean value of $2.39S_L^0$ with a standard deviation of $1.8S_L^0$. Although the reason why the standard deviation of the conditional velocity has large value can be explained as the instantaneous flame position is fluctuating in time, another explanation can be thought as small-scale structures on the flame base exist. Favier and Vervish (1998) [12] investigated the interaction of a triple flame and small scale pinched vortices using the numerical simulation, as they suggested that the assembly of small triple flamelet exist on the flame base of the lifted jet flame and small triple flames are projected in the unburnt mixture by pinched small vortices, In case of the LES, the projection of triple flames will occur in the subgrid scale.

In this research, it is assumed that the assembly of small triple flamelet exists on the flame base and the scale of triple flamelet is smaller than the subgrid scale, shown in Fig.2. In the subgrid scale, it is assumed that the subgrid burning velocity of a triple flamelet $S_{partial}^{sub}$ is nearly equal to $U_{partial}$ and the effect of the flame stretch of premixed wings is expressed by the strain rate. Instead of equation (12), $S_{partial}^{sub}$ is formulated as:

$$\frac{S_{partial}^{sub}}{S_L^0(\xi)} = \sqrt{\rho_u/\rho_b}\left(1 - C_q\left(\frac{a_l}{a_q}\right)^m\right) \quad (13)$$

where $S_{partial}^{sub}$ is the propagation velocity of subgrid triple flame, $S_L^0(\xi)$ is the laminar burning velocity of an un-stretched premixed flame which is prescribed function of the mixture fraction, a_{sub} is the strain rate in the subgrid scale, a_q is the strain rate with flamelet quenching of diffusion flame and C_q and m are model constant.

The effect of filtering the wrinkled flame base is modeled as the subgrid burning velocity using Damköhler's assumption.

$$\frac{S_T}{S_L} = \left(1 + C_{pg}\left(u_{sgs}/S_{L\max}^0\right)^n\right) \quad (14)$$

Im et al. (1994) [13] proposed the dynamic procedure to decide model constant C_{pg} in equation (14) for a wrinkled premixed flame. Park (2000) [14] have been performed LES of turbulent wrinkled premixed flames stabilized by the backward facing step or the flame holder with dynamic-subgrid-burning-velocity model using equation (9), (14) and reported results of the LES was good agreement with experimental data. The constant C_{pg} resulted in near 0.5 in his calculation.

It is assumed $S_L = S_{partial}^{sub}$ in the partially premixed flame front of turbulent lifted jet flame, the subgrid burning velocity on a partially premixed flame front results in:

$$\frac{S_T}{S_L^0(\xi)} = \sqrt{\rho_u/\rho_b}\left(1 - C_q\left(\frac{a_l}{a_q}\right)^m\right)\left(1 + C_{pg}\left(u_{sgs}/S_{L\max}^0\right)^n\right) \quad (15)$$

In this model, two effects in partially premixed flame propagation exist: subgrid propagation of the triple flame and the effect of filtering wrinkled flame.

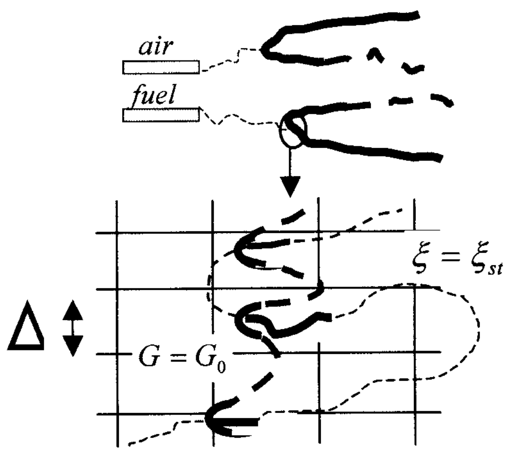

Fig.2 Schematic illustration of triple flamelet on the flame base and length scales of SGS fluctuation

Mass Fraction Model Near The Flame Front For Partially Premixed Flame

In order to close this combustion model, the mass fraction model near the flame surface is needed.

It is assumed that the flame front thickness is smaller than the filter width and the variation of G near the flame front is similar to the variation of the reaction progress variable c. The mass fraction of chemical species α are modeled as

$$G \sim c = \frac{Y_\alpha(x_i,t) - Y_{\alpha,u}(\xi)}{Y_{\alpha,b}(x_i,t) - Y_{\alpha,u}(\xi)} \quad (16)$$

where c is the reaction progress variable, Y_α is the mass fraction of species α, $Y_{\alpha,u}$ is the mass fraction of chemical species of un-burnt gas and $Y_{\alpha,b}$ is the mass fraction of chemical species inside of burnt gas.

Inside of the burnt region, it is assumed that combustion products are approximated as those of a diffusion flame. In this assumption, $Y_{\alpha,b}$ is modeled by prescribed function of the mixture fraction such as the flamelet model of the diffusion flame.

In LES formulation, Favre filtered mass fractions of chemical species α near the flame surface can be modeled using sub-grid presumed Probability Density Function (PDF) model for the non-premixed combustion [1-3]. In this paper, the presumed PDFs of scalar G and the mixture fraction ξ are assumed to be independent. Filtered mass fraction $\widetilde{Y_\alpha}$ is given as:

$$\widetilde{Y_\alpha} = \int_\xi \int_G Y_\alpha(\xi,G)\widetilde{P}(\xi)\widetilde{P}(G)d\xi dG \qquad (17)$$

where $\widetilde{P}$ is presumed Favre PDF. The beta PDF is used for $\widetilde{P}(\xi)$ [1] and the delta PDF is used for $\widetilde{P}(G)$. The effect of the fluctuation of G is neglected as the formulation become simple.

Using the equation (16) and (17), Favre filtered mass fraction model results in :

$$\widetilde{Y_\alpha} = \{1-\widetilde{G}\}Y_{\alpha,u}(\widetilde{\xi}) + \widetilde{G}\int_0^1 Y_{\alpha,b}(\zeta)\widetilde{P}(\zeta,\widetilde{\xi},\xi'^2)d\zeta \qquad (18)$$

In this formulation, $\widetilde{G}$ is expected as the switching parameter near the flame base and the mixing parameter where the burnt and unburnt gas is mixed away from the flame base.

COMPUTATIONAL CONDITIONS

Governing equations of 2-scalar flamelet LES model are equations (1), (2), (8), (9), (15) and (18). In order to close model, the filtered enthalpy transport equation and the filtered equation of state of gas are coupled. As the low Mach number approximation is assumed, governing equations are solved using incompressible 3D LES code considering variable density [3].

Present calculation is compared with the experiments of methane-air lifted non-premixed flames [8]. In the experiments, A diameter of the fuel tube D=0.0048 [m]. The calculation is performed on a cylindrical domain of 60 nozzle diameters D length and radius 20D. The numerical grid consists of 200x86x32 cells (axial, radial, circumferential direction, respectively). The smallest grid spacing of radial direction is 0.05D on the center of fuel inlet and the smallest grid spacing of axial direction is 0.05D on the inlet.

As respects model constants, Smagorinsky parameter Cs, turbulent Prandtl number and turbulent Schmidt number are assumed constant and equal to 0.10, 0.5 and 0.5 respectively. The model constants in equation (6), C_{pg} is assumed constant as 0.5, which is nearly equal to the value of wrinkled premixed flames. a_q is 550 [1/s] of quenching value of the counter-flow laminar methane-air flame and $m = n = 1$ is used in this paper. C_q is optimized as 0.3 based on the experimental results that the maximum value of the propagation velocity at the flame base was near $3S_L^0$

Inlet condition of the axial velocity is determined as:

$$u_{axial} = \langle u \rangle + \left\langle \sqrt{u'^2} \right\rangle F_m \qquad (19)$$

$$F_m = \sum_{m=0}^{6}\left[\sin(m\theta - 2\pi \cdot f_F \cdot t) + 0.05\sin(m\theta - 2\pi \cdot f_U \cdot t)\right] \qquad (20)$$

where $\langle u \rangle$ and $\left\langle \sqrt{u'^2} \right\rangle$ are time averaged axial velocity and intensity, determined to assume that the inside flow of fuel tube is fully developed turbulence, m is mode number, θ is azimuth, f_F and f_U are the frequency of the inlet instability.

The perturbed axial velocity is obtained by superimposing rotating helical and axial instability. It is well known that a length of core region of the jet is dominated by the inlet condition. The instability mode is added in the present work. f_F and f_U are determined as Strouhal number is 0.65 and 0.25 respectively [15].

Zero-gradients are posed for the mixture fraction and the pressure on the side boundary and slip wall conditions are used for velocity components. The entrainment on the side boundary is assumed to be negligible because of a co-flowing air stream in the present calculation. The outlet boundary condition of the pressure p is set to the zero-gradient and the outlet boundary of transport variables is obtained from the convective boundary conditions.

In this paper, 3 conditions are taken as test case shown in table.2.

where $Ujet$ is the fuel jet velocity, Uco is the co-flowing air velocity.

Table 2 Test case

FLAME A:	$Ujet = 15[m/s], Uco = 0.74[m/s], \mathrm{Re} = 4100$
FLAME B:	$Ujet = 25[m/s], Uco = 0.74[m/s], \mathrm{Re} = 6900$
FLAME C:	$Ujet = 15[m/s], Uco = 0.34[m/s], \mathrm{Re} = 4100$

In order to verify the prediction of lift-off heights, it is needed the condition of the co-flowing air velocity constant (FLAME A-B) and the condition of the fuel jet velocity constant (FLAME A-C).

RESULTS

Lift-Off Height and Flame Shape

The computed and experimental results in terms of the lift-off height and the fuel jet velocity are shown in Figure 3.

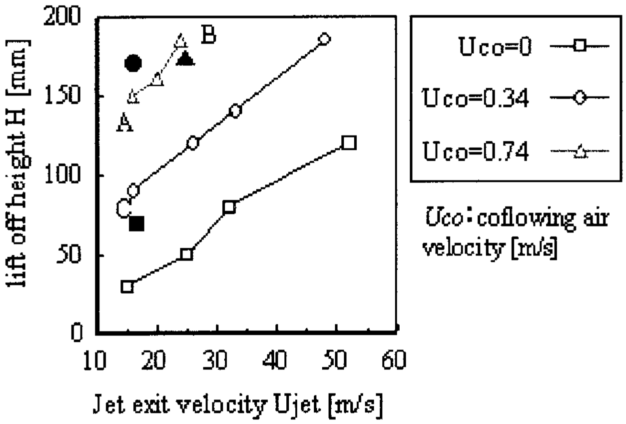

Fig.3 Lift-off point of present calculation
(Present :●FLAME A, ▲FLAME B, ■FLAME C)

Instantaneous distributions of the mixture fraction and the iso-surface of G=0.5 for the cases A and C are shown in Figure 4 and 5, respectively. It is seen that a value of the co-flowing velocity has significant effect on the flame-front position. According to the classification [10] of lifted jet flames by the flame base position shown in Fig.6, it seems that FLAME A and B is to be in the state of the triple flame propagation, whereas FLAME C is close to the state of the edge flame extinction.

In the present work, the calculation of the subgrid burning velocity was made of equation (15), in which the parameters m and n were merely set to 1.0. No attempts to adjust these parameters were undertaken. It is thought parameter n may relate to the Fractal dimension of a wrinkled turbulent premixed flame. The Direct Numerical Simulation of a lifted jet flame could provide data for correcting values of all the parameters n, m and Cq.

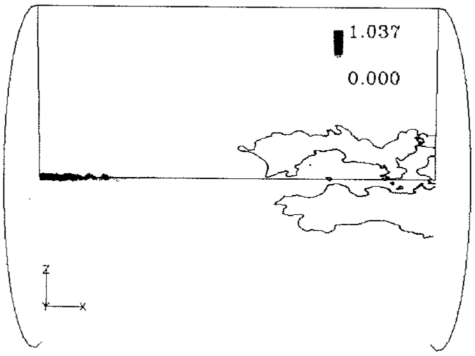

Fig.4 Instantaneous distribution of mixture fraction and wrinkling flame iso-surface G=0.5 ,FLAME A

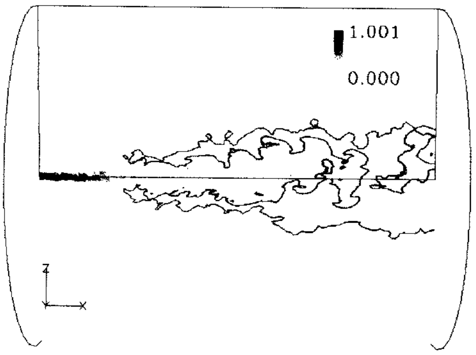

Fig.5 Instantaneous distribution of mixture fraction and wrinkling flame iso-surface G=0.5 ,FLAME C

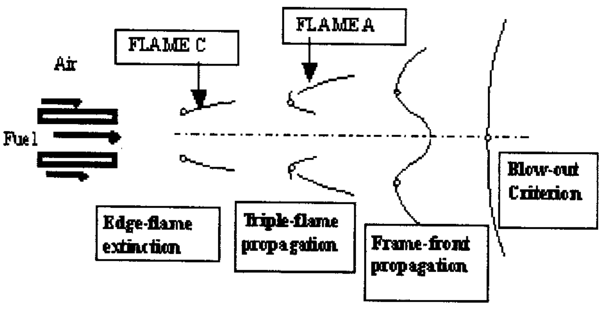

Fig.6 Classification by the position of the flame base [10]

Conditional Velocity On The Flame Base

It is thought that the balance of conditional axial velocity and subgrid burning velocity is important for a stabilization of a lifted non-premixed flame. The condition of G=0.01 and $S_T/S^0_{L\max} > 0$ is chosen as the surface index of flame base. In the present modeling, the thermal expansion occurs in the region of 0<G<1 because of the assumption that the reaction progress variable c has the same profile as the scalar G. On the surface of G=0.01, the temperature is about 18[K] higher than the inlet temperature. The conditional averaged axial velocity component on the flame base of FLAME A and C are shown Fig .7 and 8, respectively. The averaged value of the conditional axial velocity and the standard deviation σ are shown in Table 3. The conditional velocity in the case of FLAME A is mainly scattered in the range of $U_X/S^0_{L,\max} < 3$, while $U_X/S^0_{L,\max} < 2$ corresponds to the case of FLAME C. These results are in an agreement with the experimental data of Múniz and Mungal [8], Han et al [11].

In Fig.9, the conditional axial velocity data are shown versus the conditional subgrid burning velocity in the case of FLAME A. The points in the region $S_T > U_X$ correspond to forward flame propagation. It can also be seen that many points correspond to cases when the subgrid burning velocity is smaller than the axial velocity. In total, we can see that the points with coordinates (S_T , U_X) group near the line S_T = U_X in the wide region. In addition, it should be noted the number of points in the region under the line S_T = U_X is larger than that for the other region. This clearly indicates that a leading edge flame on **the grid scale** contributes into the flame stabilization similarly to that for a laminar triple flame, that is, the propagation velocity of the flame base in the present result is larger than the subgrid burning velocity.

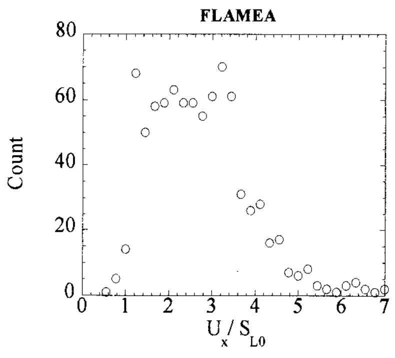

Fig.7 conditional axial velocity component near the flame base G=0.01(FLAME A)

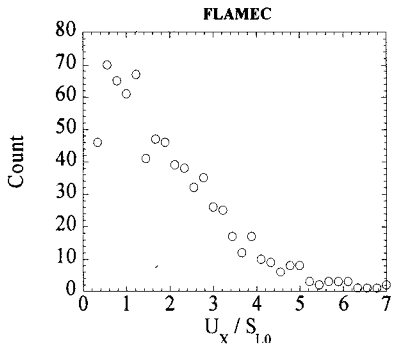

Fig.8 conditional axial velocity component near the flame base G=0.01(FLAME C)

Table 3 Cond. axial velocity near the flame base

A: $\left\langle U_X / S^0_{L,\max}\big\|_{G=0.01} \right\rangle = 2.69$, $\sigma = 0.68$, *total* : 842*counts*
C: $\left\langle U_X / S^0_{L,\max}\big\|_{G=0.01} \right\rangle = 1.84$, $\sigma = 0.99$, *total* : 786*counts*

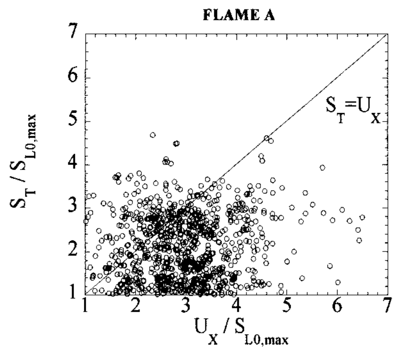

Fig.9 conditional axial velocity component and conditional subgrid burning velocity near the flame base G=0.01 (FLAME A)

SUMMARY

This paper concerned with LES of methane-air lifted jet flames. The two-scalar flamelet model was used for simulating partially premixed flames. The subgrid burning velocity model was proposed. It assumes that small triple flames take place on the subgrid scale level. Simulation results show that the difference of the lift-off height and the flame-shape with the variation of the co-flowing velocity can qualitatively be predicted. It have been also confirmed that the conditional axial velocity near the flame base is of two - three times of that for the laminar burning velocity, which agrees well with the experimental data.

Our approach to modeling the lifted jet flames based on the assumption associated with the flame stabilization mechanism. -The existence of small structure of triple flames on the flame base and their projection into unburnt gas are assumed on the subgrid scale level-. Calculation results indicate that the present modeling expresses not only that effect but also a contribution of a leading edge flame into the stabilization mechanism similar to that for a laminar triple flame on the grid scale level.

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