The Manifestation of Eddy Shocklets and Laminar Diffusion Flamelets in a Shear Layer

Richard S. Miller
Department of Mechanical and Aerospace Engineering
State University of New York at Buffalo
Buffalo, New York 14260

Abstract

Results obtained by Direct Numerical Simulations (DNS) are used to investigate several aspects of three dimensional shear layers under both non-reacting and reacting conditions. This includes: (1) the examination of the global flow structures, (2) the manifestation of shocklets, and (3) the assessment of the extent of validity of the laminar diffusion flamelet model in describing complex turbulent flames. At sufficiently low Mach numbers, many of the characteristics commonly associated with the secondary instability of the incompressible layer are distinguishable. These include the formation of vorticity tubes and the appearance of mushroom like structures for conserved scalar quantities. Compressibility effects on these structures are then investigated. In both 2D and 3D simulations, at sufficiently high Mach numbers, eddy shocklets are found and are confirmed to display the characteristics of an oblique shock wave. However, in the 3D simulations these shocks are somewhat weaker. The existence of shocks has not been reported in any previous 3D shear layer simulations. It has been proposed that the structure of turbulent diffusion flames is composed of an ensemble of laminar diffusion flamelets. Here, preliminary tests are made by considering a simple reaction of the type $A + rB \rightarrow (1 + r)Products$. The results generated by DNS of a low Mach number, high Damköler number flow compare reasonably well with predictions based on a 1D laminar opposed jet flame.

Scope

The scientific community has experienced a tremendous boom in interest, within the last decade, on high speed reacting flows [1]. This increase in research has been spurred by government plans to develop advanced air-breathing propulsion systems for use within the next century. The understanding of the mechanisms which control mixing and combustion in highly compressible shear layers are of utmost importance in achieving these goals. In order to simplify the problems involved with studying these complex flow fields, much progress has been made in the analysis of non-reacting mixing layers. There have been relatively few studies of reacting flow fields, and these have typically been limited to two dimensional simulations (for recent reviews see [1,2,3,4]). The scope of the current research presented here entails reacting mixing layers under the assumption of a simple chemistry. Direct numerical simulations [3] are used to investigate two controversial issues of current research interest; the existence of eddy shocklets in three dimensional shear layers, and the extent of validity of laminar diffusion flamelet modeling in complex turbulent combustion systems.

Background

Brown and Roshko [5] found that a mixing layer is dominated by large scale coherent vortical structures. While experimental studies do show the presence of such structures in supersonic layers, they are much weaker and have a markedly reduced rate of growth as compared to their subsonic counterparts. Brown and Roshko studied the effects of density fluctuations on the growth rate of mixing layers. They found that density effects alone cannot explain the slow growth rate of the supersonic shear layer. Papamoschou and Roshko [6] studied the compressible shear layer and found that the compressibility effects play a dominant role in the slow growth rate of the layer.

Oh [7] suggested that in supersonic shear layers, some of the turbulence energy in the flow is generated by shocks that formed above the large eddies. As a result, the eddies are decelerated on passing through these shocks, and the resulting disturbance produces pressure fluctuations. Favorable correlations between pressure fluctuation and velocity gradient created relatively large values of the pressure dilatation term. Oh then reasoned that the pressure dilatation term could reduce the turbulent shear level in high Mach number mixing layers, thereby slowing the rate of growth. Other studies [8,9] have linked the decreased growth rate at supersonic convective Mach numbers to the existence of shocks and shocklets. These shocks were hypothesized to hinder the growth rate by both the production of counter vorticity, and by reducing the turbulence scales.

Two dimensional simulations of incompressible shear layers have long been performed due to their ease and relatively low computational expense [10]. These simulations are capable of capturing the formation and rollup of the two dimensional coherent vortical structures. The existence of shocklets in two dimensional simulations of compressible shear layers has been well documented for $M_c > 0.7$, where M_c denotes the "convective Mach number" [11,12,13]. These simulations have also correlated well with experimental measurements of the growth rate in such layers. However, in order to truly capture the physics of these flows, complex three dimensional effects must be taken into account.

Pioneering 3D large eddy and direct numerical simulations of incompressible mixing layers were performed by Mansour et al. [14], Cain et al. [15], and Metcalfe et al. [16]. Evidence of spanwise rollers and rib vortices have been observed. Most simulations of 3D mixing layers are temporally developing, due to the much higher computational cost of spatial simulations (see [3] for a review). In such temporally developing flows, Lin and Corcos [17] showed that the streamwise vorticity in the braid region "collapses"

into an axisymmetric vortex. These vortices are responsible for the generation of the mushroom shapes found in 3D simulations.

Lee et al. [18] have found shocklets can be formed in three dimensional homogeneous turbulence simulations. They concluded that the presence of shocklets is important due to the conversion of turbulent kinetic energy to internal energy via the pressure dilatation correlation. Zeman [19] has proposed a model based on turbulence dissipation enhancement due to eddy shocklets. This model has the rather unique advantage in that it is able to predict the reduced growth rate of compressible mixing layers. However, no such shocklets have previously been observed in three dimensional mixing layer simulations [20].

A diffusion flame, as its name implies, is one in which the reactants are originally segregated, and the major mechanism of reactant conversion to product is through diffusion. In a turbulent diffusion flame, the major mechanism of reactant conversion is through turbulence. However, before the conversion to product, the reactants must mix at the molecular level. Currently, several methods are being used to model these flames with complicated chemistry kinetics models. In particular these include the chemistry models of Miller et al. [21]. However, these models are typically complex and difficult to employ in DNS [3]. It is of great practical importance to find a simple model which may be used for true complex turbulent reactions occurring at realistic reaction rates.

Peters [22,23,24] has proposed that a turbulent diffusion flame is composed of an ensemble of laminar diffusion flamelets. This is a reasonable assumption in reacting systems in which the chemistry is sufficiently fast such that the flame occurs in an asymptotically thin layer. These flamelets can be assumed one dimensional with a quasi steady structure. In chemical reactions within a turbulent flow under these conditions, the mixing could be calculated to obtain the local mixture fraction ratio and the scalar dissipation. With this information, the flame characteristics would then be known from comparison to an appropriate simple 1D laminar flame configuration. The laminar flow model may be as simple as possible. Peters suggests that a suitable configuration is that produced by a 1D opposed jet system. This proposal has been the center of some controversy. Bilger [25] has disputed the necessary condition that flamelets become asymptotically thin in the limit of increasing Damköler numbers.

Mell et al. [26] have made comparisons of the laminar flamelet model with two dimensional isotropic reacting turbulence, with fairly promising results. However, 2D simulations are poor models for true three dimensional turbulent flows. Before implementation for practical use, strict comparisons with 3D turbulent reacting flows must be made for a variety of circumstances including flows with more complex chemistry, and heat releasing reactions. Here, preliminary results concerning the extent of validity of the model are provided by examining a complicated three dimensional turbulent reacting mixing layer.

Computational Approach

A three dimensional, time developing, planar mixing layer is simulated using an explicit finite difference scheme. The temporal reference frame has been chosen since it appears to capture all of the pertinent physics of the mixing process. Temporal development differs from that of spacial development in that the asymmetric effects of a growing mixing layer cannot, due to periodic boundary conditions, be studied. However, these effects are not the object of the present investigation. The Navier Stokes equations are solved in full. Two species equations are also solved, which allows for the introduction of a simple finite rate, non-heat releasing, reaction of the type $A + rB \rightarrow (1 + r)Products$. No turbulence or subgrid models are used. The thermo-chemical properties of the upper and lower fluids are the same for ease of calculation and modeling. The viscosity, and thermal conductivity are both assumed constant. Both the Prandtl and the Schmidt numbers are set equal to unity.

The numerical method is based on an explicit finite difference scheme which is second order accurate in time and fourth order accurate in space. The scheme is a monotone Flux Corrected Transport (FCT) algorithm, which is extremely accurate in capturing steep gradients (e.g. shocks) within the flow field [27]. Both 2D and 3D simulations are performed. The grid used is either $80 \times 80 \times 45$ or $128 \times 128 \times 64$ in 3D, while 2D simulations are performed on either 128^2, or 256^2 grids. All simulations are performed on Cray-2 or Cray-YMP supercomputers. Computations are made for convective Mach numbers in the range of 0.2 to 2.5, with corresponding Reynolds numbers from 70 to 350. The Reynolds number is defined as:

$$Re = \frac{\rho_\infty U_\infty \delta_\omega|_0}{\mu}$$

where ρ_∞ is the free stream density, U_∞ is the free stream velocity, μ is the viscosity, and $\delta_\omega|_0$ is the initial vorticity thickness based on the mean streamwise velocity $< U >$:

$$\delta_\omega = \frac{2U_\infty}{\frac{\partial <U>}{\partial y}|_{max}}$$

The vorticity thickness is typically normalized with respect to its value at time $t^* = 0$, where the dimensionless time is defined as:

$$t^* = \frac{tU_\infty}{L_x}$$

and L_x is the streamwise length of the computational domain.

Forcing techniques for the inducement of rollup and pairing in planar mixing layers have been the focus of many studies. This has been done analytically [28], experimentally [29], and computationally [30]. Here, the initial velocity profile is taken to be a hyperbolic tangent function. Low amplitude forcing is used at both the most unstable mode and the second harmonic in order to simulate the interaction between vortices. Disturbance amplitudes are typically ten percent of the free stream velocity. The use of forcing greatly reduces the computer time required to achieve full rollup along with the typical 3D structures.

The computational domain is defined such that the streamwise direction is the x-coordinate, the spanwise is the z-coordinate, and y is the vertical. Figure 1 shows a schematic of the shear layer. The top half

of the domain ($+y$) is initially inhabited by species A, and has velocity $+U_\infty$. The bottom half of the domain initially contains species B with velocity $-U_\infty$. The product mass fraction, P, is initially zero everywhere by definition. The numerical grid is compressed in the y axis near the region of high initial gradients. This allows for finer resolution where a significant amount of the mixing and reaction occurs.
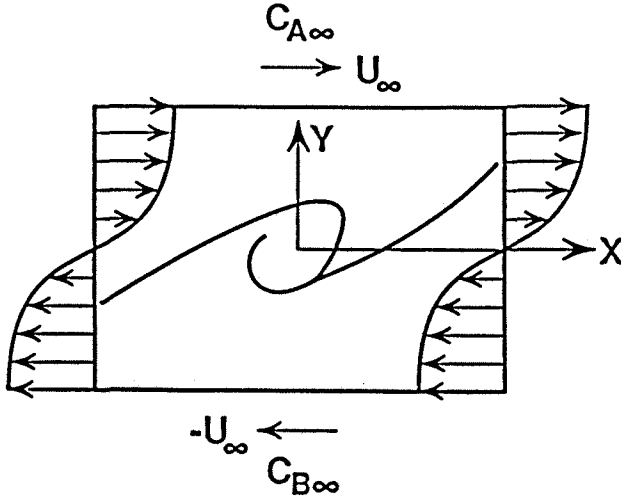
Figure 1: Schematic diagram of a temporally evolving mixing layer.

Presentation of Results

Flow Structures: Three different cases are examined. These correspond to 3D finite rate reaction simulations with Da=30, at M_c=0.4, M_c=0.8, and M_c=2.0. The only variable which is altered in these simulations is the free stream velocity. All other flow parameters, including those in the forcing procedure, remain constant for all cases. These ranges allow for the study of low compressibility, mild compressibility, and finally an extremely high compressed case where shocks are found. It is desired to investigate the degree of actual mixing of the two streams which is accomplished by the shear layer. Figure 2 shows the normalized total product formation vs. time. As the figure clearly shows, mixing at low compressibility is much more efficient than that at high compressibility. In fact, more than five times as much product is
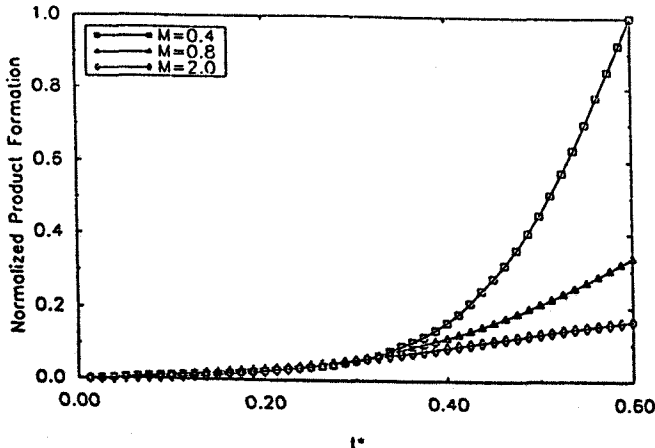
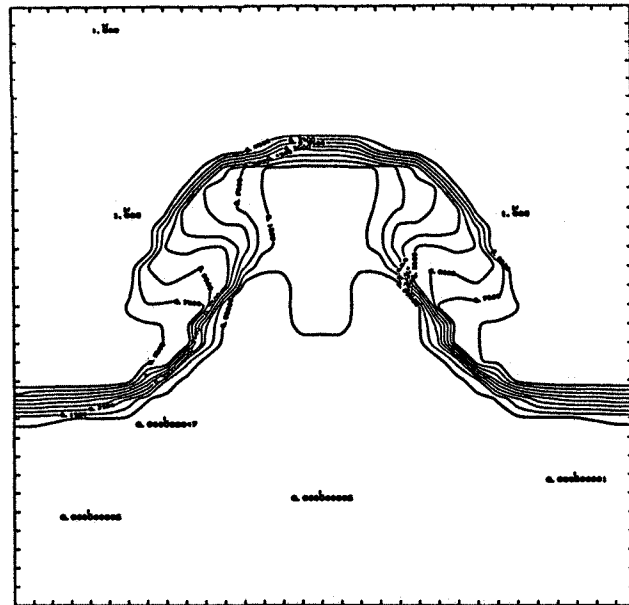Figure 2: Normalized product vs. dimensionless time

Figure 3(a): Scalar contours, M_c=0.4

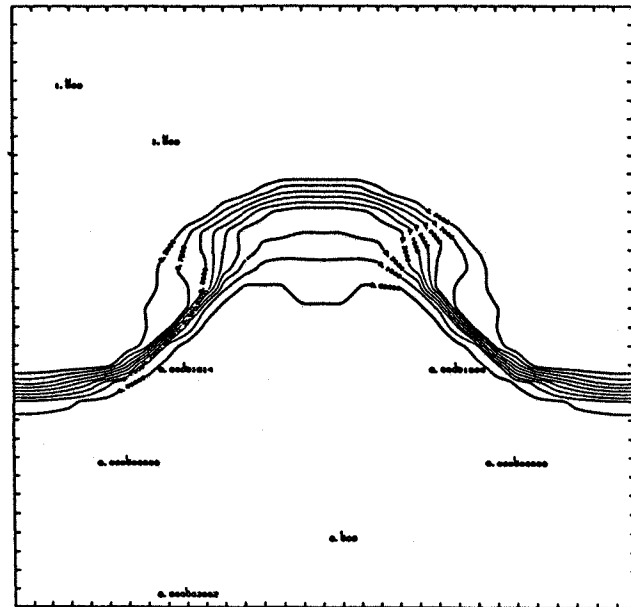Figure 3(b): Streamwise vorticity contours, M_c=0.4

Figure 4(a): Scalar contours, M_c=0.8

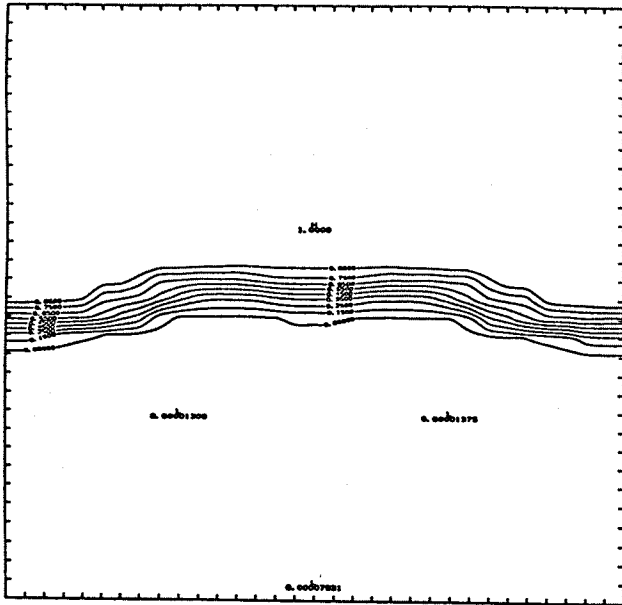Figure 4(b): Streamwise vorticity contours, M_c=0.8

Figure 5(a): Scalar contours, $M_c=2.0$

Figure 5(b): Streamwise vorticity contours, $M_c=2.0$

formed for the $M_c=0.4$ case than for mixing at the $M_c=2.0$ case. Since at low compressibility vortical structures form and grow faster, more mixing occurs at low Mach numbers than at high Mach numbers.

In Figs. 3, 4, and 5, specific 3D structures are examined as they pass from low to high compressibility levels. These structures are depicted here by examining the contours of a conserved scalar variable in a streamwise plane. Figures 3(a) and 3(b) show the fully developed mushroom structure, and the streamwise vorticity contours for $M_c=0.4$, respectively. In this low compressibility level, the mushroom structure is typical of those observed experimentally even at very low Reynolds numbers [30]. Figure 3(b) displays a cross section in the braid plane between rollers for which contours of the streamwise component of vorticity are presented. The solid lines represent positive vorticity while the dashed lines represent negative vorticity. The vorticity braids are shown to be slightly elliptical with the major axis almost completely vertical. Figures 4(a) and 4(b) are taken at exactly the same locations as those in Fig. 3, but now the convective Mach number is $M_c=0.8$. The mushroom shape is still intact, but has been rather smoothed. The alternating positive and negative streamwise vorticity braids have retained their shape and increased their magnitude from those at the $M_c=0.4$ case. However, the major axis of the ellipse is now inclined at approximately a 45° angle with the horizontal. Finally, Figs. 5(a) and 5(b) make the same comparisons for $M_c=2.0$. The mushroom shape has disappeared, leaving only a small wave in the scalar contours. However, the braids, though thinner, contain much stronger vorticity than those in the previous two cases. They still

maintain their elliptical shape, but now the major axis is almost completely horizontal.

Shocks: For the first time, our results indicate that shocks are indeed observed in 3D simulations at high Mach numbers. To establish whether a region of steep gradient does contain a shock, the density, pressure, and temperature ratios across the region were compared with the corresponding values of calorically perfect air. It was found that the jumps in the thermodynamic variables across this region are in good agreement with the values across a shock. It is observed that although the flow is strongly supersonic on either side of the shock wave, the normal components of velocity exhibit the expected change from supersonic to subsonic speeds on passing through the shock wave. Figures 6(a) and 6(b) show density contours for 2D and 3D simulations at $M_c=2.5$, respec-
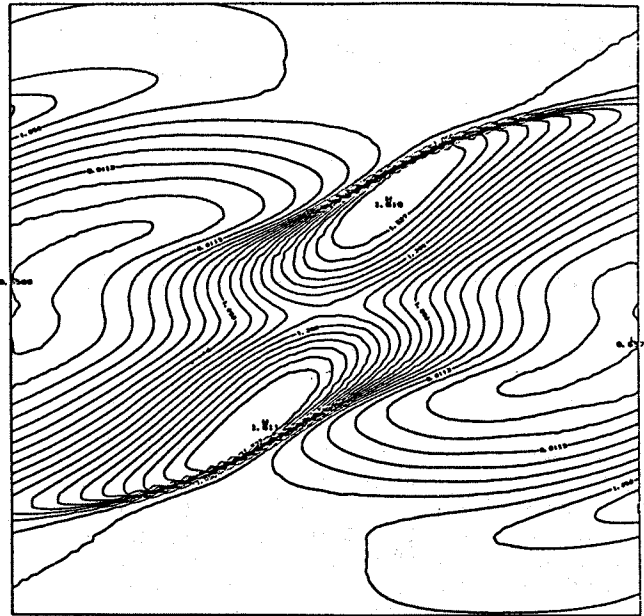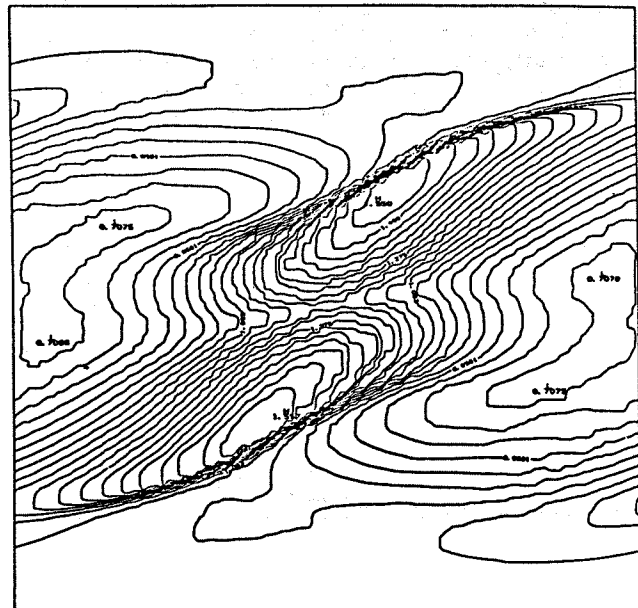

Figure 6(a): Density contours, 2D $M_c=2.5$

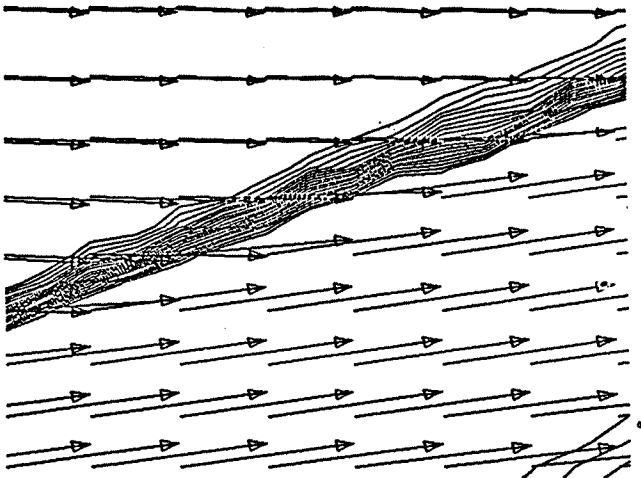Figure 6(b): Density contours, 3D $M_c=2.5$

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Figure 7: Closeup showing shock and velocity vectors

tively. For the 3D case, the contours are shown along a spanwise plane. As can be noticed by examining the density magnitudes on either side of shocks, the 2D simulations show stronger shocks in comparison with those in the 3D case. A plausible explanation for this is that in the 3D case, the flow has a third dimension along which it can change direction to avoid the high pressure regions created by the presence of the vortical structures. Figure 7 shows a close up of shock wave density contours with velocity vectors superimposed. It is clearly shown that the velocity vectors are turned towards the shock wave on passing through it.

Flamelet Model: Here, we consider a simple reaction of the type $A + rB \rightarrow (1 + r)P$. A, B, P denote reactants A, B, and the product P, respectively, and r is a stoichiometric coefficient which may be varied to simulate different reactions. Two equations are then needed for the mass fraction of the two species.

$$L(\rho A) = \omega, \tag{1}$$

$$L(\rho B) = r\omega, \tag{2}$$

where L denotes the convection-diffusion operator, ρ is the density, and ω is the chemical reaction rate. Assuming that the two species have the same thermochemical properties, with the single-step chemistry model considered, a conserved Shvab Zeldovich scalar variable may be defined as [32]:

$$F = \frac{A - B/r + 1/r}{1 + 1/r} \tag{3}$$

$$0 \le F \le 1$$

One simple approach to account for the effects of the reaction is with the assumption of infinitely fast chemistry, $i.e.$ the flame sheet model [32]. This assumption implies that the flame is an infinitely thin sheet located along the stoichiometric surface, $F_s = 1/(1+r)$. For this model, instead of solving equations (1) and (2), only one species conservation equation need be solved, namely;

$$L(\rho F) = 0 \tag{4}$$

Because under this type of reaction the two species A, B cannot coexist, the knowledge of F is sufficient

to determine A, B, and P. This relationship is shown graphically in Fig. 8 for the case where $r = 1$. This model provides a simplified means of simulating chemical reactions. However, this is not usually a good approximation for practical finite rate reactions. At relatively high Damköhler numbers, the reaction occurs in a thin, but finite, zone which is centered on the stoichiometric surface. Peters argues that if the reaction zone is sufficiently thin (but finite) the mean reactant conversion would only depend on the magnitudes of the conserved scalar F, and the local species dissipation:

$$\chi = 2D \mid \nabla F \mid^2 \tag{5}$$

where D is the species diffusivity, and ∇ denotes the gradient operator. Now, if the idea of laminar diffusion flamelets is valid, then the relationship between the magnitudes of the scalar variable and (F, χ) for turbulent reacting flows, is the same as that in a laminar flow flame of the same chemistry model. Following Peters' suggestion, the model is tested using the 1D laminar opposed jet system, governed by [33]:

$$\frac{d^2\phi}{dF^2} = -\frac{2}{\chi}\omega_\phi \tag{6}$$

where ϕ represents the scalar, ω_ϕ denotes its corresponding reaction term, and

$$\chi = \chi_s \exp[-2(\text{erfc}^{-1}(2F))^2] \tag{7}$$

Equation (7) is a proposed model for the species dissipation in Eq. (5) [34]. χ_s is the value of the dissipation at the stagnation region of the laminar flame, and erfc^{-1} is the inverse complementary error function. Note that nothing has been indicated as far as the chemistry is concerned. The kinetics can be very complex, but we have a closed form $\chi(F)$ relation. In order to study the validity of the laminar flamelet model, 3D direct numerical simulations are conducted
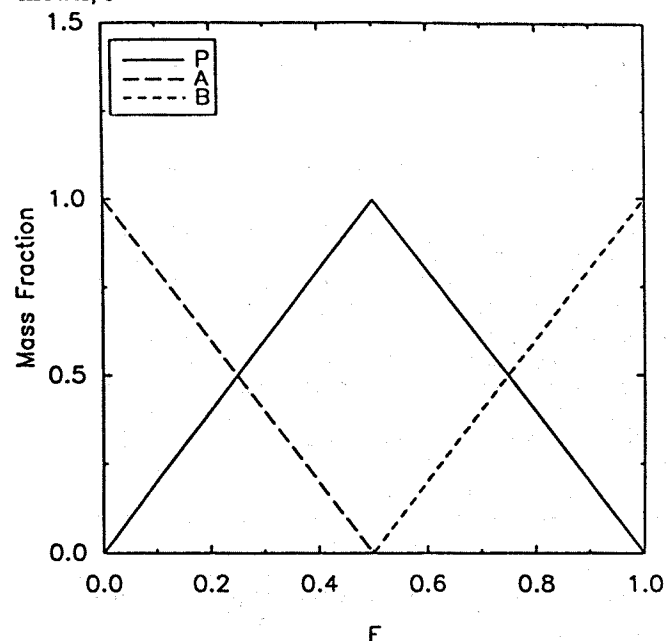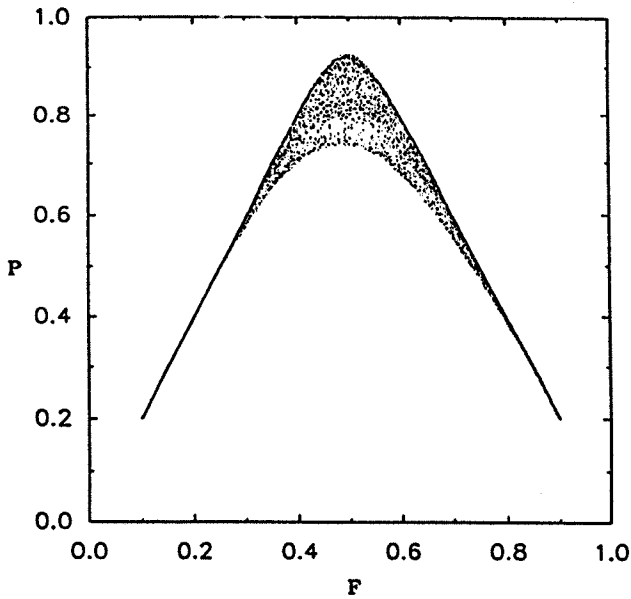

Figure 8: Flame sheet model solution, r=1

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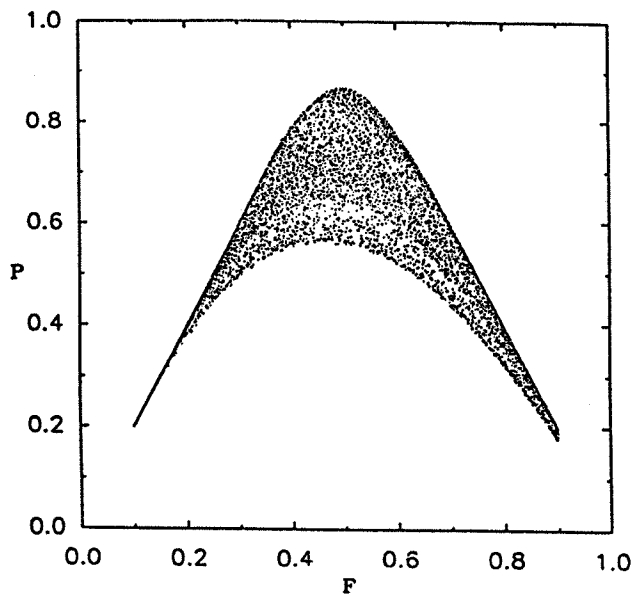
Figure 9(a): Product vs. conserved scalar, Da=150 and r=1

Figure 9(b): Product vs. conserved scalar, Da=30 and r=1

of P(F) vs. F would coincide with the simple line shown in Fig. 8. However, for finite rate reactions a scatter plot must be made. This is shown in Figs. 9(a) and 9(b), for Da=150 and Da=30, respectively. Although the higher reaction rate plot shows closer correspondence to the infinite reaction rate solution, it is still far too slow to be modelled as such. Solutions to the 1D laminar opposed jet flame yield single curves which are functions of the parameter K_f/χ_s. One observation that can be made from Fig. 9 is that the scatter values of the product mass fraction corresponding to small and large values of the conserved scalar form a straight line which is very close to that obtained for the infinitely fast reaction. Therefore, the most severe test of the model is for the stoichiometric surface corresponding to the point of maximum scatter ($F_s=0.5$). Figures 10(a) and 10(b) show the product mass fraction at the stoichiometric surface as a function of K_f/χ_s, for both the DNS and the 1D opposed laminar jet flame. The DNS data were
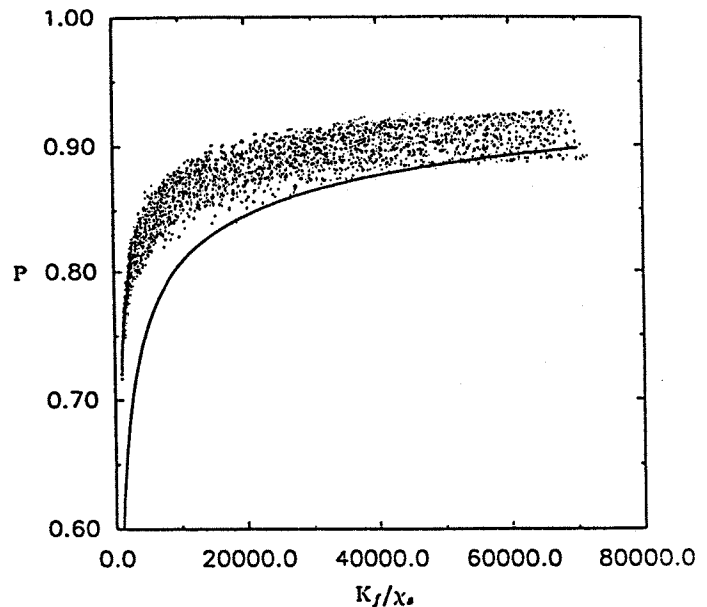

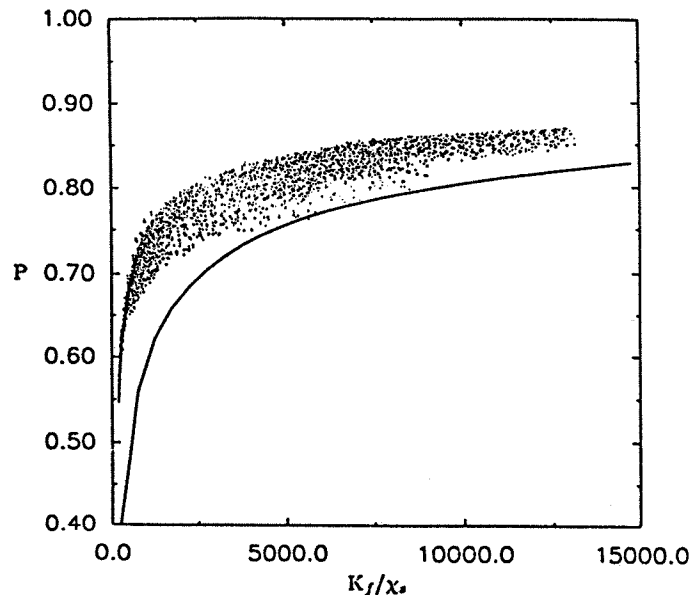Figure 10(a): Laminar flamelet model comparison, Da=150 and r=1

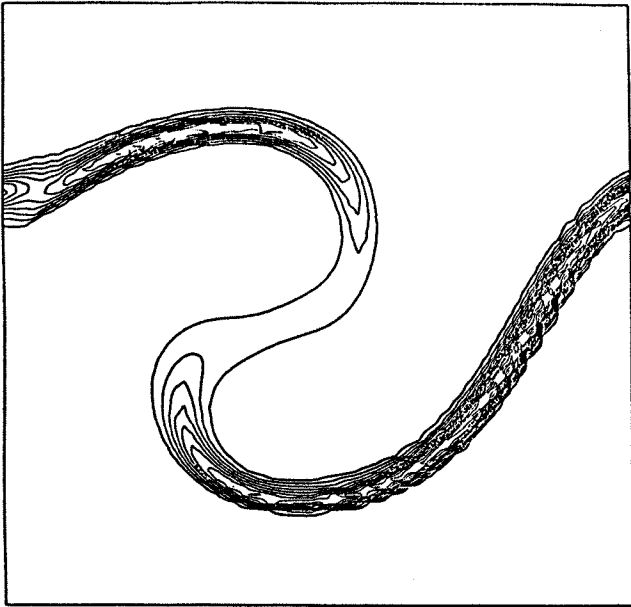Figure 10(b): Laminar flamelet model comparison, Da=30 and r=1
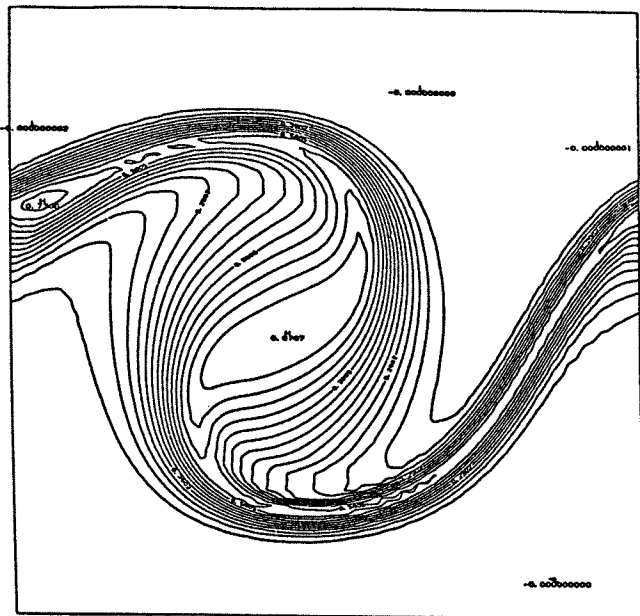
for both high and low reaction rates. In order to minimize compressibility effects, simulations are performed with a convective Mach number $M_c=0.2$. The physical flow is desired to be as "turbulent" as possible in order to test the model. Therefore, simulations are continued until $t^*=0.85$, when the flow has completely developed. Product mass fraction, conserved scalar, and the instantaneous dissipation are calculated. In order to compare the DNS to model predictions, for each grid point i, a corresponding value of $(\chi_s)_i$ is calculated from the model Eq. (10). The reaction rate coefficient (K_f) is now divided by each $(\chi_s)_i$, so that a simple reaction dependent value is obtained for comparison. We begin by considering the simple reaction in which the stoichiometric coefficient r=1, such that the stoichiometric surface is located at $F_s=1/2$. For an infinitely fast reaction rate, plots

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Figure 11(a): Reaction rate contours

Figure 11(b): Product mass fraction contours

cluded that the laminar flamelet model works best in the large scale vortical structures of the mixing layer. Comparing the two different values of Da reveals that agreement does indeed improve with increasing the value of the Damköler number. However, the difference is not very large which is promising since it is for low values of Da for which the model is intended to be used.

In Figs. 12(a) and 12(b) results are presented for a more complicated chemistry. The stoichiometric coefficient is now r=3, such that $F_s=1/4$. This is a much better approximation to true hydrocarbon chemistry which typically has low values of F_s. Again, it is the behavior of the laminar flamelet model at or near the stoichiometric surface in which we are most interested. Figures 13(a) and 13(b) show the stoichiometric product mass fraction as a function of K_f/χ_s. The agreement between the 1D opposed jet solution and the DNS is greatly improved for all ranges of K_f/χ_s. The agreement appears to hold well for the lower Damköler number simulation.
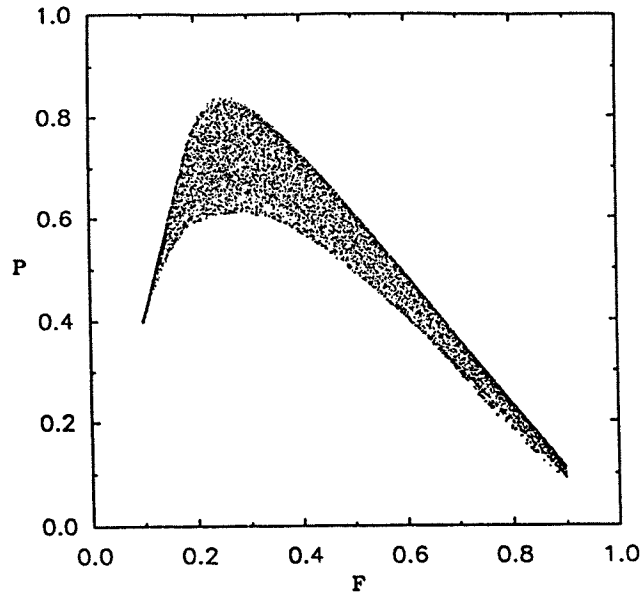

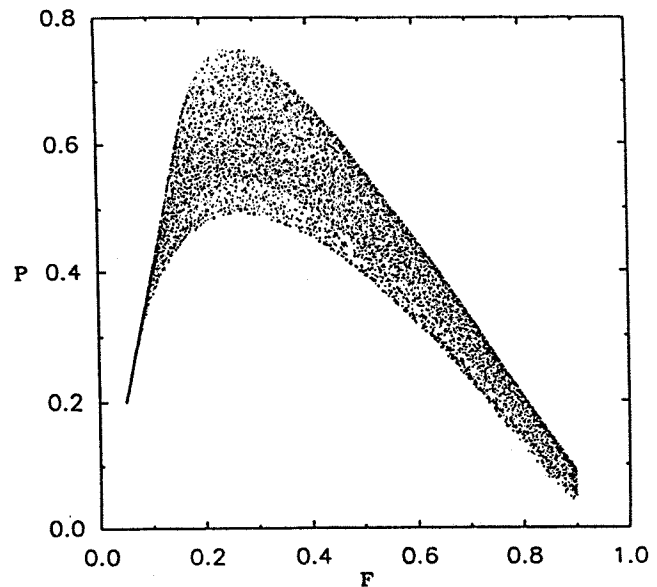Figure 12(a): Product vs. conserved scalar, Da=375000 and r=3

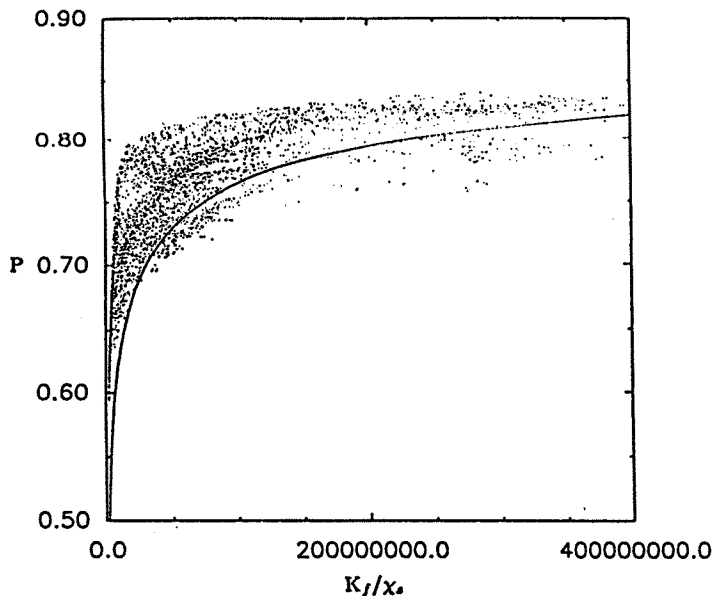Figure 12(b): Product vs. conserved scalar, Da=75000 and r=3

taken from a small range of the conserved scalar centered about F_s. These figures correspond to Da=150, and Da=30, respectively. For both of these figures, the agreement between the model and the DNS data improves as the value of the dissipation decreases (or K_f increases).

Figure 11 shows contours of reaction rate and product mass fraction for an x-y plane of the layer, for Da=30. In the large scale vortical structures, reactants have sufficient time to mix and nearly complete the reaction to form products. In this region the gradients of the conserved scalar are small, therefore the dissipation rate is low. However, in the braids, due to vortex stretching, the gradients and dissipation are at their highest and diffusion allows a continuous molecular mixing and reaction. Therefore, it can be con-

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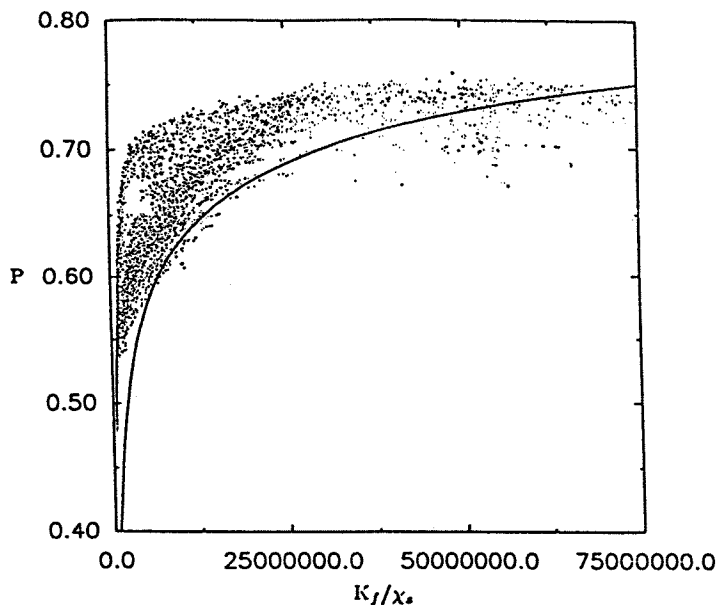Figure 13(a): Laminar flamelet model comparison, Da=375000 and r=3

Figure 13(b): Laminar flamelet model comparison, Da=75000 and r=3

Conclusions

A monotone Flux Corrected Transport numerical scheme has been employed in order to simulate a 3D mixing layer. The results of these simulations are used to study two controversial issues in such layers: (1) the existence of eddy shocklets in a 3D shear layer, and (2) the validity of the laminar diffusion flamelet model for describing non-equilibrium chemical reactions. The results are shown to correlate well with previous observations, both experimental and analytical, through study of the large scale structures and statistical characteristics of the layer. Shocks are indeed found at high Mach numbers. Their existence has never been reported before in three dimensional mixing layer simulations. Also, the results show good agreement between the simulated data and the lam-

inar flamelet model for a simple binary chemical reaction. The agreement between the model and the DNS is shown to improve by either increasing the Damköhler number, or by increasing the value of the stoichiometric coefficient r. Work is currently underway to incorporate more complex reacting systems into an analogous computational study.

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