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Laminar Diffusion Flame in the Reacting Mixing Layer

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Laminar flows in which mixing and chemical reactions take place between parallel streams of reactive species are studied numerically. The governing equations for laminar flows are from two-dimensional compressible boundary-layer equations. The relevant chemistry is a finite rate single step irreversible reaction with Arrhenius kinetics. Ignition, premixed flame, and diffusion flame regimes are found to exist in the laminar reacting mixing layer at high activation energy. At high Mach numbers, ignition occurs earlier due to the higher temperatures in the unburnt gas. In diffusion regimes, property variations affect the laminar profiles considerably and, thus, need to be included when there are large temperature differences. The maximum temperature of a laminar reacting mixing layer is in the almost linear relationship with the adiabatic flame temperature at low heat release, but is only weakly linearly-correlated at high heat release.

Key Words : Ignition, Premixed Flame, Diffusion Flame, Laminar Flame, Reacting Mixing Layer, Numerical Simulation

1. Introduction

Reacting free shear layers occur in many systems, including gas turbine combustors and rockets. Chemical reaction can occur when the reactants are molecularly mixed. However, short residence times require efficient mixing between the fuel and oxidizer. This is especially important for air-breathing ramjets. Fast mixing requires the flow to be vigorously turbulent, which requires the laminar flow to be unstable. The usual reacting mixing layer consists of two-fluids streams, one containing the fuel and the other, the oxdizer. The large temperature change caused by the combustion alters the thermodynamic properties of the flow considerably and produces dilatation ; both of these effects cause a strong interaction between the hydrodynamics and the chemistry, making the study of reacting flows very difficult. The degree of mixing in shear layers depends on the development of flow instabilities. Hence, understanding of the stability characteristics of reacting free shear layers would lead to techniques required for enhancing mixing or controlling the flow. Stability analysis can also be used to predict some characteristics of the turbulent reacting mixing layer. To understand the instability characteristics of the compressible reacting mixing layer, one should understand the physics of the laminar

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diffusion flame, which is the main purpose of this study.

By using activation energy asymptotics, Linan and Crespo (1976) studied the structure of a diffusion flame by only considering the one-dimensional gradient in space normal to the flow direction. They showed that ignition, premixed flame, and diffusion flame regimes exist in the laminar flame. The fuel and the oxidizer are mixed in the ignition regime and are ignited with thermal explosion after some distance. In the ignition regime, the one is higher than the stoichiometric and the other is lower. In the premixed regime, the flame extends to the fuel or the oxidizer until the mixture burns completely. After the premixed flame, there exists the diffusion flame where the fuel and the oxidizer are mixed by diffusion in the direction normal to the flame. The diffusion flame regime covers most of the reacting mixing layer whereas the ignition and the premixed flame regime span only small portion of the flow. These regimes are governed by the non-linear physics, which makes the analysis difficult. Marble and Adamson (1956) assumed the steady two-dimensional shear layer as a boundary layer, and studied the ignition and the diffusion flame by using the method of asymptotics.

In this paper, we numerically simulate laminar flows in which mixing and chemical reaction take place between parallel streams of reactive species. The computed laminar flows provide physical insight on laminar diffusion flames and can serve as inputs to the linear stability studies by Na et al. (2006). The simple model of a reacting mixing layer involves two uniform parallel streams containing both fuel and oxidizer. The chemistry considered is a finite-rate single-step irreversible reaction with Arrhenius kinetics, which is more realistic than the infinite-rate chemistry of the flame sheet model. The physical processes considered are diffusion, reaction and thermal conduction. First, we derive the governing equations for laminar flows from the two-dimensional compressible boundary-layer equations and describe the numerical methodology used to solve them. Simulation results of laminar flows will be presented to illustrate the structure of laminar diffusion flames.

2. Governing Equations and Numerical Method

We consider a plane mixing layer in which the fuel and oxidizer are initially unmixed. In this situation, density variations due to chemical heating or compressibility may affect the velocity field. For this reason, we decided to use the two-dimensional compressible boundary-layer (or thin shear-layer) equation. A schematic of the flow configuration is shown in Fig. 1. To simplify the analysis, we assume that the fast stream contains the fuel and the slow stream, the oxidizer ; U_1 and U_2 represent the free-stream velocities. We also assume the Prandtl and Lewis numbers are unity, which means that temperature and species diffuse at the same rate as momentum. We assume the following power laws in temperature T and pressure P for the transport properties :

$$\mu \propto P^0 T^{0.7}, \ \kappa \propto P^0 T^{0.7}, \ D \propto P^{-1} T^{1.7} \qquad (1)$$

where μ is the viscosity, κ the thermal diffusivity, D and the mass diffusivity. To emphasize the importance of using variable properties, we will compare otherwise identical constant and variable property cases. Chemistry part is treated by a single step irreversible scheme, involving fuel F and oxidizer O, reacting to yield a product P as follows :

$$\nu_F F + \nu_O O \rightarrow \nu_P P \qquad (2)$$

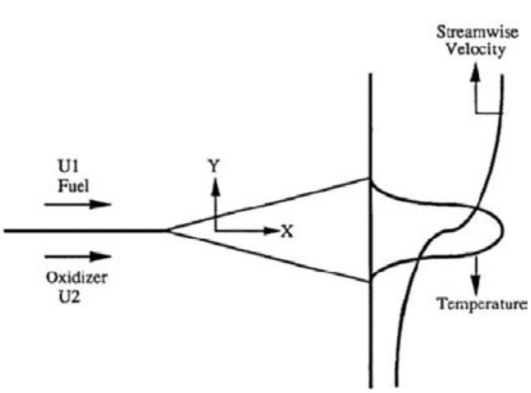


Fig. 1 Schematic diagram of spatially developing shear layer

where ν_F, ν_O, and ν_P are the stoichiometric coefficients for fuel, oxidizer, and product, respectively. For the reaction rate, we assume the Arrhenius law.

The boundary-layer equations for the two-dimensional flow of a compressible perfect gas with zero streamwise pressure gradient and chemical reaction form the basis for the computation. The non-dimensional equations for continuity, momentum, energy and species are given as follow:

$$\frac{\partial \rho u}{\partial x}+\frac{\partial \rho v}{y}=0 \tag{3}$$

$$\frac{\partial \rho u^2}{\partial x}+\frac{\partial \rho v u}{\partial y}=\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right) \tag{4}$$

$$\frac{\partial \rho u T}{\partial x}+\frac{\partial \rho v T}{\partial y}=\frac{1}{PrRe}\frac{\partial}{\partial y}\left(\kappa\frac{\partial T}{\partial y}\right)+\frac{M_1^2(\gamma-1)}{Re}\mu\left(\frac{\partial u}{\partial y}\right)^2 Da\omega_T \tag{5}$$

$$\frac{\partial \rho u y_i}{\partial x}+\frac{\partial \rho v y_i}{\partial y}=\frac{\partial}{\partial y}\left(\rho D\frac{\partial y_i}{\partial y}\right)+\omega_i \tag{6}$$

$$\rho T=1 \tag{7}$$

All varialbles are non-dimensionalized by dividing each dimensional quantity by its corresponding value on the fuel side of the mixing layer and the vorticity thickness. Here, ρ, u, v and T denote the density, velocities in x and y direction, and temperature, respectively. y_i represents the mass fraction of the fuel, air and product. The vorticity thickness of the initial velocity profile, δ_ω, is defined as the reference length scale:

$$\delta_\omega^*=\frac{U_1^*-U_2^*}{|du^*/dy^*|_{\max}} \tag{8}$$

The superscript $*$ means that the variables are dimensional and non-dimensional parameters Re, Pr, Sc and Da are the Reynolds number, the Prandtl number, the Schmidt number and the Damkhöler number, respectively. γ is the specific ratio and M_1 is the Mach number of the fuel stream. The rate of heat release, ω_T and the reaction rate ω_i of species i, are defined as follows:

$$\omega_T=\frac{Q}{W_F\nu_{iF}}(\rho y_F)^{\nu_F}(\rho y_O)^{\nu_O}\exp\left[-\beta'\left(\frac{1}{T}-1\right)\right] \tag{9}$$

$$\omega_i=\frac{W_i(\nu_i''-\nu_i')}{W_F\nu_{iF}}(\rho y_F)^{\nu_F}(\rho y_O)^{\nu_O}\exp\left[-\beta'\left(\frac{1}{T}-1\right)\right] \tag{10}$$

W_i represents the molecular weight and ν_i' and ν_i'' represent the stoichiometric coefficients of the species when appearing as a reactant or product, respectively; thus ν_O' is ν_O, while ν_O'' is zero for the scheme in equation (2). Q is the non-dimensional heat release parameter and can be expressed as follows.

$$Q=\frac{[h_F^0 W_F\nu_F+h_O^0 W_O\nu_O-h_P^0 W_P\nu_P]}{C_P T_{ref}} \tag{11}$$

h_i^0 is the standard heat of formation of species i, C_P is the specific heat of species i and T_{ref} is the reference temperature. The non-dimensional adiabatic flame temperature, T_{ad}, is related to Q in the following manner:

$$T_{ad}=Q+1 \tag{12}$$

The Damkhöler number, Da, and the non-dimensional activation energy parameter, β' are defined by

$$Da=\frac{\delta_{\omega 0}^*}{U_1^*}\Big/\left[\frac{W_F\nu_F}{W_F^{\nu_F}W_O^{\nu_O}}B\rho_1^{*(\nu_F+\nu_O-1)}\exp(-\beta')\right]^{-1} \tag{13}$$

$$\beta'=\frac{E^*}{R_u^* T_1^*} \tag{14}$$

The Damkhöler number is the ratio of a characteristic flow time to a characteristic chemical reaction time. β is the frequency factor, E^* is the activation energy of the reaction and R_u^* is the universal gas constant. In all cases reported here, the stoichiometric coefficients, ν_F and ν_O are equal to 1, the specific heat ratio, γ is set to 1.4, and the non-dimensional activation energy parameter, β' is chosen to be 6 and 20 for comparison.

The above governing equations are mathematically parabolic in both the temporally and spatially developing layers. To solve the equations, we use one of the implicit methods, Crank-Nicolson, which has the second order accuracy with respect to both independent variables. As for boundary conditions, we specify μ, ρ, y_F and as constants as $y \rightarrow \pm\infty$.

$$u=\rho=y_F=1,\ y_O=0,\ \text{as } y\rightarrow\infty \tag{15}$$

$$u=U_2,\ \rho=\rho_2,\ y_F=0,\ y_O=1,\ \text{as } y\rightarrow-\infty \tag{16}$$

Also we need to specify the initial flow field. For a non-reacting compressible mixing layer, we can use self-similar solutions (Sandham and Reynolds, 1989). The initial reactant mass fraction profiles are chosen to be normalized error functions.

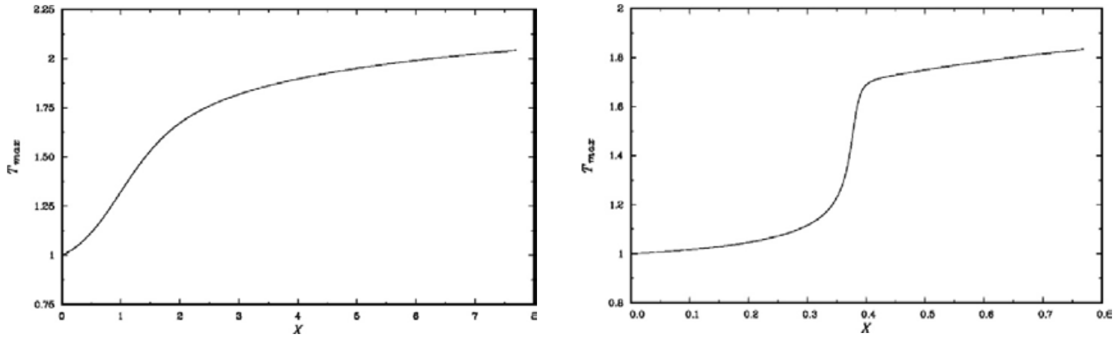
3. Laminar Diffusion Flame

3.1 Ignition, premixed flame, and diffusion flame regimes

By using the method of activation energy asymptotics, Linan and Crespo (1976) investigated the structure of a diffusion flame. They showed that ignition, premixed flame, and diffusion flame regimes exist in the laminar flame. These findings were also confirmed by Jackson and Hussaini (1988) in high speed flow by using the same activation energy asymptotics. In the present work, we also studied these regimes in the compressible reacting mixing layer by taking two different values for the non-dimensional activation energy parameter, $\beta'=6$ and 20. Fig. 2(a) shows the maximum temperature $T_{\max}$ in the profile as a function of streamwise location x for $\beta'=6$, $T_{ad}=4$, $M_1=0$ and $Da=10$. At this level of activation energy, $T_{\max}$ changes smoothly from the initial temperature at $x=0$ to the characteristic value of a diffusion flame. Fig. 2(b) shows the results with the same parameters except now $\beta'=20$. There is a sudden change in the maximum temperature in a thin region around $x=0.37$, which defines the location of a premixed flame ignition zone. At the beginning of this ignition region, the reactants have been mixed but the low temperature is maintained. This implies that there is little reaction taken place. As the reaction begins to take place, the temperature rises and at the same time the reaction rate increases rapidly, creating a premixed flame. Premixed combustion continues until all the premixed gas is consumed. Since the boundary layer equations have parabolic nature, these ignition and premixed flames are not the ones established by heat transfer from the burnt to the unburnt gas region. Thus, the premixed flame is established from the mixing and chemical reaction between the fuel and the air. The similar results have been reported by Linan and Cresop (1976) and Marble and Adamson (1956). These ignition and premixed flame regimes occupy a very small portion of the flow field. A diffusion flame is established just downstream of the premixed flame. This flame occupies the most of the mixing layers.

Figure 3 shows the similar results obtained with $M_1=5$. Theses figures show that the ignition regime exists in supersonic flows if the activation energy is high. They also show the premixed flame regime and the diffusion flame regime. Note that at high Mach numbers the temperatures at $x=0$ increase considerably due to viscous heating.

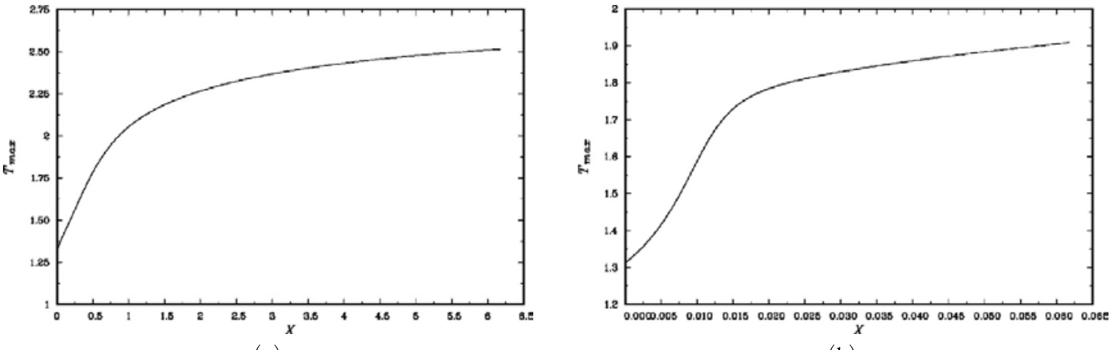
Figure 4 shows contours of temperature, reaction rate and the mass fractions for the conditions of Fig. 2(a). The reaction rate is defined as the consumption rate of the fuel, $Da\omega_F/\rho$. At this level of activation energy, it is hard to distinguish the ignition and premixed flame regimes. Super-



(a) (b)

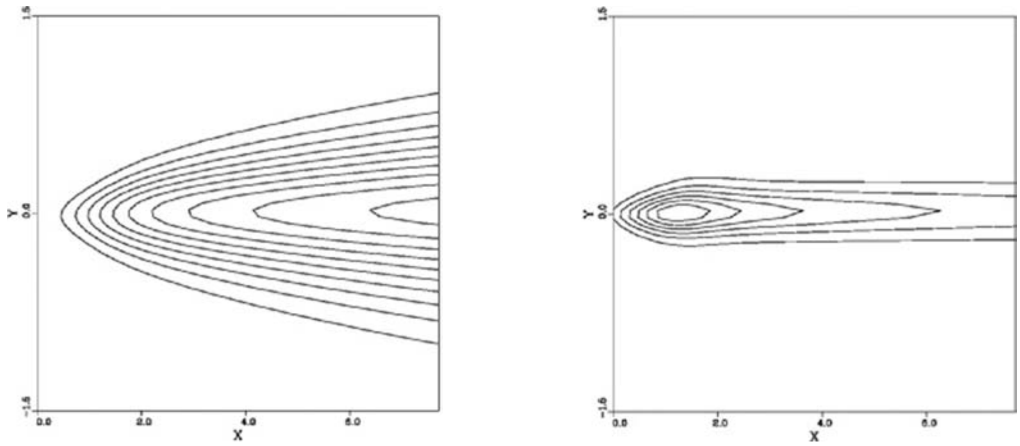
Fig. 2 $T_{\max}$ vs. x. $M_1=0$, $T_{ad}=4$. (a) $\beta'=6$ (b) $\beta'=28$

sonic flows with $\beta'=6$ do not produce qualitatively different results. However, Fig. 5(a) shows the rapid rise of the temperature over a narrow range of x at high activation energy ($\beta'=20$); this is the premixed flame zone. The reaction rate contours show clearly the existence of the three

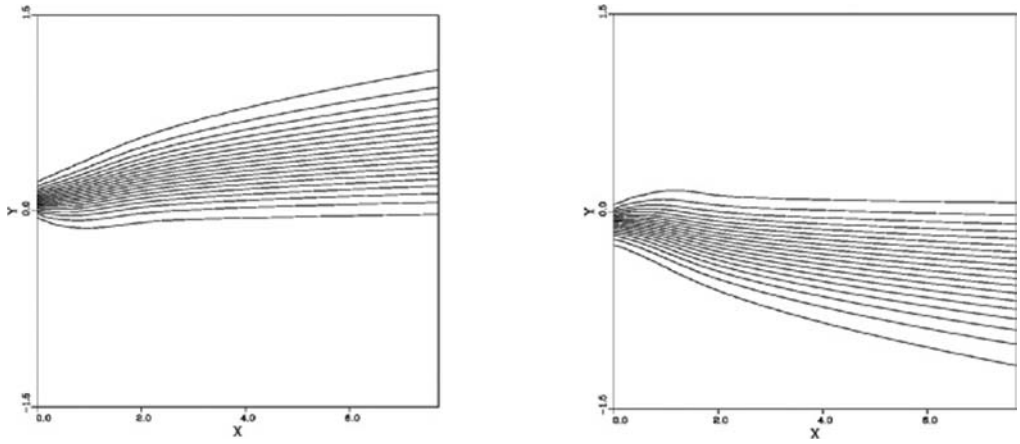


(a) (b)

Fig. 3 $T_{\max}$ vs. x. $M_1=5$, $T_{ad}=4$. (a) $\beta'=6$ (b) $\beta'=20$



(a) min=1, max=2 (b)

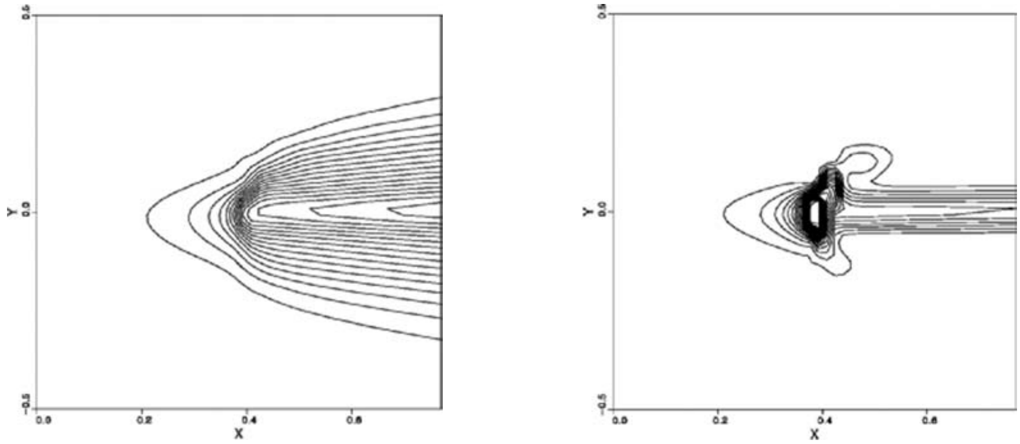


(c) min=0, max=1 (d) min=0, max=1

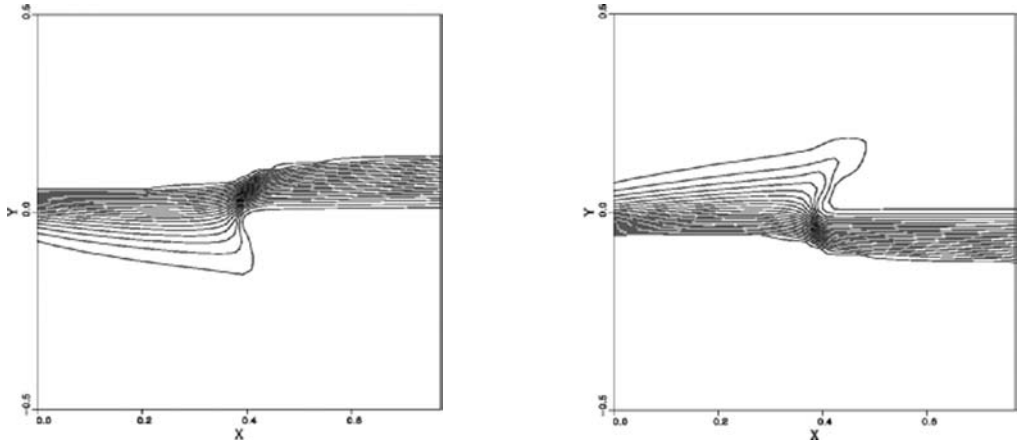
Fig. 4 Contours of the (a) T (b) $Da\omega_F/\rho$ (c) y_F (d) y_O. $\beta'=6$, $M_1=0$, $T_{ad}=4$

regimes. Fig. 5(b) shows that the ignition occurs at about $x=0.37$; this gives rise to an oblique premixed flamelet. This premixed flamelet propagates outward until all of the mixed reactants are consumed. The region of high reaction near the center of the layer just beyond the ignition region is the place for the onset of the diffusion flame. From there on, the diffusion flame behavior is dominant and the flame location is at the centerline of the flow. Fig. 5(c) shows the contours of the mass fraction of the fuel. The mass fraction of the fuel varies from 1 at $y=+\infty$ to 0 at $y=-\infty$. Prior to the ignition, the fuel diffuses from the upper stream into the lower stream. At the premixed flame ($x=0.37$), the premixed fuel is consumed. After the premixed flame, no fuel is found below $y=0$. Fig. 5(d) shows the contours of the mass fraction of the oxygen; its behavior is the reverse of the fuel. Fig. 6 shows the similar results but for $M_1=5$. The behavior described $M_1=0$ also occurs for $M_1>0$. The temperature contours do not exhibit a sharp temperature rise. The reaction rate contours show that the ignition occurs earlier due to the higher temperatures and the premixed flame is less oblique than at low Mach numbers. The mass fraction contours clearly show the existence of the premixed flame regime.

From the above results, we found the ignition, premixed flame, and diffusion flame regimes to exist in the laminar reacting mixing layer at high activation energy. We also found that the ignition

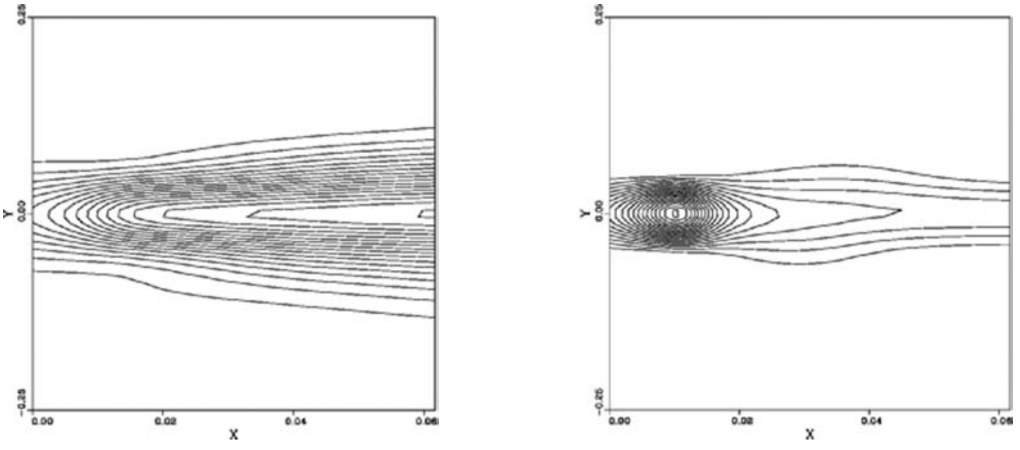


(a) min=1, max=1.6 (b)

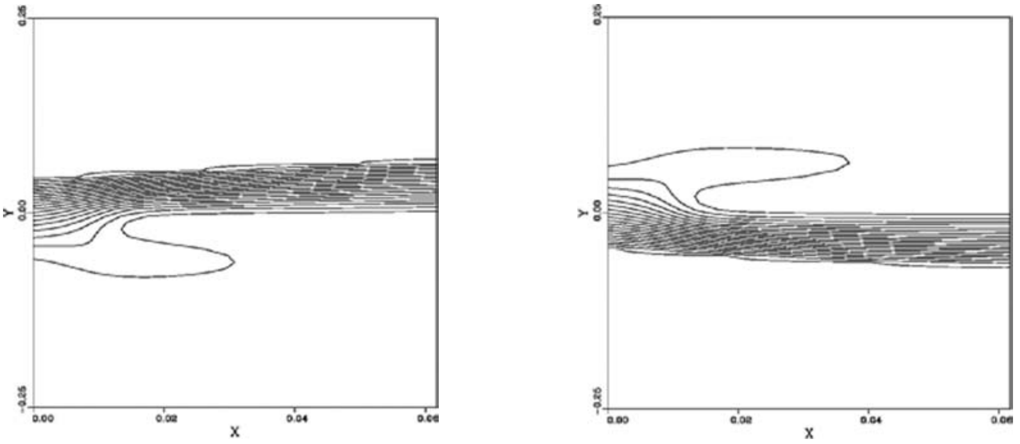


(c) min=0, max=1 (d) min=0, max=1

Fig. 5 Contours of the (a) T (b) $Da\omega_F/\rho$ (c) y_F (d) y_O. $\beta'=20$, $M_1=0$, $T_{ad}=4$



(a) min=1.32, max=1.9 (b)



(c) min=0, max=1 (d) min=0, max=1

Fig. 6 Contours of the (a) T (b) $Da\omega_F/\rho$ (c) y_F (d) y_O. $\beta'=20$, $M_1=5$

occurs earlier due to the higher temperatures in the unburnt gas. In the next section, we will discuss about the structure and characteristics of the diffusion flame zone which occupies most part of the compressible reacting mixing layer.

3.2 Effect of properties and heat release

In order to see the importance of variable properties, a constant property case is compared with the corresponding variable property one for the same inlet profiles. Fig. 7 shows the vorticity thickness versus heat release at the same streamwise location, $x=7.7$. The figure suggests that variable properties affect the profiles considerably and need to be included when there is a large temperature variation. These flows may have significantly different Reynolds numbers, depending on the choice of characteristic shear layer thickness and viscosity.

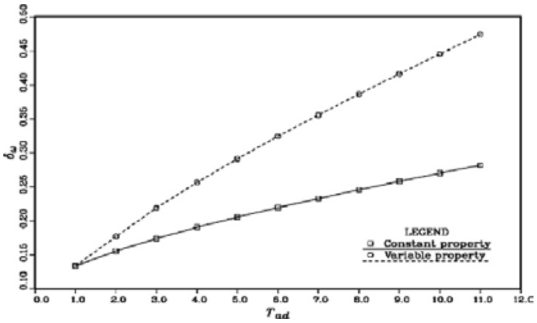


Fig. 7 The growth of vorticity thickness vs. T_{ad}. $Da=10$, $M_1=0$, $x=7.7$

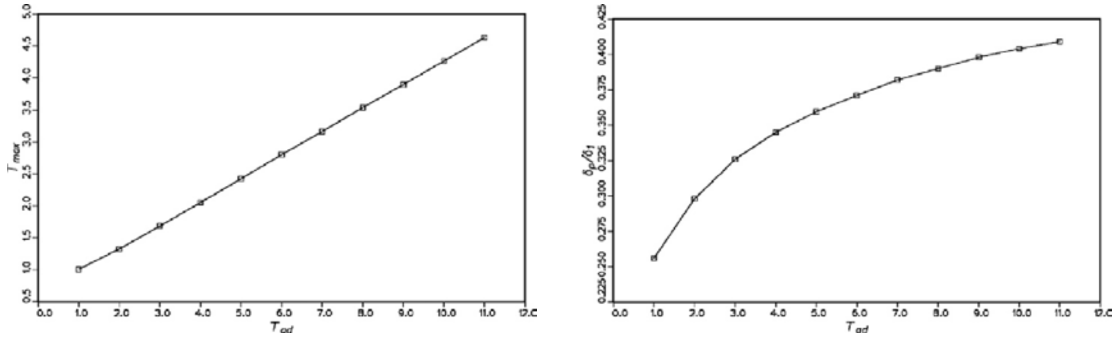
Figure 8 shows the variation of the maximum temperature and normalized product thickness with heat release. The maximum temperature of the layer at a given x changes almost linearly with the adiabatic flame temperature. The product thickness,

$$\delta_P(x) = \int_{-\infty}^{+\infty} y_P(x,y)\,dy \qquad (17)$$

is a good measure of the size of the region occupied by reaction product. We normalize this product thickness with respect to 1% thickness of the layer at the same location, δ_1 (the distance between the points at which the mean product concentration is 1% of its maximum value) ; this has been used as a reference length by various researchers (Mungal and Dimotakis, 1984 ; Hermanson and Dimotakis, 1989 ; Heidainejad and Ghoniem, 1989). Unlike the maximum temperature, the change of δ_P/δ_1 with T_{ad} is not linear. At low heat release, product formation is strongly affected by T_{ad}. The effect is weaker at high heat release.

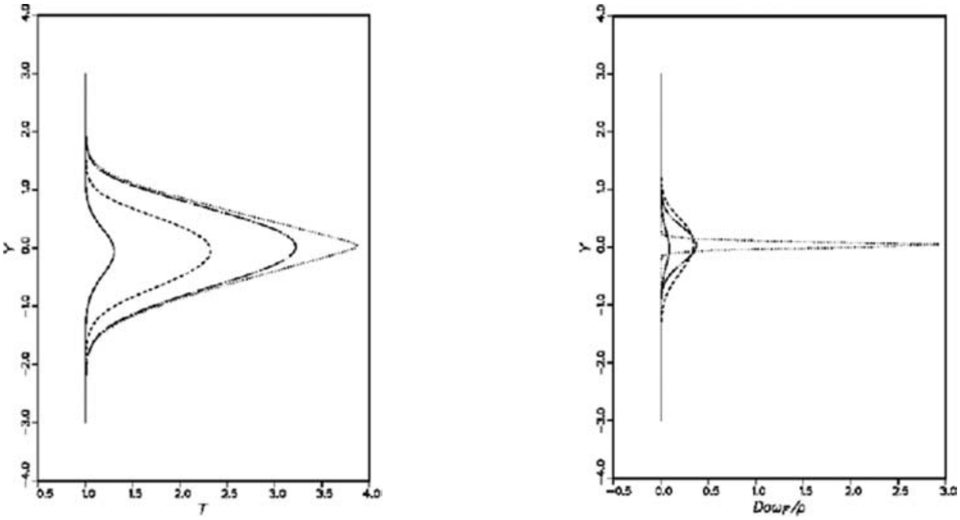
3.3 Effect of damköhler number

In Sec. 2.1, the Damköhler number was defined as the ratio of the convective flow time scale to the chemical reaction time scale. It is expected that as



(a) (b)

Fig. 8 The variation of the maximum temperature and normalized product thickness with heat release. (a) T_{max} (b) δ_P/δ_1. $Da=10$, $M_1=0$, $x=7.7$



(a) (b)

Fig. 9 Effect of the Damköhler number. $T_{ad}=8$, $Da=10$, $M_1=0$, $x=7.7$.
(a) T (b) $Da\omega_F/\rho$. ———, $Da=0$; -----, $Da=0.5$; -·-·-·-, $Da=2$; ········, $Da=1000$

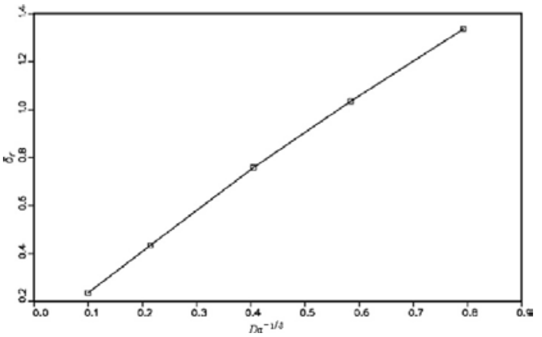


Fig. 10 Reaction zone thickness vs. $Da^{-1/3}$. $T_{ad}=8$, $M_1=0$, $x=7.7$

Da increases, the rate of product formation and heat release also increase. In Fig. 9, we show temperature profiles and reaction rate for $M_1=0$ and $T_{ad}=8$ for various Damköhler numbers. The effect of the Damköhler number is strongest for $Da<1$, where the rate of product formation and heat release increase rapidly with the speed of the chemical reaction ; an asymptote is reached for $Da>2$. Mungal and Frieler (1988) and Heidarinejad and Ghoniem (1989) reported similar results based on experiments and simulations (vortex method) respectively, but their results were limited to low heat release. We here used a very high Da (~ 1000) to study the fast chemistry limit. For large Da, the reaction zone is very thin and the region in which the fuel and oxidizer co-exit is very small. In the limit of $Da \rightarrow \infty$, the fuel and oxidizer co-exist nowhere and the reaction zone becomes an infinitesimally thin flame sheet.

The thickness of the reaction zone, the distance between the points at which the reaction rate is 10% of its maximum value, is expected to vary as $Da^{-1/3}$ for large values of the Damköhler number (Gibson and Libby, 1972) and Fig. 10 indicates that the flow exhibits the expected behavior.

5. Summary

The governing equations for laminar flows are derived from the two-dimensional compressible boundary-layer equations and are computed to illustrate the structures of laminar diffusion flames. The chemistry considered in the present work is that of a finite rate single step irreversible reaction with Arrhenius kinetics. Ignition, premixed flame, and diffusion flame regimes are found to exist in the laminar reacting mixing layer at high activation energy. At high Mach numbers, ignition occurs earlier due to the higher temperatures in the unburnt gas. In diffusion regimes, property variations affect the laminar profiles considerably and need to be included when there are large temperature differences involved. The maximum temperature of a laminar reacting mixing layer changes almost linearly with the adiabatic flame temperature ; the normalized product thickness depends strongly on the adiabatic flame temperature at low heat release, but only weakly at high heat release. Compressibility hardly changes the structure of the laminar layer when the heat release is high.

Acknowledgments

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References

Gibson, C. H. and Libby, P. A., 1972, "On Turbulent Flows with Fast Chemical Reaction. Part II. The Distribution of Reactants and Products Near a Reacting Surface," *Comb. Sci. Tech.*, Vol. 6, pp. 29～35.

Heidarinejad, G. and Ghoniem, A. F., 1989, "Vortex Simulation of the Reacting Shear Layer : Effects of Reynolds Number," AIAA Paper No. 89-0573.

Hermanson, J. C. and Dimotakis, P. E., 1989, "Effects of Heat Release in a Turbulent Reacting Shear Layer," *J. Fluid Mech.*, Vol. 199, pp. 333～375.

Jackson, T. L. and Hussaini, M. Y., 1988, "An Asymptotic Analysis of Supersonic Reacting Mixing Layers," *Comb. Sci. Tech.*, Vol. 57, pp. 129～140.

Linan, A. and Crespo, A., 1976, "An Asmymptotic Analysis of Unsteady Diffusion Flames for Large Activation Energies," *Comb. Sci. Tech.*, Vol. 14, pp. 95～117.

Marble, F. E. and Adamson, T. C., 1954, "Ignition and Combustion in a Laminar Mixing Zone," *Jet Propulsion*, Vol. 24, No. 85.

Mungal, M. G. and Dimotakis, P. E., 1984, "Mixing and Combustion with Low Heat Release in a Turbulent Shear Layer," *J. Fluid Mech.*, Vol. 148, pp. 349～382.

Mungal, M. G. and Frieler, C. E., 1988, "The Effect of Number in a Turbulent Shear Layer," *Comb. Flame*, Vol. 71, pp. 23～34.

Na, Y., Lee, S. and Shin, D., 2006, "Linear Stability Analysis of the Reacting Shear Flow," *Journal of Mechanical Science and Technology*, Vol. 20, No. 8, pp. 1309～1320.

Sandham, N. D. and Reynolds, W. C., 1979, "A Numerical Investigation of the Compressible Mixing Layer," *Dept. of Mechanical Engineering*, Stanford Univ., Stanford, CA, TF-45.