

A NUMERICAL STUDY ON FLAME STABILITY AT THE TRANSITION POINT OF JET DIFFUSION FLAMES

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Flame stability of a fuel jet diffusion flame was studied numerically by using finite rate chemistry. The flow is time dependent and plane two-dimensional, and the chemical reaction is described by simplified, overall one-step kinetics. The variable parameters are the jet Reynolds number, Re_0 , and Damköhler number, Da_0 ; and three types of flame stability behavior were observed depending on values of these parameters. The first one is the local and occasional extinction at the transition point from a laminar to a turbulent flame. When Re_0 is kept at a rather high value and Da_0 is decreased, local extinction at the transition point begins to occur at a certain critical value. The occasional extinction is caused at the instant when the local scalar dissipation rate in the reaction zone becomes too large, producing a rupture in the reaction zone layer. The rupture is quickly connected again to recover the continuous reaction zone layer. As Da_0 is decreased further, however, the frequency of rupture increases, and at another critical value, complete extinction is produced at the transition point, leaving a short, residual rim flame immediately downstream of the injector. This is the second type of flame stability. As Da_0 is decreased further, the third and final flame stability characteristic is observed: the blow-off of the whole flame from the injector rim. When the flame is extinguished completely at the transition point, most of the injected fuel flows downstream as a fuel jet entraining the surrounding air to produce a lifted, turbulent diffusion flame in the downstream flow. This study of the structure of the flame has shown that it is actually an ensemble of instantaneous local premixed, diffusion, and partially premixed flames.

Introduction

The fuel jet diffusion flame is one of the most important flames in terms of fundamental and practical interests. In particular, the flow stability and the flame stability in this flame have been the subjects of many investigations. We have studied numerically the flow stability problem to show that the decreased density and the accelerated transport properties in the flame play significant roles in the transition from a laminar to a turbulent flame [1]. Furthermore, the subsequent study has made clear that the behavior of the induced flow and flame fluctuations in the downstream flow are crucially affected by the same effects [2]. These studies are concerned mainly with the flow problem: the stability of eventually laminar jet flow and the behavior of large-scale fluctuations in the transitional region. The direct effects of chemical reactions are not important in these problems. It is the resulting variations in temperature and density that play decisive roles. The flame surface model of infinite reaction rate has been successfully applied, since time scales of molecular transport processes and of the flow processes are much larger than those of chemical reactions [3]. A similar approach has been successfully applied to the understanding of time-dependent behavior of a buoyant jet diffusion flame [4].

Now, we turn to the flame stability problem. Our old experiment [5] and recent experiments by other investigators [6–8] have shown that there are three types of flame stability: the local and occasional extinction at the transition point, the complete extinction at this point leaving a small residual flame immediately downstream of the fuel injector, and the blow-off of the whole flame from the injector rim. In the present study, a numerical study will be made to understand this stability behavior. Since the extinction is caused as a result of finite rate chemistry, we cannot adopt the simplified flame surface model. However, we are interested only in elucidating essential features of the phenomena, and hence, need not be involved in detailed chemical kinetics. The simple, overall one-step kinetics should be enough. In addition, we make a plane, two-dimensional flow calculation, in spite of the fact there are no strictly two-dimensional jets. We believe that the underlying physics should remain the same for planar and three-dimensional flame jets, and we want to understand this physics through making a numerical experiment [2,3].

The main parameters in the nondimensional flow system are the jet Reynolds number and Damköhler number. The former determines the intensity of induced-flow fluctuations at the transition point, while

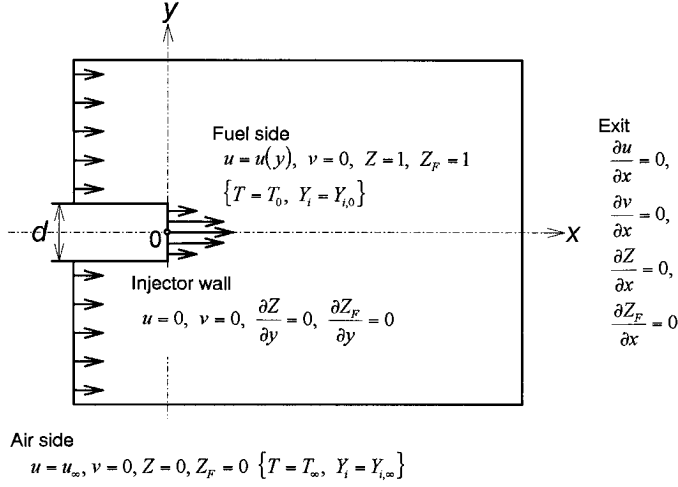


FIG. 1. Theoretical model of plane, two-dimensional jet diffusion flame and boundary conditions.

the latter represents the ratio of flow time to reaction time, and hence, the flame strength against the flow fluctuation. The combination of these two parameters will determine the flame stability. However, the extinction at the transition point is an instantaneous and local phenomenon, and we need another physical quantity to describe this phenomenon. The instantaneous and local flame stretch is one possibility. However, the flow velocity is a vector quantity and it is rather difficult to evaluate accurately the stretch in the calculation. Instead, we adopt the scalar dissipation rate [3,9,10]. This is a scalar quantity and is relatively easy to calculate. In addition, it has a definite physical significance: the inverse of the characteristic diffusion time in the outer diffusion layer surrounding the narrow reaction zone [3]. In this study, therefore, we try to understand the extinction phenomenon at the transition point in terms of this quantity. In addition, we will try to understand the turbulent flame structure in the downstream flow when the flame is extinguished completely at the transition point, and for that purpose we will introduce another physical quantity. The stability and combustion mechanism of this lifted flame is controversial and has been the subject of recent concern [11,12].

Model and Assumptions

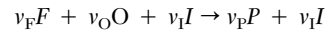
The model and assumptions are the same as those of the previous studies [1,2] except for the finite rate chemistry, and so will be described here very briefly. The analytical model is shown in Fig. 1. The flow is time dependent and plane two-dimensional. A Cartesian coordinate system is taken such that x is the principal flow direction, y is the transverse direction, and the origin is at the center of the injector exit plane. The fuel is injected through an injector of

width d with a fully developed velocity distribution with mean velocity u_0 , uniform temperature T_0 , and mass fraction $Y_{i,0}$ of species i , into a coflowing air stream of velocity u_∞ , temperature T_∞ , and mass fraction $Y_{i,\infty}$. The thickness of the injector plates separating air from fuel is assumed to be zero, and the boundary layer is developed naturally on the air side as it flows along the plates. To stabilize the diffusion flame, an ignition source is placed at the injector rim, and the temperature of the source is set equal to the adiabatic flame temperature of the stoichiometric mixture. The blow-off of the flame from the injector rim depends crucially on this ignition source.

The boundary conditions are the ordinary ones and are described in Fig. 1. The initial condition is that the fuel is injected suddenly at time 0. First, under this initial condition, the calculation with sufficiently large Damköhler number is performed to produce the stable flame. Then Damköhler number is decreased to a specified value, and the calculation is continued until we obtain the flame behavior in the later stage when sufficient time has elapsed for the effects of the initial condition and the excessive Damköhler number to have worn off completely. No artificial disturbances are added to the flow, and the fluctuations appear spontaneously if the flow is unstable [1].

The actual calculation was done in terms of non-dimensional quantities, in which the reference length is d , the reference velocity is u_0 , the reference time is d/u_0 , and the values of the injected fuel are used as reference for other dependent variables.

The mixture undergoes an overall, one-step irreversible reaction with a finite reaction rate described by



where v_i is the stoichiometric coefficient of species i .

The species F, O, I, and P represent fuel, oxygen, nitrogen, and product, respectively. The nondimensional reaction rate w_F is given by the following expression in terms of the Damköhler number, Da_0 , and nondimensional activation energy ε :

$$w_F \equiv -\frac{m_F v_F \hat{\omega}}{\rho_0 u_0 d} = -Da_0 \rho^{v_F + v_O} Y_F^{v_F} Y_O^{v_O} \exp\left(-\frac{\varepsilon}{\theta}\right)$$

$$Da_0 = \left(\frac{d}{u_0}\right) B_1 \frac{\rho_0^{v_F + v_O - 1} v_F}{m_F^{v_F - 1} m_O^{v_O}}$$

$$\varepsilon = E_1 / R^0 T_0$$

where m_i is molecular weight of species i , R^0 is the universal gas constant, B_1 and E_1 are the frequency factor and the activation energy, respectively, for the overall one-step reaction.

The dependent variables are the axial velocity u , the transverse velocity v , the mixture fraction Z , and the normalized fuel mass fraction Z_F . The mixture fraction Z is defined as

$$Z \equiv \frac{Y_I - Y_{I,\infty}}{Y_{I,0} - Y_{I,\infty}} = \frac{Y - Y_\infty}{Y_0 - Y_\infty} = \frac{h - h_\infty}{h_0 - h_\infty}$$

where Y is given by the coupling functions

$$Y = \frac{Y_F}{m_F v_F} - \frac{Y_O}{m_O v_O} = \frac{1}{m_F v_F} (Y_F - Y_O / j) \text{ or}$$

$$Y = \frac{Y_F}{m_F v_F} + \frac{Y_P}{m_P v_P} = \frac{1}{m_F v_F} \{Y_F + Y_P / (j + 1)\}$$

$$j = m_O v_O / m_F v_F$$

and h is the sum of the thermal and chemical enthalpy. The apparent flame surface location is defined with the position where Z becomes equal to Z^* , given by the equation

$$Z^* \equiv -\frac{Y_{F,\infty} - Y_{O,\infty}/j}{(Y_{F,0} - Y_{O,0}/j) - (Y_{F,\infty} - Y_{O,\infty}/j)}$$

The normalized fuel mass fraction Z_F is defined as

$$Z_F \equiv \frac{Y_F - Y_{F,\infty}}{Y_{F,0} - Y_{F,\infty}}$$

Only concentration diffusion, with the same diffusion coefficient for all species, is considered. The specific heat at constant pressure is assumed constant, and the Lewis number $Le = \lambda / \rho c_p D$ is equal to unity. The nondimensional viscosity coefficient μ and the nondimensional diffusion coefficient D depend on the nondimensional temperature θ in the following manner [13]:

$$\mu = \theta^{0.7}, D = \theta^{1.7}$$

The conservation equations for mass and momentum and the equations for Z and Z_F are given in the following nondimensional forms:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial(\rho u_m)}{\partial t} + \nabla \cdot (\rho \mathbf{v} u_m) - \frac{1}{Re_0} \nabla \cdot (\mu \nabla u_m)$$

$$= -\frac{\partial P}{\partial x_m} + \frac{1}{Re_0} \left(-\frac{\partial \mu}{\partial x_m} \frac{\partial u_i}{\partial x_j} + \frac{\partial \mu}{\partial x_j} \frac{\partial u_i}{\partial x_m} \right)$$

$$\frac{\partial(\rho Z)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Z) - \frac{1}{Re_0 Sc_0} \nabla \cdot (\rho D \nabla Z) = 0$$

$$\frac{\partial(\rho Z_F)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Z_F) - \frac{1}{Re_0 Sc_0} \nabla \cdot (\rho D \nabla Z_F)$$

$$= \frac{w_F}{Y_{F,0} - Y_{F,\infty}}$$

where Reynolds number and Schmidt number are defined by $Re_0 = \rho_0 u_0 d / \mu_0$ and $Sc_0 = \mu_0 / \rho_0 D_0$. The equation of state is

$$p = \rho R^0 T \sum_i \frac{Y_i}{m_i}$$

The local and instantaneous nondimensional scalar dissipation rate is defined by $D|\nabla Z|^2$ in terms of the gradient of mixture fraction and the nondimensional diffusion coefficient.

Numerical Method

The numerical calculation was done by using the finite-difference approximation. The technique adopted was the SIMPLE method developed by Patankar, and the QUICK scheme was used for convective terms [1,2]. The time advance was made by using the implicit method with second order precision, and an interval of the nondimensional time is 0.2. The iteration was made by the SOR method. The grid numbers were 221 and 141 in the x and y directions, respectively. The computation domain is $x = -28.4$ to 50.0 and $y = -14.9$ to 14.9 .

The fuel adopted was methane, and air was assumed to be composed of 79% N_2 and 21% O_2 by volume, to give $j = 4.0$, $Y_{I,\infty} = 0.767$, and $Y_{O,\infty} = 0.233$. The pressure was atmospheric, and the co-flowing air and the injected fuel were at room temperature. The velocity ratio was $u_\infty / u_0 = 0.1$, the Schmidt number was $Sc_0 = 0.7141$, and the nondimensional activation energy was fixed at $\varepsilon = 52.3$ corresponding to $E_1 = 31.2$ kcal/mol [14].

Results and Discussion

The variable parameters are the jet Reynolds number, Re_0 , and Damköhler number, Da_0 . The calculation was done for $Re_0 = 1000$ to 2000 and $Da_0 = 10^4$ to 10^9 .

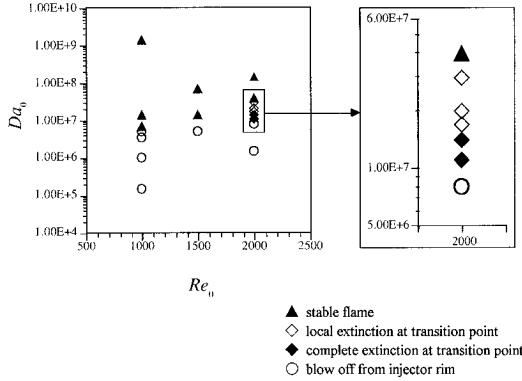
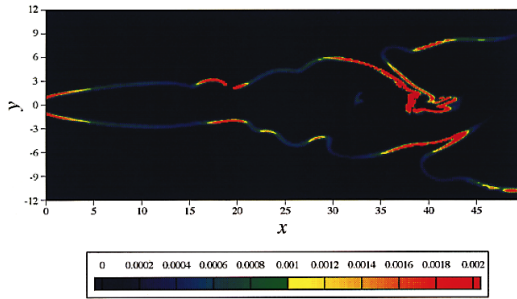


FIG. 2. Flame stability diagram.

FIG. 3. Instantaneous distribution of reaction rate for $Re_0 = 2000$ and $Da_0 = 2.0 \times 10^7$.

Flame Stability

Three types of flame stability behavior were observed, in agreement with the experimental observations, in the range of variable parameters in the present calculation as shown in Fig. 2. The first one is the local and occasional extinction at the transition point from laminar to turbulent flame, and the second one is the complete extinction at this point, leaving a stable, short, residual rim flame immediately downstream of the injector. The third one is the blow-off of the whole flame from the injector rim. All three types of flame stability behavior occur in the case of $Re_0 = 2000$. In the cases of $Re_0 = 1000$ and 1500 , however, the local and the complete extinction at the transition point do not occur, and the flame blows off directly from the injector rim, because for these rather small Reynolds numbers the fluctuation induced by the flow instability at the transition point is not large enough to quench the flame, and the effect of the velocity shear layer at the injector rim is stronger. For a fixed value of $Re_0 = 2000$, the local extinction begins to occur at a certain critical value of Da_0 , and the complete extinction is caused at another smaller critical value. As Damköhler number is decreased further, the flame blows

off at a third critical value. The critical values increase with Re_0 . These stability behaviors correspond to the earlier experimental observation [5].

Local Extinction

The instantaneous distribution of reaction rate for $Re_0 = 2000$ and $Da_0 = 2.0 \times 10^7$ is shown in Fig. 3. As can be seen in this figure, the chemical reaction is concentrated in rather narrow reaction zone layers. In the part of this layer in the upstream portion of the laminar flame, the reaction rate decreases gradually toward the downstream direction, while it increases and decreases locally near the transition point. In the vicinity of this point, local extinction is observed at the upper reaction zone layer ($x = 19$ and $y = 2$). To show how this extinction is produced, the time sequences of relative velocity vectors, reaction rate, temperature, and scalar dissipation rate are shown in Fig. 4 where the time advances to the right with a nondimensional time interval $\Delta t = 3.2$. In the figures, the solid curves represent the loci of the position where the reaction rate is one-tenth of the maximum reaction rate.

The arrows in Fig. 4a indicate the velocity vectors relative to an arithmetic average of maximum and minimum velocities at each x cross section, and we can see how the vortex-like convective flow fluctuations are induced by the flow instability. These fluctuations produce the local and occasional increase in the concentration gradients of fuel and oxygen in the vicinity of the reaction zone layer. Then fuel and oxygen supplies to the reaction zone increase accordingly to yield an increase in the reaction rate. However, since the temperature gradient simultaneously becomes larger, if the increase becomes too large, the heat flow by heat conduction to both sides of the flame can no longer be balanced by heat release due to the reaction, leading to a local extinction [9]. This process is shown in Fig. 4b,c, and it can be seen more clearly in Fig. 4d, in which the scalar dissipation rate SDR is shown. The latter represents the gradients of concentrations and temperature. As is described before [3,10], the large scalar dissipation rate is produced in the diffusion layers inside the portion of upstream laminar flame to make two parallel layers of high dissipation rate. At the transition point, the layers are broken off to produce islands shedding downstream, like Karman's vortex street. In the shedding islands, the dissipation rate decreases gradually by molecular diffusion on one hand, but on the other hand it increases drastically by convective flow fluctuations to shake the movement of the islands. The local extinction is caused at the instant when this island hits the thin reaction zone outside the diffusion layers to yield a rupture in the continuous reaction zone layer. However, the extinction is occasional and the extinguished zone is connected again quickly to recover a continuous

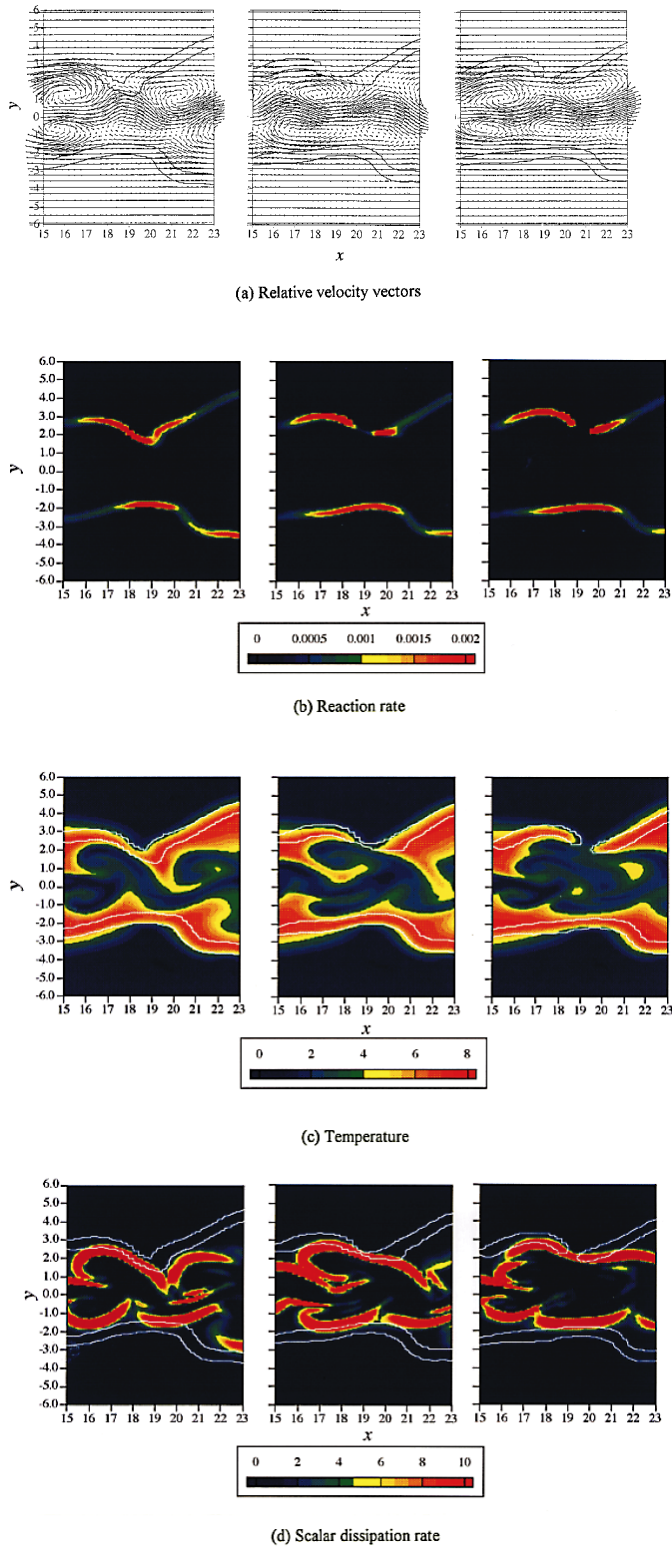


FIG. 4. Time sequence leading to local extinction for $Re_0 = 2000$ and $Da_0 = 2.0 \times 10^7$. (a) Relative velocity vectors; (b) reaction rate; (c) temperature; (d) scalar dissipation rate.

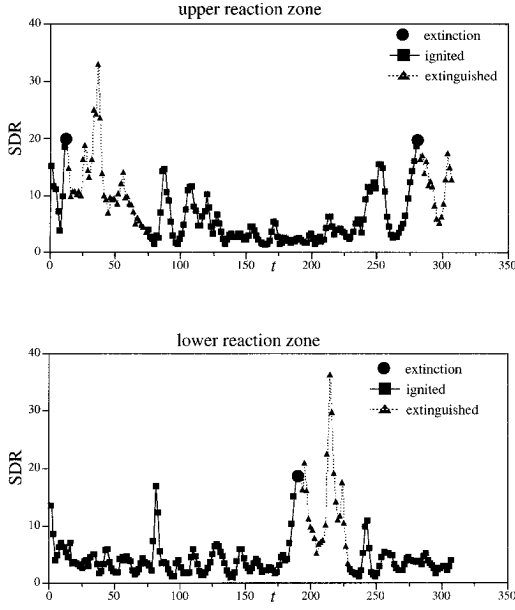


FIG. 5. Time history of maximum scalar dissipation rate near transition point for $Re_0 = 2000$ and $Da_0 = 2.0 \times 10^7$.

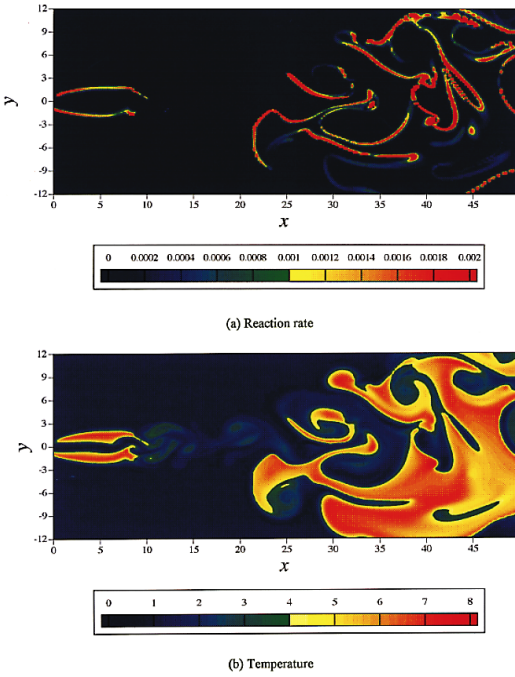


FIG. 6. Instantaneous distributions of reaction rate and temperature for $Re_0 = 2000$ and $Da_0 = 1.4 \times 10^7$. (a) Reaction rate; (b) temperature.

layer. This behavior of local extinction is actually observed in a recent experiment [8], as well as in our old experiment [5]. In this way, the extinction at the transition point is closely related to the dynamics of the island of high scalar dissipation rate.

The time history of maximum scalar dissipation rate at the apparent flame surface, defined by $Z = Z^*$, near the transition point is shown in Fig. 5. The upper and the lower figures correspond to the upper and the lower flame surfaces. The symbol \bullet represents the instant when the extinction occurs. The symbols \blacksquare and \blacktriangle represent the ignited and the extinguished states. It was found that the local extinction at the transition point is caused at the instant when the local scalar dissipation rate at the apparent flame surface exceeds a certain value (the critical value is approximately 20), and the unburned mixture is ignited again to resume the continuous reaction zone when the local scalar dissipation rate becomes fairly small.

Complete Extinction and Convective Turbulent Flame

The instantaneous distributions of reaction rate and temperature for $Re_0 = 2000$ and $Da_0 = 1.4 \times 10^7$ are shown in Fig. 6. As Da_0 is decreased, the frequency of the rupture in the reaction zone at the transition point increases, leading finally to the complete extinction. Then, the short laminar flame remains at the injector rim, most of the injected fuel flowing downstream without combustion, and a convective turbulent flame is produced in the downstream region. Although the detailed flame structures are unsteady and move back and forth incessantly, the flame as a whole remains stationary at a certain fixed position. The flame corresponds to a lifted flame, the stability and the combustion mechanism of which have been the subject of recent interest [11,12]. To understand the structure of the flame, we introduce two parameters Z_{FO} and G_{FO} defined as

$$Z_{FO} = \frac{Y_O}{j} \quad \left(\frac{Y_O}{j} \leq Y_F \right)$$

$$\text{or } Z_{FO} = -Y_F \quad \left(\frac{Y_O}{j} \geq Y_F \right)$$

$$G_{FO} = \text{grad}Y_F \cdot \text{grad}Y_O$$

Z_{FO} may be interpreted as a measure of mixedness of unburned fuel with oxygen coming from the surrounding air. Z_{FO} is positive for the fuel-rich mixture and negative for the fuel-lean mixture, and the absolute value of Z_{FO} increases as the mixedness of mixture increases. G_{FO} may be interpreted as a flame index to distinguish premixed flames from diffusion flames. G_{FO} is positive for a premixed flame and negative for a diffusion flame, and the absolute

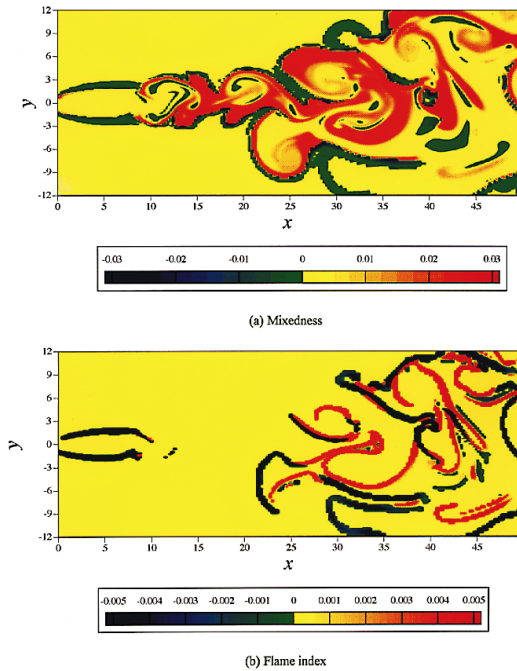


FIG. 7. Instantaneous distributions of mixedness and flame index for $Re_0 = 2000$ and $Da_0 = 1.4 \times 10^7$. (a) Mixedness; (b) flame index.

value increases as the supplying rate of fuel and oxygen by molecular diffusion increases. The instantaneous distributions of Z_{FO} and G_{FO} corresponding to Fig. 6 are shown in Fig. 7. As shown in Fig. 7a, when the flame is extinguished completely at the transition point, the unburned fuel flows downstream as a fuel jet entraining the surrounding air to produce a lifted turbulent diffusion flame in the downstream flow. The present study has revealed that the entrainment of the air is made mostly by a large-scale vortex motion, resulting in a variety of separated fuel-rich, well-mixed, and fuel-lean regions of vortex size. As shown in Fig. 7b, the convective turbulent flame in the downstream region is composed of an ensemble of instantaneous local premixed, diffusion, and partially premixed flames.

Conclusions

The present numerical study on the flame stability of a fuel jet diffusion flame has led to the following conclusions:

1. Three types of flame stability were observed depending on jet Reynolds number Re_0 and Damköhler number Da_0 . The first one is the local and occasional extinction at the transition point from laminar to turbulent flame, and the second one

- is the complete extinction at this point, leaving a stable, short, residual rim flame immediately downstream of the injector. The third one is the blow-off of the whole flame from the injector rim.
2. For a given set of values of Re_0 and Da_0 , the local extinction at the transition point is caused at the instant when the local scalar dissipation rate at the thin reaction zone becomes large.
3. When the flame is extinguished completely at the transition point, a lifted, convective turbulent flame was produced in the downstream flow. The turbulent flame structure is an ensemble of instantaneous local premixed, diffusion, and partially premixed flames.

Acknowledgments

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COMMENTS

Yung-cheng Chen, Tchinhua University, Taiwan. You have found that local extinction can occur when the scalar dissipation rate is above certain limit. Have you also checked that flame quenching can also happen if the strain rate is above certain limit?

Author's Reply. There are great difficulties in technique and accuracy to evaluate the instantaneous and local strain rate (SR) or the flame stretch at the apparent flame surface in the unsteady and multi-dimensional flow field such as the present flame jet, because the flow velocity is a vector quantity and the determination of the velocity relative to the fluctuating flame surface is required. Therefore, we could not obtain the limit value of SR.

Moreover, it should be emphasized that the instantaneous and local scalar dissipation rate at the apparent flame surface (SDR) is the most appropriate parameter to describe the flame behavior in the general flow field where the convection tangent to the flame and the unsteady effect play an important part as well as the convection across the flame. The reason is that SDR is directly connected to the concentration and temperature field, and it is a measure of

the rate of diffusion of reactants into the reaction zone layer [1]. For example, Nishioka et al. [2] suggested that SDR is the most appropriate parameter to link the laminar jet diffusion flame with the laminar counter-flow flame.

It has been found that SR has one-to-one correspondence to SDR in the well-known flow field such as the counter-flow flame [3], and the limit of SDR corresponds to that of SR. However, such a simple one-to-one correspondence does not exist in the above-mentioned general flow field.

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