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Effects of confinement on partially premixed flames

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1. Motivation and objectives

Partially premixed combustion is an intermediate regime between the limiting cases of premixed and nonpremixed combustion. Although combustion problems are generally approached from one of these two limiting cases, there are many practical situations where flames cannot be considered as purely premixed or nonpremixed, and thus the partially premixed approach must be used.

In partially premixed combustion, mechanisms from the premixed and nonpremixed regimes can coexist, and as a result some interesting new phenomena can arise. One such phenomenon is the flame stabilization in laminar mixing layers by triple flames. One of the first observations of triple flames was made by Phillips (1965), who investigated a triple flame propagating in a methane mixing layer. Kioni *et al.* (1993) also examined triple flames both experimentally and numerically. There have also been numerous analytical studies on the shape and propagation of triple flames under various assumptions by Dold (1989), Dold *et al.* (1991), and Hartley and Dold (1991). In terms of modeling, Müller *et al.* (1994) have combined the flamelet formulations for premixed and nonpremixed combustion in order to treat lifted diffusion flames. One common feature in the analytical and numerical studies mentioned above is the assumption of zero heat release, which is necessary to make the problem tractable. The effect of heat release on triple flames was investigated by Ruetsch *et al.* (1995), where for the unconfined case, flame speeds larger than their premixed counterparts were found.

One of the most important practical situations in which these conditions arise is in lifted turbulent jet diffusion flames. At a critical velocity the burning zone of a fuel jet lifts offfrom the nozzle, moves to increasing distances as the jet velocity increases, and finally blows off. The mechanisms that control these phenomena, i.e. that determine the *stability* of these flames, are still not understood.

In addition to regions where diffusion flame stabilization takes place, partially premixed conditions also exist during the ignition process in nonpremixed systems. Numerical simulations by Réveillon *et al.* (1994) of the ignition process in a weakly stirred mixture of fuel and oxidizer show that triple flames propagate along lines of stoichiometric mixture fraction throughout the fluid. In addition, Peters (1994) notes that NO_x emissions are likely to be large in such transient cases, and therefore an understanding of triple flames can provide information concerning pollutant formation.

This study extends the work previously done and examines the effects of lateral confinement on partially premixed flames. Once again, we study both the flame structure and propagation.

1.1 Numerical simulation and flow configuration

We use direct numerical simulations to solve the fully compressible Navier-Stokes equations. The simulation uses a two-dimensional version of the code developed by Trouve (1991). This code uses the high-order compact finite difference scheme of Lele (1992) for spatial differentiation, the third order Runge-Kutta scheme of Wray for time advancement, and the Navier-Stokes characteristic boundary conditions method of Poinsot and Lele (1992). Below we summarize some of the important features and assumptions of the code relevant to this work; for further details on the numerical method readers are referred to Lele (1992) and Poinsot and Lele (1992).

The chemical scheme we consider is represented by a one-step global reaction between a fuel and oxidizer:

$$F + O \longrightarrow P$$

where we have assumed unity stoichiometric coefficients for simplicity. The reaction rate behaves according to the Arrhenius form:

$$\dot{w} = K\rho Y_F \rho Y_O \exp\left(-\frac{T_{ac}}{T}\right)$$

where ρ is the density, T_{ac} is the activation temperature, K is the pre-exponential factor, and Y_F and Y_O are the fuel and oxidizer mass fractions. Following Williams (1986), we can write this reaction rate as

$$\dot{w} = \Lambda\rho Y_F \rho Y_O \exp\left(-\frac{\beta(1-\theta)}{1-\alpha(1-\theta)}\right)$$

where the reduced pre-exponential factor(Λ), heat release parameter(α), Zel'dovich number(β), and reduced temperature(θ) are defined by:

$$\Lambda = K\exp(-\beta/\alpha); \quad \alpha = \frac{T_f - T_0}{T_f}; \quad \beta = \frac{\alpha T_{ac}}{T_f}; \quad \theta = \frac{T - T_0}{T_f - T_0}$$

with T_f being the adiabatic flame temperature and T_0 taken in the ambient flow. In this study we hold the Zel'dovich number constant at $\beta = 8$ and use a heat release parameter of $\alpha = 0.75$.

The transport coefficients in the simulations are temperature dependent. This temperature dependence is expressed through the molecular viscosity, μ, given by:

$$\mu = \mu_0 \left(\frac{T}{T_0}\right)^a$$

with $a = 0.76$. The temperature dependence of the thermal conductivity, λ, and the mass diffusivities, $\mathcal{D}_k$, are obtained by requiring the Lewis and Prandtl numbers to be constant:

$$Le_k = \frac{\lambda}{\rho \mathcal{D}_k c_p}; \qquad Pr = \frac{\mu c_p}{\lambda},$$

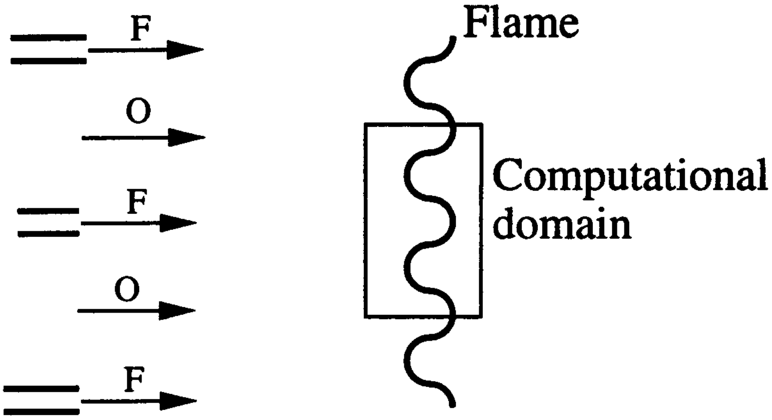

FIGURE 1. Computational domain used in the simulations. This domain represents a portion of a flame subjected to a periodic lateral variation in mixture fraction. The confinement is therefore accounted for by the periodic lateral boundary conditions.

where $k = F, O$ refers to either the fuel or the oxidizer species. We assume unity Lewis numbers throughout this study.

We solve the compressible Navier-Stokes equations in the two-dimensional domain depicted in Fig. 1. At the boundaries in the horizontal direction we use an inflow boundary condition on the left and nearly-perfect reflective boundary conditions, required to avoid pressure drift, at the outflow. In the lateral direction, in order to simulate the effects of confinement, we use periodic boundary conditions. This is in contrast to previous work on triple flames, which used nonreflecting boundary conditions in the lateral direction.

Within this domain we initialize the flow with a planar premixed flame, where the mixture fraction, defined as

$$Z = \frac{1 + Y_F - Y_O}{2},$$

is everywhere equal to its stoichiometric value, $Z_s = 0.5$. The incoming flow is uniform and set equal to the premixed laminar flame speed, S_L^0, which is maintained throughout the simulation. Also associated with the flame is the premixed flame thickness, δ_L^0.

After the flow and flame are initialized, a sinusoidal perturbation is added to the uniform stoichiometric mixture fraction. This perturbation is not small, as we consider values for the overall range of Z at the inlet from $\Delta Z = 0.2$ to $\Delta Z = 1.0$. In all cases, we maintain a overall equivalence ratio of one.

1.2 Calculation of the instantaneous flame speed

A useful diagnostic is the instantaneous flame speed at any point in the flow. We compute this by a method previously used to stabilize triple flames (Ruetsch *et al.* 1995), which is summarized below. The basis of this method comes from the the Hamilton-Jacobi equation for the G-field developed by Kerstein *et al.* (1989):

$$\rho\frac{DG}{Dt} = \rho V|\nabla G|.$$

Here G is the field variable whose level surfaces represent the interfaces or flame surfaces, and V is the local propagation of these surfaces, or local flame speed.

The finite thickness flames with heat release we consider in this study do not obey the G-equation; however, we can apply the Hamilton-Jacobi equation in our simulations if we construct an appropriate G field. We should remark here that the G-equation applies to premixed flames; therefore, G can be interpreted as a progress variable in finite thickness flames. We therefore define the progress variable c as:

$$c = 1 - (Y_F + Y_O)$$

which ranges from zero in the unburnt gases to unity in completely burnt gases. From the convective-diffusive equation for a scalar field we then obtain:

$$\rho\frac{Dc}{Dt} = \frac{\partial}{\partial x_i}\left(\rho\mathcal{D}\frac{\partial c}{\partial x_i}\right) + \dot{w}_c$$

where $\dot{w}_c = -(\dot{w}_F + \dot{w}_O)$. Equating $\rho Dc/DT$ and $\rho DG/Dt$ along with $|\nabla G|$ and $|\nabla c|$, and solving for the relative progression velocity of the iso-progress variable surface, V, we obtain:

$$V = \frac{1}{\rho|\nabla c|}\frac{\partial}{\partial x_i}\left(\rho\mathcal{D}\frac{\partial c}{\partial x_i}\right) + \frac{1}{\rho|\nabla c|}\dot{w}_c$$

This relation gives the propagation speed of a progress variable isosurface along its normal oriented towards the unburnt gas. Thus the components of the progress variable isosurface propagation are given by:

$$\mathbf{v} = -\frac{\nabla c}{|\nabla c|}V$$

The sum of the local fluid velocity, $\mathbf{u}$, and the progress variable isosurface velocity, $\mathbf{v}$, indicates whether the flame is progressing or receding.

At this point we should clarify some terminology regarding flame speeds. Poinsot *et al.* (1991) showed that there are several flame speeds which describe flame propagation in a premixed laminar flame tip. Ruetsch *et al.* (1995) also indicated that there are also different flames speeds depending on whether or not one includes the flow redirection in front of the flame resulting from heat release. In this study we are concerned with two flame speeds. The local flame speed is simply $|V|$, whereas the propagation speed, assuming the configuration in Fig. 1, is defined as:

$$S_L = U_{INLET} - (u_x + v_x)$$

where the x-components of the $\mathbf{u}$ and $\mathbf{v}$ fields are u_x and v_x, and $U_{INLET} = u_x$ evaluated at the inlet. It is important to differentiate between these two flame speeds, since the local flame speed is important in terms of the chemistry, and the propagation speed determines how the flame moves as a whole.

2. Accomplishments

We begin our study of partially premixed flames by first reviewing characteristics of unconfined flames, followed by a qualitative comparison between the unconfined and confined cases. We then focus on the global propagation of confined flames, which is followed by a discussion of the mechanism for flame stabilization in the regions farthest from stoichiometry.

2.1 Review of unconfined partially premixed flames

In this section we briefly review material associated with the unconfined partially premixed flames. For a more thorough review see Ruetsch *et al.* (1995). In the unconfined case, where lateral flow out of the side boundaries occurs, we subject a premixed flame to a gradient in Z (using a *tanh* profile), which results in a single triple flame composed of two premixed and one diffusion wing. Aside from the change in the flame structure, the flame speed also changes when the flame is subjected to a gradient in mixture fraction. The increase in flame speed is a direct result of heat released in the flame. For thin flames, the flame speed and expansion ratios scale as:

$$\frac{S_L}{S_L^0} \sim \sqrt{\frac{\rho_U}{\rho_B}}; \qquad \frac{\delta_B}{\delta_U} \sim \frac{\rho_U}{\rho_B}$$

where the subscripts U and B refer to the unburned and burned regions of the flow, and δ denotes the lateral distance between a pair of streamlines. These relations were derived for the two-dimensional case. In general, however, one expects fluctuations of the mixture fraction to be three-dimensional. The analysis performed in the planar two-dimensional case can be redone for the axisymmetric case. This results in the following relations:

$$\frac{S_L}{S_L^0} \sim \sqrt{\frac{\rho_U}{\rho_B}}; \qquad \frac{r_B}{r_U} \sim \sqrt{\frac{\rho_U}{\rho_B}}.$$

where r is the radial coordinate of a streamline. Therefore, for the unconfined case we obtain the same increase in flame speed for a given amount of heat release, or density ratio. The only difference is in the length scale ratio for streamline divergence.

2.2 Confined vs. unconfined flames

Figure 2 compares the streamline, pressure field, and reaction rate for both confined and unconfined cases. Because the confined case uses a sinusoidal perturbation in mixture fraction about stoichiometric conditions, we observe two lateral locations where the mixture is at stoichiometric values, hence two triple flames. Because the lateral expansion observed in the unconfined case is absent in the confined case, the streamline patterns are substantially different. Because the streamlines can diverge in the unconfined cases, the pressure can recover laterally, and no global pressure drop is observed across the flame. For the confined flame, this is not the case. The major pressure difference occurring in this case is the drop across the flame, similar to that of a planar premixed flame. In addition to the pressure drop across the

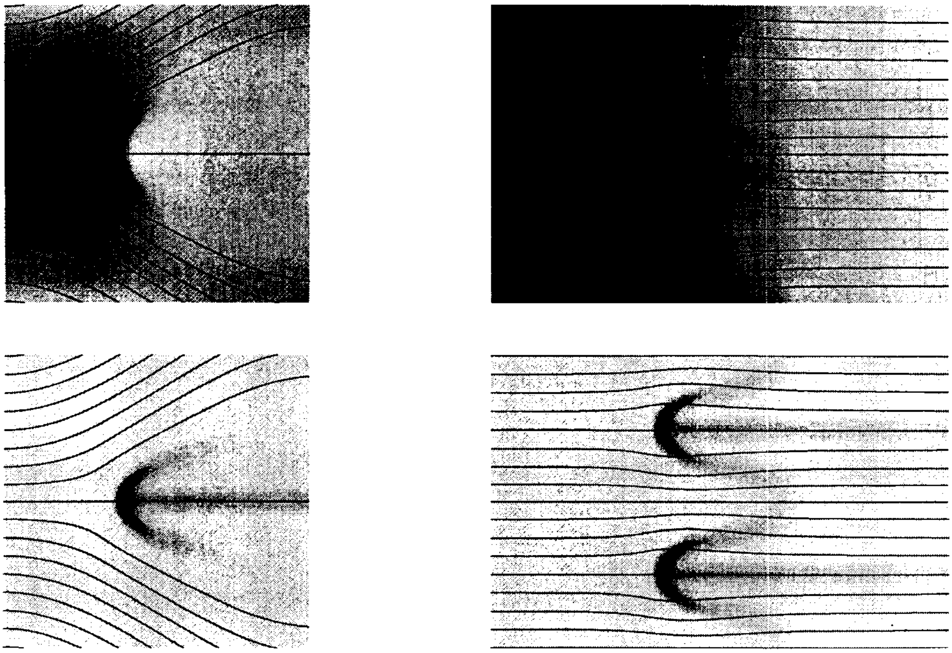

FIGURE 2. Pressure (top) and reaction rate (bottom) gray scale images with streamline superposed for the unconfined (left) and confined (right) cases. (Higher values correspond to darker regions.) The global divergence of streamlines in the unconfined case is absent in the confined runs, where only a small local divergence in front of the flame is observed. The global pressure drop across the flame in the confined case is absent in the unconfined results.

flame, we observe a pressure rise in front of the flame centered around the stoichiometric streamlines. This is similar to the region in front of the triple point of the unconfined flame, but is much smaller in magnitude. In the unconfined case, this pressure rise is associated with a deceleration of the horizontal velocity that is directly responsible for the increase in propagation of the triple flame structure as a whole. The main question here is whether or not the confined flame observes an increase in flame speed.

2.3 Propagation of confined flames

Time series of the propagation speeds at the stoichiometric point, or leading edge, and the point farthest from stoichiometry, or flame trough, are given in Fig. 3. When the premixed flame is initially subjected to the variation in mixture fraction, the flame response is qualitatively similar to an unconfined flame at the leading edge, in that the propagation speed increases. The flame trough experiences the opposite trend; the flame speed decreases. This behavior is necessary for the flame shape to change, but is only a transient feature. As the flame has time to adjust to the change in mixture fraction gradient, the flame speed returns to that of the premixed case in both the leading edge and trough. The transient time scale for

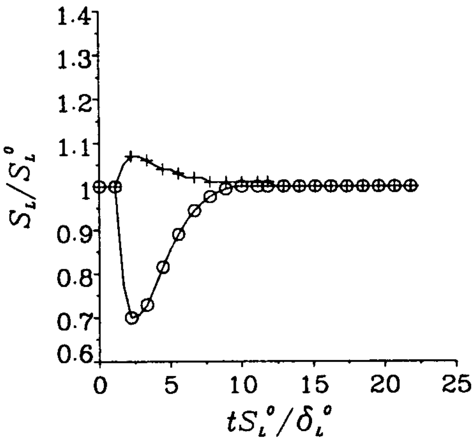

FIGURE 3. Time series of flame speed at the leading edge (+) and flame trough (o) when exposed to a variable mixture fraction. When the mixture fraction is first felt by the flame, the leading edge's flame speed increases, and the trough's flame speed decreases. After some time, both converge to the premixed planar flame speed, S_L^0. The values of Z in the troughs are 0.44 and 0.56.

the change depends on the value of ΔZ, where the larger values require a longer times to relax to the premixed flame speed.

The mixture fraction varies from $0.4 < Z < 0.6$ at the inlet. Simulations with larger ranges of the mixture fraction were performed up to and including $0 < Z < 1$ at the inlet. However, it is important to realize that these values correspond to inlet conditions. Because of the diffusive nature of the flows we consider, these ranges in mixture fraction are greatly reduced by the time the flow reaches the flame. As a result, values ranging from $.29 < Z < .71$ were achieved at the flame surface, and in all cases the flame speeds in both the leading edge and trough converged to the same values, indicating a saturation of flame deformation. Furthermore, these values are within three percent of the premixed laminar flame speed. Thus, for the confined case, no long term change in flame speed occurs when exposing the flame to a perturbation in the mixture fraction.

2.4 Stabilization of the flame trough

Of particular interest is how the flame in the trough is stabilized. To aid in exploring this phenomenon, it is instructive to compare what occurs in the trough of a partially premixed flame to its one-dimensional counterpart. Figure 4 compares the velocity, reduced temperature, and reaction rate in the trough of a partially premixed flame with the same profiles for a one-dimensional flame stabilized with the same reactant composition. There are several differences between these two cases. From the velocity profiles, it is apparent that the flame in the trough of the two-dimensional flow is stabilized in a higher velocity than the one-dimensional

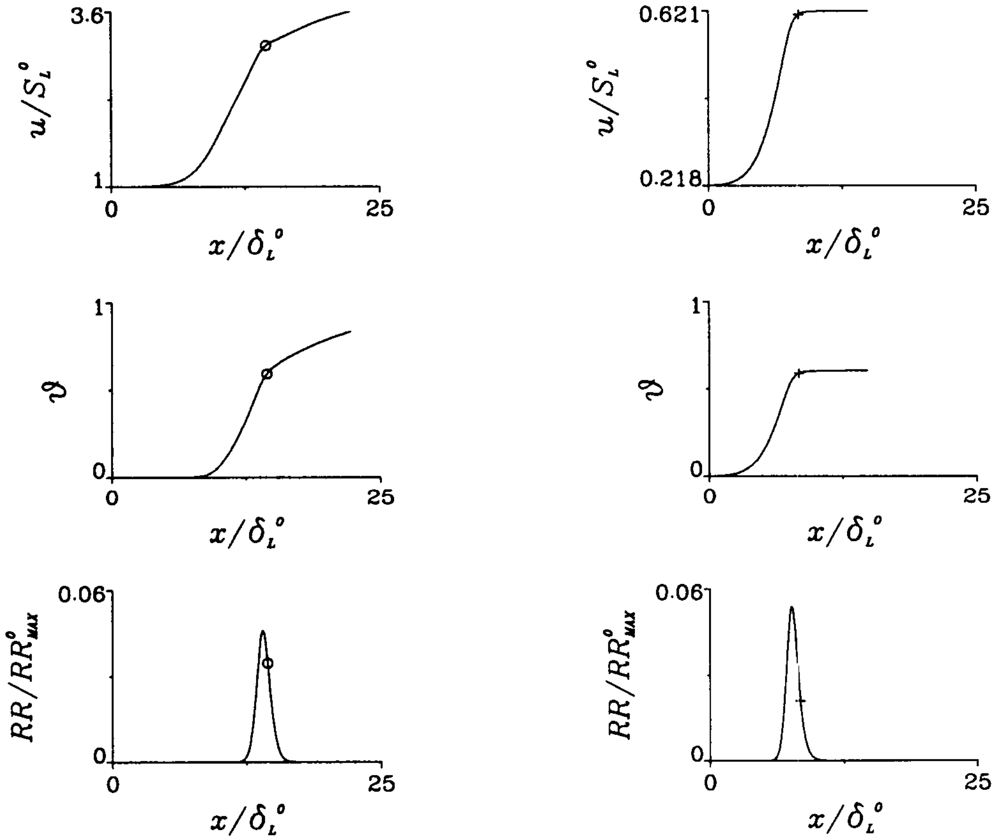

FIGURE 4. Velocity, reduced temperature, and reaction rate through the flame trough of a two-dimensional flame (left) and for a one-dimensional flame under with the same mixture fraction as in the trough of the two-dimensional case (right). The velocity in the two-dimensional case is larger than in the one-dimensional case. The velocity and temperature profiles in the two-dimensional case show and increase through the flame front, and then a smaller rate of increase afterwards, due to the lateral diffusion of temperature and species.

flame. In addition to the magnitude difference, the shapes of the profiles also differ. The increase in the velocity and reduced temperature can be broken into two regions in the two-dimensional case. The transition between these two regions is marked in Fig. 4. The first region corresponds to the one-dimensional flame, where the chemical reaction is responsible for the increase in these properties. The second region, where the velocity and temperature increase more slowly, is absent in the one-dimensional case. This region results from the lateral conduction of temperature and species into the trough region. The diffusion of reactants into this region shifts the reaction rate back relative to the transition point marked in the figure.

The comparison between one-dimensional flames and slices though the trough of two-dimensional flames can be extended to examine the effect of the mixture

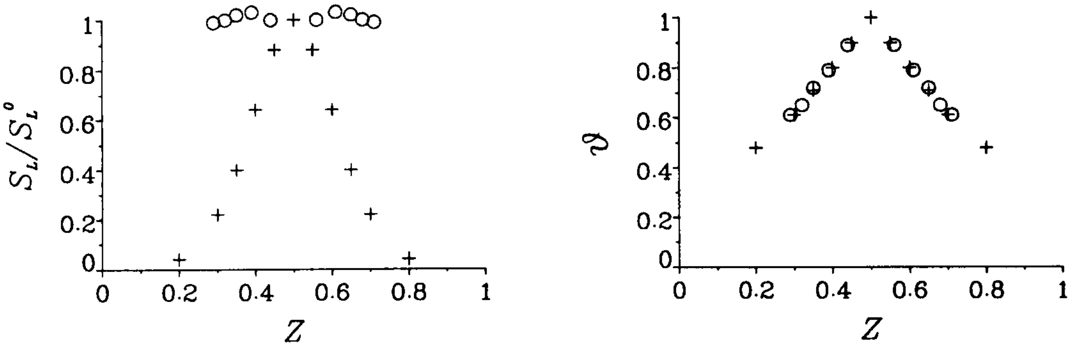

FIGURE 5. Flame speed (left) and reduced temperature (right) in the trough of two-dimensional partially premixed flames (o) and for stabilized one-dimensional flames (+) at various mixture fractions.

fraction range on flame speed. The transition points for the temperature profiles were calculated for several values of ΔZ at the inlet, along with stabilized one-dimensional flames at various ΔZ. These are displayed in Fig. 5, along with the propagation speed of the flames, i.e. the velocity at the inlet, not at the transition point. The propagation speed plot shows that the two-dimensional cases maintain a flame speed close to the planar premixed flame speed at stoichiometric conditions. One possible mechanism for maintaining this flame speed is that the lateral heat conduction is driving the temperature at the transition point higher, which, for Arrhenius kinetics would exponentially increase the flame speed. However, this appears not to be the case, as we see that the one- and two-dimensional reduced temperatures collapse well onto the same curve. Furthermore, the reaction rates are roughly equal in these two cases, as is evident from Fig. 4.

We can utilize concepts from premixed combustion concerning the laminar flame tip by Poinsot *et al.* (1991) to aid in understanding the stabilization process in the trough region. In their investigation, they identified three mechanisms which may increase the flame speed: the chemical, diffusive, and hydrodynamic mechanisms. For unity Lewis numbers they found the chemical mechanism, which is related to the reaction rate, is small. This is apparent in our case from the reaction rate plot in Fig. 4. The diffusive mechanism corresponds to a leakage of fuel across streamtube boundaries. This mechanism is present; however, the fact that we are using a two-species reaction complicates its interpretation. Furthermore, the diffusion process causes a "leakage" across streamlines in a direction that would tend to decrease the propagation speed. The hydrodynamic mechanism is related to an isothermal area expansion and is signified by a lateral flow divergence. From the streamline pattern in Fig. 2, we see that this does occur in the trough region. One can also see the effect of the hydrodynamic mechanism on the temperature profile in Fig. 4 for the two-dimensional and one-dimensional cases. The flame thickness, based on the maximum temperature gradient, is much larger due to the lateral heat conduction in the two-dimensional case. This larger flame thickness also indicates the presence of the hydrodynamic mechanism, (cf. Fig. 7 of Poinsot *et al.* 1995). The hydrodynamic mechanism of flame stabilization in the trough region is aided in the confined case by the fact that the streamtubes must return to their original thickness behind the flame. Since an expansion occurs in front of the leading edge, the contraction along the streamline furthest from stoichiometric conditions must occur at that horizontal location. This contracted region then expands farther downstream, through the flame trough, thus enhancing the hydrodynamic mechanism.

2.5 Relevance to turbulent jet flames

In this last section we digress from confined flames and discuss recent experimental work on turbulent jet flames and the applicability of triple flames in turbulence. The recent study of Schefer *et al.* (1994) of lifted flames at Reynolds numbers of 7,000 to 12,000 have found that the reaction zone is a smooth, thin, connected sheet surrounding the jet. Furthermore, measurements of the fuel concentration fields show that the flame lies on or near the stoichiometric contour in a region where the velocity significantly exceeds the laminar premixed flame propagation speed. All of these observations are consistent with the conclusion that the flame is, at least at these Reynolds numbers, a triple flame. Strong support for this conclusion is provided by the preliminary PIV experiments by Muñiz and Mungal (1995) of a methane jet burning in coflowing air. They find that the flame is stabilized in a region in which the measured velocity is approximately the triple flame speed for these gases. Therefore, it appears that triple flames are likely candidates for diffusion flame stabilization.

3. Future work

The ability to calculate partially premixed flames in a confined flow presents opportunities to study many different phenomena. To this point we have considered flows with overall equivalence ratios of unity. We can extend the study to examine extinction phenomena with global equivalence ratios far from stoichiometric conditions. To explore this regime, one would have to abandon the single-step chemistry model for a multistep reduced chemical scheme.

Another phenomenon that can be investigated in partially premixed combustion is the effect of non-unity Lewis numbers on flame speed. The confined partially premixed simulations provide and effective and efficient means of achieving large flame curvature. Simulations in this area are currently under way.

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