NUMERICAL STUDY OF TURBULENT COMBUSTION IN A SHEAR LAYER

by

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Submitted to the Department of
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ABSTRACT

A numerical methodology is introduced which enables the study of turbulent combustion in a shear layer over a substantial range of the governing parameters. The Transport–Reaction Element Method (TREM), a scheme capable of resolving an exothermically reacting scalar field, is developed and is used with the Vortex Element Method (VEM) which yields the flowfield. The two schemes are Lagrangian, grid-free and adaptive and solve the unaveraged, time dependent and coupled scalar transport-reaction and Navier-Stokes equations respectively, in their scalar-gradient and vorticity forms. The TREM exploits the Shvab-Zeldovich formulation to provide solutions for both moderately fast and infinitely fast reactions. For finite reaction speeds, Arrhenius kinetics are used.

The methodology is first implemented in the numerical simulation of the turbulent non-reacting variable density spacial shear layer, i.e. the flow evolving between two streams of fluids of different velocities and densities. This flow enables an independent study of baroclinic vorticity generation, which is one of the mechanisms of flowfield modification in the presence of combustion. The variation of the growth rate, entrainment ratio and speeds of vortical structures (eddies) with the free stream density ratio, follow experimentally established trends. It is also found that the layer growth behavior can be altered via external forcing of the flow instability.

The turbulent non-premixed reacting shear layer is then simulated with the aim of investigating the effects of the combustion heat release. Calculations for finite and infinite reaction speed and for different values of the enthalpy of reaction are carried out. They are compared with calculations for which the effects of the reacting field on the flowfield are removed by keeping the density uniform. Combustion heat release decreases the shear-mixing region size via both a delay in the onset of the flow instability and a suppression of eddy pairing. This, together with the decreased density within the mixing region leads to reduced product formation. External forcing of the flow instability does not eradicate these trends. Pairing of eddies continues to be resisted and is altered into tearing of smaller eddies by adjacent larger neighbors. Explanations for these effects are established by analyzing the mechanisms by which the flow and reacting fields interact. It is found that the initial delay of the flow instability is a result of volumetric expansion, while the alteration of the eddy interaction mechanism is a result of baroclinic vorticity generation.

Finally, the basis of an alternative methodology relying on the concept of the Lagrangian strained diffusion flamelet is introduced to deal with fast but finite reaction speeds. The part of the scheme solving the flamelet reacting field is developed and is used in a study of diffusion flames subjected to steady and oscillating strains. Results indicate that unsteady strains strongly influence the flame mean burning rate if abrupt, transient phenomena such as quenching, extinction and re-ignition are at least partially experienced.

Thesis Committee:  Prof. A. F. Ghoniem (Chairman)
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1. INTRODUCTION

1.1. Background

Turbulent combustion is of fundamental importance to most energy conversion processes occurring in propulsion and power generation systems. It has long been recognized that fast and efficient burning, with enhanced rates of chemical energy release can be achieved if turbulence is properly employed to promote mixing among the reacting species, without causing quenching of the reaction zone or the generation of unwanted instabilities. On the other hand, combustion itself can have a significant impact on turbulence since it causes substantial changes in the density and transport properties of the mixture. Hence, a thorough understanding of the interactions between turbulence and combustion is necessary in the effort to optimize energy conversion. Stringent pollutant emission standards offer additional motivation for the closer scrutiny of the phenomenon. The origins of these emissions are subtle and are commonly linked to local unsteady and non-equilibrium phenomena which in order to be accurately predicted require a detailed analysis of the turbulent combustion field.

Predicting the results of the interactions between a turbulent flowfield and a reaction zone is extremely difficult and involves a detailed examination of the convective and diffusive transport processes, coupled with the combustion kinetics and dynamics. A major source of difficulty is the fact that these processes are inherently unsteady and are strongly coupled. Turbulence influences combustion via enhanced mixing and reaction zone stretch and curvature, all of which result from the evolution of a highly concentrated and oscillating vorticity field. Combustion, on the other hand, influences the turbulent flowfield through thermal expansion, baroclinic vorticity and the variation of the thermodynamic and transport properties of the fluids involved. The first two mechanisms are linked to changes in the density field which are attributed to the heat release and the change in chemical composition occurring during combustion.
In this work, turbulent combustion is studied in the context of a non-premixed shear layer. Turbulent reacting shear layers have commonly been used for this purpose [1]. The flow configuration, shown in figure 1.1, results from the amplification of the shear instability between two parallel streams of fluids initially flowing at different velocities, and possibly, densities, downstream of a splitter plate. It represents a generic model of many mixing and combustion systems. It is also simple enough to allow accurate and detailed experimental measurements, which in turn can be used to validate theoretical and numerical models. Experimental studies for both reacting and non-reacting shear layers [2-6] have yielded flow-visualizations of the type shown in figure 1.1 and have revealed that the flow is essentially two dimensional at its early stages and is dominated by large-scale vortical structures (eddies). These structures which are present even at very high Reynolds's numbers originate via the Kelvin-Helmholtz instability and persist through successive downstream interactions. They also coincide with the region where product exists and hence they represent the prime mechanism by which reactants from the free streams mix and burn.

Significant effort has been expended to develop models which can predict turbulence and combustion in reacting shear layers. Success, however, has been limited. Even after extensive simplifications of the chemical kinetics and of the effect of combustion on the thermodynamic and transport properties, the problem is far too complex to allow analytical solutions. Phenomenological models based on the closure of a system of time-averaged transport equations which describe the statistical behavior of the aerothermodynamic variables have been used to obtain results which exhibit some agreement with experimental measurements. Examples of such models include moment methods [7,8], assumed probability density functions (PDF) shape methods [9], solutions based on modeled joint PDF of scalar [10,11] and solutions based on modeled joint PDF of velocity [12]. However, such models suffer from a number of significant limitations. The modeling assumptions for the turbulent correlations, the origins of which can usually be
traced to the study of homogeneous, small-scale turbulence in a uniform density field, is questionable. It is not apparent whether such correlations can be applied in a non-homogenous turbulent flow dominated by large scale structures like a shear layer. Furthermore, the variable density field present in mostcombusting flows raises further questions about the applicability of correlations obtained in a uniform density field. Additionally, solutions obtained from phenomenological models are strongly dependent on empirical coefficients which limit their generality and most importantly, their predictive capability.

Closure models are further limited by the time averaging itself, a process which masks some of the pertinent information in the governing equations. The significant unsteadiness of the turbulent flow, coupled with the strong non-linearity of the reaction source term, e.g. the Arrhenius form, imply a strong dependence of the phenomenon on instantaneous values of the variables involved, rather than the time-averaged ones. Furthermore, time averaging of the source term itself, except of the case of an assumed PDF of the gas dynamic variables, leads to a divergent model of the average reaction rate. Moreover, since some of the interesting dynamics of turbulence-combustion interactions are hypothesized a priori, e.g. assumed PDF's, solutions do not provide better insight into the phenomena. For all these reasons, phenomenological models are bound to be limited in their success in analyzing this flow.

Recent advances in numerical methods, combined with the exponential growth in computer power, have enabled the numerical study of turbulent combustion in shear flows via the integration of the governing transport equations over some limited parameter range, without the need for time-averaging or large scale modeling. These time-dependent, spacially resolved solutions attempt to reproduce the phenomenon in its full complexity and can, hence, be used to gain a better understanding of the underlying physical mechanisms. They also promise to enable general predictability thus substituting, at least partially, for experimental investigations.
Finite-difference methods [13,14], spectral methods [15-18] and Lagrangian vortex/transport (flowfield/scalar-field) element methods [e.g 19-21] have been utilized in numerical simulations of non-reacting and reacting shear layers in two and three dimensions. The idealized temporal evolution approximation, which is significantly less expensive computationally than the actual spacial evolution, is almost exclusively invoked, particularly in three dimensional calculations. The severe limitations inherent in this idealized representation of the flow are discussed in the following paragraphs. The first two methods are based on an Eulerian description of the flowfield and require grids which cover the computational domain. Finite-difference methods use grids to discretize gradients of the aerothermodynamic variables, a process inherently impaired by numerical diffusion. Grid resolution also defines the size of the smallest possible scales and thus limits the range of possible Reynolds numbers in the simulation. Spectral methods employ grids to expand the aerothermodynamic variables in harmonic functions. This makes these methods prone to the use of periodic boundary conditions. The accuracy of the discretization, as well as the range of the Reynolds number, are dependent on the number of harmonic modes used. This allows simulations at higher Reynolds numbers than the ones performed using finite-difference methods but which are currently still limited to relatively low values. Vortex/transport element methods, on the other hand, are grid-free, Lagrangian schemes which enable solutions at high Reynolds number. This is because flow gradients are not discretized on a fixed grid and convection is implemented by translating these gradients along particle trajectories. This approach limits numerical diffusion and endows the algorithm with spacial adaptivity. Discretization of the gradients on a computational particle field which is convected along particle trajectories captures the large scale structure, while the effect of the small scales, for the sake of economy, can be modeled based on understanding of "substructural phenomena". The high Reynolds number capability of the method is a critical reason for its selection for the study of turbulent combustion.
Vortex/transport element methods of various forms have been used to simulate reacting shear layers. The combustion kinetics have been simplified to a single-step Arrhenius type and the Damkohler number (comparison of combustion and diffusion speeds) has been kept very low. These two simplifications can only model distributed reaction phenomena and avoid resolution problems accompanying the formation of thin reaction zones. For the spacially developing shear layer case [22,23] calculations have been restricted to two dimensions and the hydrodynamic field has been decoupled from the reacting field by assuming low (negligible) combustion heat release. Thus, the effect of combustion on the flow is removed. This is a major simplification contradicted by experimental evidence [6] which indicates substantial alterations of the flow structure due to the presence of the reaction exothermicity. For the idealized temporal evolution case, simulations have been carried out in both two [24-26] and three [27,28] dimensions. Finite (but small) combustion heat release, was allowed in some of these calculations. Three-dimensional calculations, though, also incorporate the extra simplifying assumption of infinite activation energy. Such an assumption removes the exponential nature of the reaction rate and thus reduces the stiffness of the governing equations.

As will be shown in later parts of this work (see Chapter Three), the applicability of the idealized, temporally evolving flow model, is severely limiting for reacting shear layers. The temporal model aims at approximating the shear layer flow via a Galilean space-time transformation: a computational domain is selected which is moving with the mean flow velocity and which describes a small section of the flowfield. This section is defined by the flow time scale in such a way as to include one or two vortical structures. The small size of the domain, as compared to that necessary in a spacial layer simulation, is the major source of the savings mentioned earlier. The problem with the use of temporal layers lies in the fact that the boundary conditions in the streamwise direction (i.e. at the inlet and exit) of the domain are not explicitly known. For this reason, artificial periodic boundary conditions are imposed. As a result the actual flow cannot be reproduced exactly from such a
calculation. For example, the asymmetry imposed by the velocity ratio, which results in the tendency of the uniform density shear layer to intrude more into the slower of the two streams, cannot be captured. Additionally, the streamwise asymmetry in the shape of the vortical structures is also lost. For the reacting field, the limitations are more devastating. The periodic boundary conditions remove any spacial evolution of the combustion-related properties of material which crosses the domain in the streamwise direction; only temporal evolution is permitted. On the other hand, the same material experiences significant flow-related evolution. This is an uncommon situation since it requires the flow speed to be higher than the combustion speed, i.e. high Karlovitz number. For a real fuel, characterized by a high Damkohler number, such a condition would unavoidably lead to quenching (termination of the reaction due to excessive flow stretch). In the temporal simulations noted above, this problem does not arise due to the low Damkohler number assumption. What is evident from the above discussion though, is that the applicability of temporal simulations is in fact restricted to low Damkohler number combustion and unphysical solutions would result if higher values of this parameter were to be used.

For all these reasons, the temporal layer idealization is avoided in this work. Rather, a numerical methodology for the study of the spacial two dimensional post-transitional shear layer is developed. In contrast to previous work, this methodology enables the incorporation of the effects of the combustion heat release on the flow. Hence, results obtained are used to investigate flow-combustion interactions of significant complexity. The Damkohler number is raised to moderate values and models dealing with very high values of this parameter are proposed.

1.2 Objectives

The objectives of this thesis are to:
(i) Develop and implement a numerical methodology which enables the simulation of a two-dimensional, spatially evolving, post-transitional, exothermically reacting, non-premixed shear layer over a wide range of the governing parameters.

(ii) Utilize the results in a study of flow-combustion interactions to:

(a) Analyze the effects of post-transitional flow on combustion by considering the distortion of the reacting field via the hydrodynamic strain.

(b) Investigate the effects of combustion on the flow by considering the effects of the heat release and of the associated variable density field.

1.3. Organization

To achieve these objectives, the Lagrangian Transport–Reaction Element Method (TREM), a scheme which deals with an exothermically reacting scalar field, is developed and used in conjunction with the variable density Vortex Element Method (VEM) to simulate the flow. The new scheme exploits the use of Shvab-Zeldovich variables and can perform a highly accurate calculation of one reacting scalar. It provides solutions for both moderately fast and infinitely fast reactions. The details of the formulation are presented in Chapter Two. The description and analysis of the scheme is given in Chapter Three.

In Chapter Four the developed methodology is implemented in the simulation of a two-dimensional, spatially developing, non-reacting, variable density -but incompressible-shear layer, i.e. the shear layer evolving between two fluids (gases) of different velocities and densities. This is an intriguing flow which has received significant attention experimentally [29-32], and which before this work had not been successfully simulated. In the context of the main objectives of this thesis, its simulation is motivated by the fact that in it, the hydrodynamic effect of the density variation is manifested only through the generation of baroclinic vorticity. Since this mechanism is also active in the presence of combustion, studying this non-reacting flow can lead to a better understanding of the effects of the combustion-related variable density field in a reacting flowfield.
In Chapter Five the calculations are extended to the non-premixed reacting spacial shear layer with significant heat release. The two streams, each carrying one of the reactants, mix downstream of the splitter plate and burn to yield a single product. Simulations for both finite and infinite speed of reaction are performed. Flow-combustion interactions are studied in detail. Particular emphasis is placed on the effects of combustion heat release on the flowfield.

As a first step for future work, the basis for a new scheme addressing the high but still finite reaction speed domain is presented in Chapter Six. It has been recognized that under these conditions the reaction zone becomes exceedingly thin and highly stretched by the hydrodynamic strain. On the other hand, it is clear that important combustion-related phenomena occur within this thin zone. The new scheme internalizes these concepts by treating the reaction zone as a flame-sheet when dealing with the hydrodynamic field and as a finite region when dealing with the combusting field. This is achieved by segmenting the flame-sheet along its length into small, flat flamelets. In this thesis a program module is developed which resolves the reacting field in the neighborhood of these flamelets, given the local hydrodynamic strain. In future work this module is to be used to provide the global reacting field by introducing mechanisms of interaction between the flamelets. The transport of the flame-sheet by the flow is to be accomplished using the Vortex Element Method. Herein, the flamelet module program is used in a study of flat, strained diffusion flames which are subjected to steady and periodic strains.

Finally, the main conclusions of this work are presented in Chapter Seven.
(a) Non-reacting shear layer

(i) He

(ii)

N₂

(a) The turbulent, non-reacting variable density shear layer set up by a fast stream of Helium and a slow stream of Nitrogen - free stream density ratio equal to seven. (i) and (ii) represent cases with different Reynolds number: Re(ii) > Re(i) (Brown and Roshko 1974 [30])

(b) Reacting shear layer

2% F₂

2% H₂

(b) The turbulent, reacting shear layer set up by a fast stream of 2% F₂ in N₂ and a slow stream of 2% H₂ also in N₂. The combustion heat release is relatively low with an adiabatic temperature change of ΔTf = 186K (Hermanson and Dimotakis 1988 [61])
2. FORMULATION

2.1. Governing Equations–Primitive Variable Form

The equations governing the evolution of the turbulent reacting shear layer are derived under the continuum flow model and are simplified by a number of assumptions. The resulting non-dimensionalized equations, in primitive variable form, are shown in table 2.1. The details of the simplifying assumptions are discussed in the following paragraphs.

Gravitational effects are considered negligible. This assumption is justified by the fact that the shear layer flow which is studied here is of small length scale and of reasonably high speed. Hence, the resulting Froude number is large, suggesting that inertial forces dominate over gravitational forces.

The flow is assumed to be two dimensional. As pointed out in the previous chapter, such an assumption is justified by the flow configuration. Admittedly, the three dimensional nature of turbulence is in conflict with this assumption, particularly at the small scales. The resulting errors, however, are expected to be small. This is supported by a number of previous numerical studies of two dimensional non-reacting shear layers [19,20], which have shown that this approximate model is able to reproduce most of the flow features accurately.

The Mach number is assumed to be negligibly small. According to this assumption, the flow speed is much smaller than the speed of sound (speed of pressure wave propagation). Hence, spacial pressure variations, resulting from combustion and flow evolution, reach equilibrium rapidly (infinitely fast in the limit of zero Mach number) when compared to the flow timescale. Thus, for fluid motion, pressure variations would appear small when compared to the total (thermodynamic) pressure, i.e. thermodynamically, spacial pressure variations can be considered negligible. This can easily be seen by considering that the momentum equation for this case, reduces to the statement that spacial gradients of the thermodynamic pressure are equal to zero. While the pressure variations are small when compared to the thermodynamic pressure, they are not
negligible when compared to the other forces governing fluid motion. Thus by rescaling the pressure variations with the flow dynamic pressure one can ascertain their effect on the flowfield. This is expressed in the more traditional momentum equation shown in table 2.1. (This distinction between the thermodynamic and dynamic pressure in a low Mach number combusting system was initially proposed in ref.[16] where a detailed derivation of the approximate equations of motion is presented.)

While, under the low Mach number assumption, combustion has an insignificant effect on the spacial thermodynamic pressure variation, it can substantially alter this pressure in time. This is certainly true in a constant volume domain where the overall density is constant and substantial pressure changes take place as combustion heat is released and the fluid temperature is raised. In an open (infinite volume) domain, on the other hand, combustion primarily alters the fluid temperature and density resulting to approximately constant pressure. In this work the flow is partially confined (see Chapter Three). Nevertheless, constant pressure combustion is still assumed since in the cross-stream direction the confining walls are substantially far from the combusting region and in the streamwise direction the domain is relatively short. The validity of this assumption is further assessed from the results by comparing the streamwise dynamic pressure change of each fluid stream to the corresponding inlet dynamic pressure. Thus, in this formulation the thermodynamic pressure is treated as a constant both in space and time and hence it is absent from the non-dimensionalized equations. The pressure appearing in the momentum equation is the flow dynamic pressure.

Combustion is assumed to take place according to a single step reaction which consumes two reactants, one from each stream, to yield a single product. The chemical kinetics are of the Arrhenius type. The transport properties are constant. All species are assumed to behave as perfect gases with equal molecular weights, specific heats and mass diffusion coefficients. The Lewis number is equal to unity (equal heat and mass diffusion coefficients). Diffusion effects are assumed small (high Reynolds and Peclet number flow).
This allows higher order diffusion mechanisms to be neglected. Hence, thermal diffusion (Soret effect), second order diffusion terms in the scalar equations arising from products of density and scalar gradients, and heat production due to fluid dynamical viscous dissipation, are all neglected.

Non dimensionalization is carried out using a length scale, $\tilde{L}_o$, a velocity scale, $\tilde{U}_o$ and temperature, $\tilde{T}_o$, and density, $\tilde{\rho}_o$, scales. (The tildes indicate dimensional variables. In what follows, absence of the tilde denotes a non-dimensionalized variable). The actual values of these scales are specified in later chapters. The simultaneous use of density and temperature scales allows for the different scaling of the thermodynamic pressure as compared to that of the dynamic pressure which is scaled via the density and the velocity scales.

Hence, the non-dimensionalized governing equations are:

\textbf{Table 2.1}

\begin{align*}
\text{Continuity} & \quad \frac{dp}{dt} + \rho \nabla \cdot \mathbf{u} = 0 & (2.1) \\
\text{Momentum} & \quad \frac{d\mathbf{u}}{dt} = -\frac{\nabla p}{\rho} + \frac{1}{Re} \nabla^2 \mathbf{u} & (2.2) \\
\text{Equation of State} & \quad \rho \ T = 1 & (2.3) \\
\text{Chemical Reaction} & \quad \phi \chi_1 + \chi_2 \rightarrow (1+\phi) \chi_p & (2.4) \\
\text{Temperature-Species} & \quad \frac{ds_j}{dt} = \frac{1}{Pe} \nabla^2 s_j + Q_j \frac{\dot{w}}{\rho} & (2.5) \\
\end{align*}

with

\[
\begin{array}{|c|c|c|c|c|}
\hline
j & 1 & 2 & 3 & 4^{(*)} \\
\hline
s_j & T & Y_1 & Y_2 & Y_p \\
Q_j & Q_0 & \phi & -1 & 1+\phi \\
\hline
\end{array}
\]

\[ (+) \ Y_1 + Y_2 + Y_p = 1 \] \hspace{1cm} (2.6)

and where \[ \dot{w} = A_f \rho^2 Y_1 Y_2 \exp\left(-\frac{T_a}{T}\right) \] \hspace{1cm} (2.7)
The symbols used in table 2.1 are defined as follows: $u = (u,v)$ is the velocity vector in a right-handed Cartesian coordinate system $x = (x,y)$ and $t$ is the time. $\nabla = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right)$ is the gradient operator and $\frac{d}{dt} = \frac{\partial}{\partial t} + u \cdot \nabla$ the Lagrangian-material derivative. $p$ is the dynamic pressure and $\rho$ and $T$ are the fluid mixture density and temperature respectively. $\chi_i$ denotes species $i$, $i=1,2$ being the reacting species and $i=p$ being the product. $Y_i = \frac{\rho_i}{\rho}$ is the mass-fraction for species $i$ ($\rho_i$ is the species’ partial density) and $\dot{w}$ is the reaction rate. Re is the Reynolds number, $Re = \frac{\tilde{U}_o \tilde{L}_o}{\nu}$, with $\nu$ being the kinematic viscosity. Similarly, Pe is the Peclet number $Pe = \frac{\tilde{U}_o \tilde{L}_o}{\tilde{\alpha}}$. $\tilde{\alpha}$ is the thermal diffusivity, which under the unity Lewis number assumption is equal to the mass diffusivity $\tilde{D}$ which, in turn, is the same for all species. $A_f$ is the frequency factor, $A_f = \frac{\tilde{A}_f \rho_o \tilde{L}_o}{\tilde{U}_o}$, $\phi$ and $\phi$ are the molar and mass stoichiometry ratios respectively ($\phi = \phi \frac{\tilde{M}_1}{\tilde{M}_2}$, $\tilde{M}_i$ being the molar mass of species $i$). $Q_o$ is the enthalpy of reaction, $Q_o = \frac{\Delta h_f}{\tilde{c}_p T_o}$, where $\tilde{c}_p$ is the mixture specific heat. $T_a$ is the activation temperature $T_a = \frac{\tilde{E}_a}{\tilde{R} T_o}$, where $\tilde{E}_a$ is the activation energy and $\tilde{R}$ the universal gas constant.

2.2. Non-Primitive Variable Form

These equations are strongly non-linear and coupled. They are also numerically stiff, their stiffness being a strong function of the governing parameters (Re, Pe, $A_f$, $\phi$, $Q_o$, $T_a$). Their numerical integration is expected to become exceedingly demanding as the Reynolds and Peclet numbers increase and as the reaction becomes fast and strongly exothermic.

For primarily numerical reasons, which will become apparent in the next chapter, some of the difficulty in solving these equations can be alleviated by recasting them in non-primitive variable form. The resulting equations are shown in table 2.2.
Specifically, the equations of fluid motion are recast into a vorticity-streamfunction formulation. The vorticity equation is obtained by taking the curl of the momentum equation. The streamfunction equation is a manifestation of the definition of vorticity as the curl of the velocity. Solution of these equations yields the vortical-rotational component of the velocity field. The total velocity field is obtained from the Helmholtz decomposition [33] which recognizes that irrotational components of velocity (manifestations of the continuity equation), resulting from the combustion-related volumetric expansion and from the nature of the boundary conditions, also exist.

To simplify the scalar transport equations, Shvab-Zeldovich (S-Z) non-reacting variables ($\lambda$, $\gamma$, see table 2.2) are introduced. These variables are constructed from combinations of the primitive reacting scalars in such a way that the equations governing their transport (obtained from algebraic manipulations of equations (2.5)) are void of reaction terms, and are hence much simpler to deal with: i.e.

$$\frac{d\beta}{dt} = \frac{1}{Pe} \nabla^2 \beta \tag{2.8}$$

where $\beta = \lambda$ or $\gamma$.

Depending on the application, the particular choice of these variables can also result in further simplifications. A good example of this is illustrated by the $\gamma$ variable used here. By combining the temperature with the product mass-fraction into one variable, one can capitalize on the fact that if the initial conditions imply that these two properties are initially directly related (i.e. $\gamma(x,0) = 1$), then equation (2.8) above suggests that they will remain related at all later times. This, in essence, reduces the equations to be solved by one, since the solution for $\gamma$ is trivially known (i.e. $\gamma(x,t) = 1$).

The main disadvantage in the use of Shvab-Zeldovich variables is that they impose the substantial limitations on the choice of the transport properties noted earlier. This is because in order to reduce the equations, the mass-diffusion coefficients had to be assumed equal for all species and the Lewis number had to be chosen equal to unity.
In analogy to the treatment of the Navier-Stokes equations, the Shvab-Zeldovich scalar transport equations are recast into gradient form. Evidently, integration of the solutions of the gradient equations provides the scalar field only within a constant. This constant is defined by the boundary conditions. Thus, in an approach similar to the Helmholtz decomposition of the velocity field, the total Shvab-Zeldovich scalar field solutions are obtained by adding these two components.

In the limiting case of infinite reaction rate combustion, where the reaction zone collapses onto a line and reactant coexistence is prohibited, the Shvab-Zeldovich variable solutions together with the equation of the conservation of the species mass-fractions (eq.(2.6)) are able to provide a complete description of the reacting field. i.e.

**Infinite reaction:** \[ \lambda \geq 0 \quad Y_1 = \lambda, \quad Y_2 = 0, \quad Y_p = 1 - \lambda \]  
\[ \lambda \leq 0 \quad Y_1 = 0, \quad Y_2 = -\frac{\lambda}{\phi}, \quad Y_p = 1 + \frac{\lambda}{\phi} \]  

(2.9a) \hspace{1cm} (2.9b)

The temperature field is obtained using the definition of $\gamma$. If the reaction speed is finite, on the other hand, the Shvab-Zeldovich solutions and the mass-fraction conservation equation do not contain all the information necessary to construct the reacting field. At least one reacting scalar must be explicitly obtained. In the formulation presented here, this scalar is chosen to be the product mass fraction. Once the product mass-fraction solution is known, the reacting species solutions can be constructed according to

**Finite reaction:**  
\[ Y_1 = \frac{\lambda + \phi(1-Y_p)}{1+\phi} \]  
\[ Y_2 = \frac{-\lambda + (1-Y_p)}{1+\phi} \]  

(2.10)

and the temperature solution by using the definition of $\gamma$, to completely describe the reacting scalar field. It should also be noted that the non-reacting flow case is easily included in the finite reaction speed case by simply specifying $Y_p = 0$.

Hence the governing equations become:
Table 2.2

Helmholtz Dec.

\[ \mathbf{u} = \mathbf{u}_o + \mathbf{u}_p + \mathbf{u}_e \]  \hspace{1cm} (2.11)

where

(a) \hspace{1cm} (b) \hspace{1cm} (c)

\[ \mathbf{u}_o = \nabla \times (\psi \mathbf{k}) \hspace{0.5cm} \mathbf{u}_p = \nabla \phi_p \hspace{0.5cm} \mathbf{u}_e = \nabla \phi_e \]  \hspace{1cm} (2.12)

\[ \nabla^2 \psi = -\omega \hspace{0.5cm} \nabla^2 \phi_p = 0 \hspace{0.5cm} \nabla^2 \phi_e = -\frac{1}{\rho} \frac{\mathrm{d} \rho}{\mathrm{d} t} \]  \hspace{1cm} (2.13)

Vorticity

\[ \frac{\mathrm{d} \mathbf{\omega} \times \mathbf{k}}{\mathrm{d} t} + (\nabla \cdot \mathbf{u}) \mathbf{\omega} \times \mathbf{k} = \frac{\nabla \rho \times \nabla p}{\rho^2} + \frac{1}{\text{Re}} \nabla^2 \mathbf{\omega} \times \mathbf{k} \]  \hspace{1cm} (2.14)

Equation of State

\[ \rho \ T = 1 \]  \hspace{1cm} (2.3)

Chemical Reaction

\[ \phi \ \chi_1 + \chi_2 \rightarrow (1+\phi) \chi_p \]  \hspace{1cm} (2.4)

S-Z Variables

\[ \lambda = Y_1 - \phi Y_2 \hspace{1cm} \gamma = T \cdot \frac{Q_0 \phi}{1+\phi} Y_p \]  \hspace{1cm} (2.15)

S-Z Scalar Dec.

\[ s_j = s_{gj} + s_{pj} \]  \hspace{1cm} (2.16)

with

\[
\begin{array}{c|cc}
  j & 1 & 2 \\
  s_j & \lambda & \gamma \\
\end{array}
\]

S-Z Gradient

\[ \frac{\mathrm{d} g_j}{\mathrm{d} t} + g_j \cdot \nabla \mathbf{u} + g_j \times (\mathbf{\omega} \times \mathbf{k}) = \frac{1}{\text{Pe}} \nabla^2 g_j \]  \hspace{1cm} (2.17)

where

\[ g_j = \nabla s_{gj} \]  \hspace{1cm} (2.18)

Product

\[ \frac{\mathrm{d} Y_p}{\mathrm{d} t} = \frac{1}{\text{Pe}} \nabla^2 Y_p + (1+\phi) \frac{\mathbf{\dot{w}}}{\rho} \]  \hspace{1cm} (2.19)

where

\[ \mathbf{\dot{w}} = A_f \rho^2 Y_1 Y_2 \exp(-\frac{T_0}{T}) \]  \hspace{1cm} (2.7)

\[ Y_1 + Y_2 + Y_p = 1 \]  \hspace{1cm} (2.6)

\( \mathbf{u}_o \) is the vortical-rotational component of the velocity. It is a consequence of the vorticity field and hence is obtained from the latter's definition \((\text{eq.}(2.13a))\), through the use of the streamfunction \( \psi \). \( \mathbf{k} \) is the unit vector normal to the plain of motion.) The streamfunction formulation also implies that the vortical velocity field is solenoidal, i.e. it
satisfies the incompressible continuity equation. \( u_p \) is the "potential" component of the velocity field and is added to satisfy boundary conditions. It is obtained from the incompressible continuity equation (2.13b) through the use of the "potential" velocity potential, \( \phi_p \). \( u_e \) is the expansion velocity. It is a manifestation of the change of volume of the fluid due to combustion, and hence it is obtained from the compressible continuity equation (2.13c). This is done through the use of the expansion velocity potential \( \phi_e \). \( \omega \) is the vorticity. It is defined as the curl of the velocity field, i.e. \( \omega = \nabla \times u \). As suggested earlier, this expression is equivalent to equation (2.13a) since \( \nabla \times u = \nabla \times u_\omega \).

\( \lambda \) and \( \gamma (=s_j) \) are the Shvab-Zeldovich scalars. \( s_{gj} \) is the component of the Shvab-Zeldovich scalar field related to gradient \( (g_j) \). \( s_{pj} \) is the "potential" component added to satisfy the corresponding boundary conditions. The rest of the symbols in table 2.2 are as earlier defined.
3. NUMERICAL SCHEMES

3.1. Introduction

The numerical schemes employed in the solution of the equations of table 2.2 are the Vortex Element Method (VEM) and the Transport–Reaction Element Method (TREM).

The origins of the VEM can be traced to the ideas of Rosenhead [34], but its first formal application is due to Chorin [35-37] who used it to study the unsteady wake behind a cylinder and the evolution of a vortex sheet. In its initial form the scheme solves the high Reynold's number, uniform density, time-dependent Navier-Stokes equations in their vorticity-streamfunction formulation. The scheme was later modified to account for variable density effects by Ghoniem et al. [24].

The TREM, which is developed in this work, is based on the Transport Element Method (TEM) developed by Krishnan and Ghoniem [38]. The TEM itself was based on the discretization ideas of Anderson [39] and was developed in analogy to the Vortex Method. In its basic form, this latter scheme determines a non-reacting scalar field by efficiently solving the time-dependent scalar-gradient transport equations at high Peclet number. It was used to establish the density field in a Rayleigh-Taylor flow, as well as in temporally evolving non-reacting shear layers and jets [26]. A reacting version of the TEM was also proposed by Ghoniem et al. [24] and was used to provide temperature and reacting species concentration fields in the simulation of a temporally evolving, premixed, reacting shear layer and a temporally evolving, non-premixed, reacting jet [26].

In this work it is shown that this reacting version of the TEM is not general, and that fundamental concepts in its development rely on the idealized conditions existing in temporally evolving flows. Therefore it cannot be applied in the more realistic spacially evolving flows, like the one considered here. Furthermore, it is pointed out that even in temporal calculations the scheme is valid only when combustion is extremely slow when compared to the flow. These severe limitations necessitated the development of the TREM which is a new reacting version of the TEM. It solves the gradient transport equations of
non-reacting Shvab-Zeldovich scalars as well as the transport-reaction equation of one
primitive scalar.

3.2. The Variable Density Vortex Element Method (VEM)

3.2.1. Governing Equations

As already noted, this scheme solves the variable density fluid motion equations in
their vorticity-streamfunction formulation. For a two-dimensional flow these equations are:
(also provided in table 2.2)

\[ \frac{d\omega \mathbf{k}}{dt} + (\nabla \cdot \mathbf{u}) \mathbf{k} = \frac{\nabla \times \nabla \rho}{\rho^2} + \frac{1}{Re} \nabla^2 \omega \mathbf{k} \]  \hspace{1cm} (3.1)

\[ \nabla^2 \psi = -\omega \]
\[ \mathbf{u}_\omega = \nabla x (\psi \mathbf{k}) \]  \hspace{1cm} (3.2a,b)

\[ \nabla^2 \phi_e = -\frac{1}{\rho} \frac{d\rho}{dt} \]
\[ \mathbf{u}_e = \nabla \phi_e \]  \hspace{1cm} (3.3a,b)

\[ \nabla^2 \phi_p = 0 \]
\[ \mathbf{u}_p = \nabla \phi_p \]  \hspace{1cm} (3.4a,b)

\[ \mathbf{u} = \mathbf{u}_\omega + \mathbf{u}_e + \mathbf{u}_p \]  \hspace{1cm} (3.5)

Quantities related to the density field are provided by the scheme dealing with the scalar
field, i.e. the TREM.

The major thrust of the scheme lies in solving the vorticity transport equation,
eq.(3.1). Once the vorticity field is obtained, the vortical component of the velocity field is
established by solving the streamfunction equation, \eq.(3.2a), and using the definition of
the streamfunction (\eq.(3.2b)). Since the streamfunction equation is in fact a Poisson
equation, its solution in an unbounded domain is given by the convolution:

\[ \psi(x) = \int \overline{G}(x-x') \omega(x') \, dx' \]  \hspace{1cm} (3.6a)

where \(\overline{G}(x)\) is the Green's function of the Poisson equation. In 2-D this is given by
\[ \overline{G}(x) = -\frac{1}{2\pi} \ln(r) \]  \hspace{1cm} (3.6b)

where \( r = |x| \). Hence, the vortical velocity field is given by the Biot-Savart integral, i.e.

\[ \mathbf{u}_\omega(x) = \int \overline{K}(x-x', \omega(x')) \, dx' \]  \hspace{1cm} (3.7a)

where \( \overline{K}(x) \) is the Kernel of the Biot-Savart integral, given by

\[ \overline{K}(x) = \nabla \times \left( \overline{G}(x) \hat{k} \right) = -\frac{(y-x)}{2\pi r^2} \]  \hspace{1cm} (3.7b)

The Biot-Savart law (eq.(3.7a)), which points to the fact that the vortical velocity field is obtained via integration of the vorticity field, relates directly these two quantities and thus bypasses the need for the explicit use of the streamfunction.

To complete the flowfield solution the expansion and "potential" velocity components are established. The expansion velocity is obtained by solving the expansion potential equation (eq.(3.3a)) and by using the expansion potential's definition (eq.(3.3b)). The approach is very similar to the solution of the streamfunction equation. The expansion potential equation is also a Poisson equation and hence its solution in an unbounded domain is given in integral form by

\[ \phi_e(x) = -\int \overline{G}(x-x') \left( \frac{1}{\rho} \frac{dp}{dt} \right)(x') \, dx' \]  \hspace{1cm} (3.8)

which implies an integral solution of the expansion velocity of the form:

\[ \mathbf{u}_e(x) = \int \nabla \overline{G}(x-x') \left( \frac{1}{\rho} \frac{dp}{dt} \right)(x') \, dx' \]  \hspace{1cm} (3.9a)

where

\[ \nabla \overline{G}(x) = -\frac{(x,y)}{2\pi r^2} \]  \hspace{1cm} (3.9b)

This expression, which provides the expansion velocity by integrating the material density-derivative field, eliminates the necessity for the explicit use of the expansion potential.
The "potential" velocity is obtained by solving the equation governing the "potential" potential (eq.(3.4a)) which is a Laplace equation, under the appropriate boundary conditions and by using the definition of the "potential" potential (eq.(3.4b)).

Once all three velocity components are established, the total velocity field is obtained using the Helmholtz decomposition (eq.(3.5))

3.2.2. Scheme Features

3.2.2.1. Lagrangian Evolution

The VEM is a Lagrangian, grid-free scheme. That is, integration of the vorticity transport equation is carried out in a Lagrangian frame of reference: Points of computation are convected by the local velocity field to capture the time dependent vorticity field. Establishing fluid particle trajectories (pathlines) is an essential part of this approach and is achieved via integration of:

\[
\frac{d\chi}{dt} = u \tag{3.10}
\]

where \( \chi \) is the particle trajectory. It is also evident that such an approach would, in a straightforward way, define the topography and evolution of material lines. As will be shown, this information is of significant importance to the development of both the VEM and the TREM.

Evolving the field of computation in a Lagrangian way entails substantial numerical advantages. Most importantly, it avoids the difficulty of having to deal with the nonlinearity associated with the substantial, convective derivative in the Eulerian frame of reference. It also avoids numerical diffusion concomitant with the discretization of velocity and scalar gradients on an Eulerian grid. Furthermore, its inherent adaptability, manifested by the preferential convection of the computational points to regions of significant flow events, can be properly exploited to yield substantial numerical savings. Hence, the
number of computational points can be increased/decreased in regions of high/low strain, thus optimizing their number necessary for an accurate solution.

3.2.2.2. Fractional Step Integration

In the initial form of the VEM [35] the transport equations are integrated in two fractional steps. The first step deals with pure convection. The second step with diffusion. The mathematical proof for the accuracy and rate of convergence of this approach is given in ref.[40]. The major assumption in the derivation, and the main justification for this approach, is that the flow is convection dominated, that is, the diffusion is small. Using fractional steps is necessitated by the substantially different nature of the two processes which results in significant differences in their numerical representation. Convection, as suggested by the governing transport equation, is simply implemented by convecting the computational points using equation (3.10) while keeping the convected property constant. Diffusion, on the other hand, with its stochastic nature, poses major challenges for a Lagrangian-kinematical scheme like the VEM. A number of algorithms which attempt to provide Lagrangian modeling of this process have been proposed over the years [35,41,42]. Their success, to date, while encouraging, has not been totally satisfactory.

In the version of the VEM used in this work, where vorticity modifying processes other than convection and diffusion are also present, integration of the governing equation becomes more complicated. Nevertheless, two steps can still be distinguished. All processes other than diffusion are lumped in one step, called the non-diffusive step. The other step deals with diffusion and is, hence, called the diffusive step. The justification for this splitting is similar to that given for the convection-diffusion case above: Amongst the processes involved, only diffusion cannot be dealt-with straightforwardly in a Lagrangian frame of reference, and can, in addition, be explicitly assumed small and slow enough to be considered independently. The expanding core algorithm is used to model diffusion. The integration scheme is further complicated by the fact that the diffusion step is executed
between two parts of the non-diffusive step. As shown in ref.[40] such an approach offers higher accuracy.

3.2.2.3. Use of Vorticity

Solving the momentum equation in vorticity form involves a number of advantages which the scheme capitalizes upon. The first is the commonly acknowledged advantage of the removal of the pressure gradient term from the uniform density equation. As will be shown later, this advantage can be maintained in the variable density case as well. It is also recognized that the vorticity in two dimensions can be treated as a scalar and is, hence, easier to deal-with numerically, than the primitive variable (the velocity) which is a vector. Furthermore, it is noted that in some flows, in particular high Reynolds number flows, while the primitive variable is distributed throughout the field, the vorticity may be restricted within relatively small regions. Thus, savings in numerical effort are achieved by solving for the vorticity field and resolving only these small regions. But most importantly, solving for the vorticity field implies that the velocity field is obtained via integration, and this results in minimization of errors and of numerical noise. In fact, this integration allows even crude approximations in the discretization and evolution of the vorticity field to yield accurate solutions for the velocity field [41].

But the use of vorticity involves a potential disadvantage as well. It is noted that the vorticity equation (eq.(3.1)) displays additional convective terms (the divergence term) which should significantly complicate its numerical integration. This problem is alleviated by recognizing that in a Lagrangian frame of reference, i.e. in a coordinate system attached to material lines, this equation can be recast into a form where the extra convective terms are absent. This is achieved using basic understanding of the nature of the acting physical processes, together with kinematical relations governing the evolution of material lines.

One important kinematical relation is used. It is noted [33], that the change in length of a material line elemental segment \( \delta l \) is related to the velocity difference at its ends, i.e.
\[
\frac{d(\delta l)}{dt} = \delta l \cdot \nabla \mathbf{u}
\]  
(3.11)

which when considered in a frame of reference attached to the material line and split into its directional components reduces to:

1 - direction  
\[
\frac{d(\delta l)}{dt} = \delta l \frac{\partial \mathbf{u}}{\partial l}
\]  
(3.12a)

n - direction  
\[
\frac{\partial \mathbf{u}}{\partial l} = 0
\]  
(3.12b)

where \(\delta l = |\delta l|\) and \([l,n]\) indicate directions tangential and normal to the material line.

The removal of the extra convective term from the vorticity equation is achieved by recasting it into a circulation form. While this is valid for the general vorticity equation (eq.(3.1)), here it will be demonstrated for the case where diffusion is absent. The reasoning for this approach stems from the fractional step integration of the equations noted earlier. Thus, equations derived here are used in the non-diffusive integration step.

A Lagrangian material fluid element of area \(\delta A = \delta l \delta n\) and of vorticity \(\omega\) is considered. Integration of the vorticity equation over the area of this element, which leads to the circulation form, removes the divergence-related term since this term is conservative. The physical basis for this effect is that, because the flow divergence is irrotational, it does not contribute to the element's angular momentum or equivalently - since its mass is constant - to its circulation. Thus, as the flow area increases, the vorticity proportionately decreases to keep the circulation constant. Mathematically, derivation of this effect can be obtained by using the kinematical relation above (eq.(3.12a)) in both material-line-based coordinate directions (i.e. for both \(\delta l\) and \(\delta n\)) and combining the results with the continuity equation (eq.(2.1)). This leads to

\[
\nabla \cdot \mathbf{u} = \frac{1}{\delta A} \frac{d(\delta A)}{dt}
\]  
(3.13)

which simply states that the divergence of the flowfield is related to the material change of area (2-D). Using this expression and considering that the element circulation is given as
the vorticity equation (eq.(3.1) without diffusion term) is recast into a circulation
equation in which no extra convective terms appear, i.e.:
\[
\frac{d\Gamma}{dt} = \frac{\nabla \rho \times \nabla p}{\rho^2} \delta A = - \frac{\nabla \rho}{\rho} \times \frac{d\mathbf{u}}{dt} \delta A
\] (3.14)

The version of the equation which includes the material acceleration is obtained by
substituting the pressure gradient using the corresponding momentum equation (eq.(2.2)
without the diffusion term).

3.2.3. The Scheme

3.2.3.1. Discretization

3.2.3.1.1. Vorticity

An initial smooth vorticity field, \( \omega(x,0) \), is discretized among a number of vortex
elements, \( N \), via a discretization function which characterizes each element with a finite
area, \( A_i \), and with a compact support of vorticity (strength), \( \omega_i \), locally distributed through
a radially symmetric core function, \( f_\delta \). The discretization function is also used to
reconstruct the vorticity field at later times, \( \omega(x,t) \), and is:
\[
\omega(x,t) = \sum_{i=1}^{N} \Gamma_i(t) f_\delta(x - \chi_i)
\] (3.15)

where \( \Gamma_i(t) = \omega_i(t) A_i(t) \) is the element circulation and \( \chi_i = \chi_i(x,t) \) its trajectory (location).
The core function, which physically represents a model for the smaller scales of the
flowfield is essential to the numerical stability and accuracy of the scheme [43]. This is
because it removes the singularities resulting in the velocity field when point vortices are
used. The core function is characterized by a core radius, \( \delta \), within which significant
vorticity values are encountered.

The accuracy of the discretization is controlled by the smoothness of the field, the
number and location of the vortex elements, the choice of the core function and the ratio of
the distance between neighboring elements (\( h = \Delta\chi(t=0) \)) to the core radius. Convergence
and accuracy studies [43-47] have shown that this ratio must be kept below and close to unity for high accuracy to be maintained. (This condition implies that overlap of neighboring element cores is necessary for an accurate solution.) Values of $h/\delta$ between 0.66 and 0.9 are usually chosen and are sufficient to limit the discretization error to tolerable levels. (The accuracy of discretization increases as $h/\delta$ approaches unity but this benefit comes at the disadvantage that future overlap -i.e. during transport- is more quickly destroyed) These studies have also shown that a second order Gaussian core function, i.e.

$$f_\delta(r) = \frac{1}{\pi \delta^2} \exp(-\frac{r^2}{\delta^2})$$  \hspace{1cm} (3.16)

which is used here, enables second order accuracy of discretization. Physically the use of this function implies that each element is modeled as a Gaussian vortex (see figure 3.1).

In this work the approach followed in the initial discretization of the vorticity field is the one proposed by Leonard [41] which assumes the strength of an element to be equal to the value of the vorticity at its center (i.e. $\omega(\chi_{l,0}) = \omega_l$) and uses the number and location of the elements and the core function radius as parameters to minimize the discretization error. Such an approach does not offer absolute control over this error since the minimizing parameters cannot be freely varied. The possible location of the elements is controlled by the features of the vorticity field and their number is restricted by economic reasons. The core function radius is bounded by the above mentioned criteria. But the possibility of a small initial discretization error (maximum pointwise error $O(5\%)$) does not in any significant way impair the scheme because, as already noted, the integration of the vorticity field minimizes this error and leads to a highly accurate velocity field solution (maximum pointwise error $O(0.1\%)$)

The main advantage of this discretization approach is that due of the equality of the continuous and discrete vorticity at the center of the element the two values can be interchanged in the integration of the vorticity equation (see next section).
3.2.3.1.2. Material Density-derivative

The material density-derivative field, \( -\frac{1}{\rho} \frac{d\rho}{dt} \), necessary in the calculation of the expansion velocity field is discretized in a similar fashion as the vorticity. Hence, expansion elements are constructed with a finite area and a compact support of material density-derivative (strength), \( -\frac{1}{\rho} \frac{d\rho}{dt} \), locally distributed by the core function:

\[
-\frac{1}{\rho} \frac{d\rho}{dt}(x,t) = \sum_{i=1}^{N} \left[ -\frac{1}{\rho} \frac{d\rho}{dt} \right]_{i}(t) A_i(t) f_{\delta}(|x-\chi_i|) \tag{3.17}
\]

The approach followed in the discretization is identical to that used in the vorticity case. Furthermore it is noted that, the scalar field is initiated in such a way that regions of variable density coincide with regions of finite vorticity and thus the same elements are used to discretize both the vorticity and material density-derivative fields.

3.2.3.2. Evolution in Time

The VEM only deals with the time evolution of the vorticity field. The material density-derivative field evolution is provided by the TREM.

The time-evolution of the vorticity field is established by numerically integrating the vorticity equation subject to the appropriate boundary conditions (see Section 3.4.2.1). More specifically, the vorticity equation is locally integrated for each vortex element and the updated vorticity field is obtained via summation of the contributions of all elements as suggested by equation (3.15).

The numerical integration of the vorticity equation for each vortex element is carried out in two fractional steps. The first step, the non-diffusive step, includes all processes other than diffusion i.e. convection, expansion and baroclinicity. During this step the element locations are updated by numerically integrating

\[
\frac{d\chi_i}{dt} = u(\chi_i,t) \tag{3.18}
\]
that is, the elements are advected with the local velocity vector. This defines element trajectories, as well as material lines (by keeping track of elements introduced at the same point at the inlet). The element vorticity is also updated by locally integrating the circulation equation

$$\frac{d\Gamma_i(t)}{dt} = -\frac{\nabla \rho_i(t)}{\rho_i(t)} \times \frac{d\chi_i(t)}{dt} A_i(t)$$  \hspace{1cm} (3.19)

Both equations are integrated via Euler predictor-corrector schemes and the material acceleration in equation (3.19) is established by a two-step iteration forward-difference scheme.

The core expansion scheme [41,48] is used to simulate diffusion in the second, diffusive step. As the name of the scheme implies diffusion is modeled by expanding the element core size according to:

$$\delta_i^2(t) = \delta_i^2(0) + \frac{4t}{Re}$$  \hspace{1cm} (3.20)

This expression is arrived at by using the element vorticity field, defined by the discretization function, eq.(3.15), to analytically solve the governing diffusion equation, under the assumptions that the strength and area of the element are constant and that the core radius is only a function of time.

The transport of the elements during the non-diffusive step rearranges their locations according to the local strain field. Hence in regions of high tensile strains, elements tend to move away from one another, thus failing to maintain the core overlap necessary for good solution accuracy. To overcome this problem, an element injection scheme [48] is implemented (see figure 3.2). According to this scheme a new element is injected halfway between two elements when the distance between them exceeds a specified length ($L_{inj}$) which ensures core overlap. The new strength and area of all three elements involved in each injection are determined by enforcing local conservation of both circulation and area. This is achieved by splitting the circulation and area of the two initial elements.
amongst the three resulting elements in proportion to the length of the material line associated with each element, $\delta l_i$, defined as the distance between the points located halfway between it and its two closest neighbors.

While injection improves the accuracy of the solution it increases the number of elements and hence increases the cost of the computation. This problem can be minimized by recognizing that elements can also be removed from regions of high compressive strains where they tend to over-accumulate. Thus, when two elements get closer than a specified distance ($L_{\text{com}}$) they get combined into one element. Local conservation of both circulation and area define the new element's respective quantities.

3.2.3.3. Velocity Field Reconstruction

The component of the velocity induced by the updated vortex element field is given by a desingularized, discrete Biot Savart law, obtained by substituting the discrete vorticity field (eq.(3.15)) into the Biot Savart integral (eq.(3.7a)) (for an equivalent derivation see appendix A), i.e.

$$u_\omega(x,t) = \sum_{i=1}^{N} \Gamma_i(t) K_\delta(x-\chi_i(t))$$  \hspace{1cm} (3.21a)

where $K_\delta$ is the desingularized kernel of the Biot Savart law and is given by

$$K_\delta(x) = \tilde{K}(x) \frac{F(L)}{\delta}$$  \hspace{1cm} (3.21b)

with

$$F(r) = -2\pi \int_0^{r} r f(r) \, dr = 1 - \exp(-r^2)$$  \hspace{1cm} (3.21c)

As already noted, the above expression for the vortical velocity is a manifestation of the solution of the streamfunction equation in an unbounded domain. For a bounded flow like the one simulated in this work, a system of vortex element images is employed to enforce the presence of solid impermeable boundaries. For more details on how this is achieved as well as on the nature of the specific boundary conditions applied, see Sections 3.4 and 3.5.
The expansion component of velocity is obtained in a similar fashion. The discrete material density-derivative (flow divergence) field, eq. (3.17), is substituted into equation (3.9a) to yield a desingularized, expansion velocity field (for an equivalent derivation see appendix A), i.e.

\[ u_e(x,t) = - \sum_{i=1}^{N} \left( - \frac{1}{\rho} \frac{dp}{dt} \right)_i A_i(t) \nabla G_i(x - \chi_i(t)) \]  

(3.22a)

where \( \nabla G_i \) is the desingularized gradient of the Poisson equation and is given by

\[ \nabla G_i(x) = \nabla G(x) F(i) \delta \]  

(3.22b)

Boundaries confining the flow are imposed using a system of expansion element images as explained in Section 3.5.

The "potential" component of the velocity field is obtained by solving the governing Laplace equation (eq. (3.4a)) under the appropriate boundary conditions. This is achieved by employing the Schwartz–Christoffel theorem to conformally map the physical domain onto the upper half plane of another domain. This conformal mapping, which leads to an analytic solution of the equation, is very beneficial to a Lagrangian scheme like the VEM because it enables a pointwise, grid-free evaluation of the "potential" velocity field. The characteristics of the mapping, as well as the nature of the resulting solution, are strongly dependent on the flow geometry and boundary conditions. Thus more details on the "potential" velocity solution are given in Section 3.5 after these conditions have been specified.

Upon completion of the calculation of all three components of the velocity field, the VEM approach in establishing the evolution of the flowfield is completed by establishing the total velocity field using the Helmholtz decomposition, i.e.

\[ u(x,t) = u_0(x,t) + u_e(x,t) + u_p(x,t) \]  

(3.23)
3.3. The Transport-Reaction Element Method (TREM)

3.3.1. Governing Equations

The development of the TREM as an extension of the non-reacting Transport Element Method (TEM) dealing with reacting flow, was initiated upon the realization that the existing reacting version of the TEM was not applicable for spatially evolving flows. Quite early in this endeavor it became evident that essential features of the TEM could not be extended to a flow experiencing reaction. To bypass this problem, the Shvab-Zeldovich formulation was introduced. As explained in the previous chapter, under this formulation non-reacting variables are constructed from combinations of the primitive reacting variables. Since the Shvab-Zeldovich variables do not experience reaction, then the TEM can be used to establish their evolution. In the limiting case of infinite reaction speed, where reactants are not allowed to coexist and the reaction zone becomes infinitely thin, the reacting scalar field can directly be obtained from the Shvab-Zeldovich variable field solutions. For finite reaction speed, on the other hand, these solutions do not contain all the information necessary to construct the reacting field. The field of one primitive reacting scalar still needs to be explicitly solved for. Thus, a new component is added to the scheme to accomplish this task. Numerical reasons which will be clarified later, suggest the product mass-fraction to be the reacting scalar. The equations of state and of the conservation of the sum of the species mass-fractions are used to couple the two components of the scheme.

Hence, the equations solved by the TREM are written as (also given in table 2.2):

$$\frac{dg_j}{dt} + g_j \cdot \nabla u + g_j x (\omega \hat{k}) = \frac{1}{Pe} \nabla^2 g_j \quad g_j = \nabla s_{gj} \quad (3.24a,b)$$

$$s_j = s_{gj} + s_{pj} \quad s_j \text{ is } \lambda = Y_1 - \phi Y_2 \quad \text{or} \quad \gamma = T - \frac{Q_0 \phi}{1 + \phi} \quad (3.25a,b)$$

$$\frac{dY_p}{dt} = \frac{1}{Pe} \nabla^2 Y_p + (1 + \phi) \frac{\dot{W}}{\rho} \quad \dot{W} = A_1 \rho^2 Y_1 Y_2 \exp(-\frac{T^*}{T}) \quad (3.26a,b)$$
\[ Y_1 + Y_2 + Y_p = 1 \]  
\[ \rho \cdot T = 1 \]

where quantities relating to the velocity field are provided by the VEM.

It should be noted that the Shvab-Zeldovich scalar fields are obtained from the corresponding gradient solutions via integration. This is achieved by realizing that the divergence of the scalar gradient, poses a Poisson equation for the scalar i.e.

\[ \nabla^2 s_g = \nabla \cdot g \]

Thus, in analogy to the streamfunction and expansion potential equations encountered in the VEM, the integral solution of this equation in an unbounded domain is given by

\[ s_g(x) = - \int \overline{G}(x-x') \left( \nabla \cdot g(x') \right) dx' \]

Integration by parts and use of the divergence theorem with the realization that the gradient field decays at infinity, yields the form:

\[ s_g(x) = \int \nabla \overline{G}(x-x') \cdot g(x') \ dx' \]

The solution for the Shvab-Zeldovich scalar field is completed by adding the "potential" part needed to satisfy the boundary conditions, according to equation (3.25a).

3.3.2. Scheme Features

3.3.2.1. Analogy to the VEM

The TREM (and hence the TEM) is a scheme created with strong influences from the VEM. Most predominantly, it is also a Lagrangian scheme. While the Lagrangian approach endows the TREM with the significant numerical advantages discussed earlier (see Section 3.2.2.1), it, in addition, makes it strongly compatible with the VEM. This substantially simplifies the complexity of using the two schemes together to obtain both the flow and scalar fields.
In direct analogy to the VEM, fractional step integration of the transport equations is also implemented in the TREM. All processes other that diffusion are lumped in one step, the non-diffusive step. Diffusion is carried out in the second step. The reasoning employed in explaining this splitting is similar to that used in the VEM: Compared to the other processes involved, diffusion is slow. As justification of this, it is pointed out that for gases which experience ideal-like behavior like the ones considered here, the Prandtl number is commonly of the order of unity. This implies that viscous and thermal diffusion (and mass diffusion since Le=1) manifest themselves at similar speeds.

The use of gradients of the non-reacting Shvab-Zeldovich variables (i.e. in TEM subsection of the scheme) is a direct attempt to capitalize on the type of advantages resulting from the use of vorticity in the VEM (see Section 3.2.2.3). These include the fact that for high Peclet number flows the gradients may be restricted in only small part of the domain, thus reducing the size of the spacial regions that need to be numerically resolved, and most importantly, the fact that the primitive variable fields are obtained from the gradient solutions via integration which minimizes errors and removes numerical noise.

As in the case of the vorticity though, the disadvantage of having to deal with equations which are complicated by the presence of extra convective terms is also experienced. Furthermore, it should be noted that unlike the velocity-vorticity case where a vector equation is reduced to a scalar equation, in this case quite the opposite is true, further complicating the integration of the gradient equations. The approach to avoid both of these problems is similar to that used to reduce the extra complexity of the vorticity equation in the VEM, with the addition of one important condition: Material lines need to be initialized and maintained coincidental with isoscalar lines. Thus, the gradient equations are considered in a Lagrangian frame of reference, attached to material-isoscalar lines, and are recast into forms which do not experience convective terms other than material derivatives. This approach has the added advantage of trivially establishing the
gradient direction, thus necessitating only the determination of the evolution of the gradient size, which is a scalar quantity.

In what follows, it is shown that the extra condition of coincidence of material and isoscalar lines, while relatively easily attainable for non-reacting flow, is almost impossible to maintain for reacting flow. Specialized exceptions do exist and are noted. Hence, in the presence of reaction the simplification of the gradient equation is not usually possible and the advantages of using gradients rather than primitive variables are outweighed by the above noted disadvantages. This is the reason why the TEM, with its gradient formulation, is only used for the non-reacting Shvab-Zeldovich variables and not for the reacting scalar, where a scheme with primitive variable formulation is implemented.

3.3.2.2. Gradient Equation Simplification

As noted above, the coincidence of material and isoscalar lines is an essential condition for the gradient equation simplification to be possible. In order for this condition to be maintained three subconditions must be met:

(i) Initial material lines must be chosen in such a way that the scalar is constant along them.

(ii) Physical processes acting on the scalar field should be such that they maintain spacial (i.e. not necessarily temporal) constancy of the scalar on material lines.

(iii) Newly introduced sections of material line at the boundaries should exhibit the same value of the scalar as their continuations inside the domain.

The first subcondition is in general independent of the other two and is usually easy to achieve since it can be externally enforced. The second and third subconditions, on the other hand, are related and, in general, cannot be externally enforced. Hence it is these subconditions which can mainly cause the material-isoscalar line coincidence condition to fail. Their main implication is that in order to determine the cases where the simplification of the gradient equations is possible, both the physical processes and boundary conditions determining the evolution of the flow need to be considered.
3.3.2.2.1. Non-reacting Flow

For non-reacting flow, the simplification of the gradient equations can be obtained exactly only in the purely convective case since only this case can exactly maintain the condition of material-isoscalar line coincidence. The simplification can be assumed to be approximately valid in the convective-diffusive case, when diffusion, and in particular its effects along material lines, are small. This is a reasonable assumption not only because, as noted earlier, the Peclet number is large, but also because the initial coincidence of material and isoscalar lines implies that the major diffusion flux direction is normal to these lines and not along them.

In the purely convective case the scalar \( s \) is conserved along fluid particle trajectories. i.e.

\[
\frac{ds}{dt} = 0 \tag{3.32}
\]

Thus a scalar which is initially constant along a material line will remain so at all times. This satisfies the second subcondition and, in addition, allows the third subcondition to be externally enforced. This is achieved by specifying a value of the scalar on any new piece of material line introduced at the boundary, equal to that of its continuation inside the domain, which is also equal to the initial \((t=0)\) value on that line. It should be evident that while such a boundary condition is not totally general, it, nevertheless, is appropriate for a substantial number of physically useful cases.

The simplification of the gradient equation starts by the realization that if the scalar is constant along a material line then the scalar gradient is normal to it and zero along it. Furthermore, kinematical considerations suggest that under these conditions, stretching of the material lines should be related to the gradient strength: Stretching of material fluid elements in one material-line-based coordinate direction implies, through continuity, their shrinking in the other. This effectively brings material lines closer to each other. Since the scalar values are constant on each of these lines this implies that the local gradient has been
intensified (see figure 3.3). Hence, knowledge of both the gradient size and direction should determine the gradient field.

Analytically, this is shown by first considering the gradient equation for this case (eq.(3.24a) without diffusion term) in the material-line-based coordinates, which in component form is:

\[ \frac{dp}{dt} + p \frac{\partial u}{\partial l} + q \frac{\partial v}{\partial l} = 0 \]  \hspace{1cm} (3.33a)

\[ \frac{dq}{dt} + p \frac{\partial u}{\partial n} + q \frac{\partial v}{\partial n} = 0 \]  \hspace{1cm} (3.33b)

where \( p \) and \( q \) are the components of the gradient, i.e. \( g = (p,q) \). Then, by making use of the kinematical equation governing the evolution of the material-line elemental segment \( \delta l \) (eqs.(3.12a,b)) and of the compressible continuity equation (eq.(2.1)) (it should be noted that even though the scalar dealt-with here is a non-reacting, purely convected one, other scalars may be reacting thus making the flow compressible), these equations are transformed to:

\[ \frac{d[p \delta l]}{dt} = 0 \]  \hspace{1cm} (3.34a)

\[ \frac{d[q]}{dt} + \frac{1}{\rho \delta l^2} \frac{\partial u}{\partial n} [p \delta l] = 0 \]  \hspace{1cm} (3.34b)

If the condition of material-isoscalar line coincidence is maintained as described above, and thus only gradient normal to the material line may exist (i.e. \( p=0 \)), then the gradient vector becomes

\[ g = q \hat{n} \]  \hspace{1cm} (3.35)

where \( \hat{n} \) is the unit vector normal to the material line and \( q \) becomes, for this case, the size-intensity of the gradient. Hence the gradient equations (eqs.(3.34a,b)) reduce to only one equation, the one governing the evolution of the gradient normal to the material line. i.e.

\[ \frac{d[q]}{dt} = 0 \]  \hspace{1cm} (3.36)
Thus, the gradient equation has been recast into a form where the extra convective terms are absent. This equation simply implies that along a material line

$$\frac{q}{\rho \delta l} = \text{constant} \quad (3.37)$$

which quantifies the earlier conjectured relationship between material line stretch and the gradient size, that is, as material lines get stretched the gradient normal to them intensifies.

[NB/ Another version of this relationship which indicates this effect more clearly can be established by considering that the material element mass, ($\delta m$)

$$\delta m = \rho \delta l \delta n, \quad (3.38)$$

is constant, which when combined with equation (3.37) yields

$$q \delta n = \text{constant}. \quad (3.39)$$

(To obtain this result one could have equivalently used the kinematical relation governing $\delta n$ instead of that of $\delta l$ in the derivation of equation (3.34b).)]

The above simplification of the scalar gradient equations for the convective case (and approximately for the convective-diffusive case) constitutes a fundamental part of the TEM. Evidently, under these conditions the numerical determination of the evolution of the gradient becomes trivial. Equation (3.37) is used to obtain the gradient size ($q$). The constant is established from initial conditions. The Lagrangian nature of the scheme, which supplies the topology and evolution of material lines, provides both $\delta l$ (for the gradient size calculation) and $\hat{n}$ (which defines the gradient direction). Thus the gradient field is established via equation (3.35).

3.3.2.2.2. Reacting Flow

As noted earlier, the simplification of the gradient equations for reacting flow is much more elusive. It can be achieved exactly only for the convection-reaction case, and then, only under specialized circumstances. Approximate extension to the case where diffusion exists, is also not as easily justifiable as in the non reacting case. This is because
even initially minor effects of diffusion along material lines can be amplified by combustion resulting in sizable variations of the scalar along such lines.

In particular, for the second subcondition to be valid in the convection-reaction case, material lines should at all times be coincidental with isoscalar lines not only of the particular scalar under consideration but also of all other scalars contributing to the reaction. In other words, all the scalars participating in the reaction rate, need to be spatially constant on the material line. In contrast to the non-reacting, purely convective case, the presence of combustion alters the values of these scalars in time. But under these conditions the change is uniform over the material line (i.e the reaction rate is constant there) resulting in a spatially constant value.

Unlike the purely convective case, in this case the third subcondition cannot be externally enforced without knowledge of what is taking place inside the domain. This is because the value of the scalar on the material line changes with time due to combustion. Thus, for the third subcondition to be valid, material line introduced at the boundaries must have experienced the same reacting history as its continuation inside the domain. Evidently, such a boundary condition is not only difficult to enforce, it is also not particularly useful for most realistic applications. This is definitely true of spatially developing flows like the one considered in this work where material introduced at the inlet is always characterized by a shorter burning history than its predecessor immediately downstream.

An exception to this problem is offered by temporally evolving flows (e.g. temporal shear layers and jets). In these idealized flows, the presence of periodic boundary conditions essentially reintroduces at the inlet any material exiting the domain. Thus, no new material enters the domain, or equivalently, the material line introduced at the inlet has the same burning history as its downstream continuation. It should be pointed out though, that these features of temporal flows do not only enable the simplification of the gradient equations; they also severely and artificially restrict the relevant physical phenomena. In
essence, these flows require no spacial variation of the reacting scalars along material lines spanning the whole computational domain. At the same time these material lines are substantially distorted by the flow, yielding complicated vortical structures. This can only be approximately true if the reaction time scale is much larger than the flow time scale, a condition which is, to say the least, uncommon.

Another, more realistic exception, is offered by flows which bypass the problem of material line introduced at the boundary, altogether. This can be the case if the initial material lines are closed and their evolution in both space and time is established without any new material entering the domain (e.g. atmospheric plumes in an infinite domain [49]).

The gradient equation simplification for this case starts from the same argument as that of the purely convective case: If the scalar is constant on a material line the gradient must be normal to it and zero along it (i.e. eq.(3.35) applies). Furthermore, from the above discussion, it is realized that if no gradient exists along the material line, then a convection-reaction process cannot create such gradient. This arguments together with kinematical considerations like the ones used in the purely convective case imply that the gradient in the vicinity of a material element should be related to the local stretch and to the local scalar change across it, due to combustion.

For the convective-reactive case the governing scalar equation is

$$\frac{ds}{dt} = Q \frac{\dot{w}}{\rho}$$

where $Q$ is a constant depending on the scalar. The corresponding gradient equation is

$$\frac{Dg}{Dt} + g \cdot \nabla u + g \times (\omega \hat{k}) = Q \nabla (\dot{w}/\rho) = Q \sum_{n=1}^{K} \frac{\partial (\dot{w}/\rho)}{\partial s_n} g_n$$

where $K$ is the number of scalars participating in the reaction rate. As in the purely convective case, equation (3.41) is considered in a material-line-based coordinate system and is combined with the kinematical relations governing the evolution of the material-line elemental segment $\delta l$, and the continuity equation to yield (in component form):
1 - direction
\[ \frac{d}{dt} \left[ \rho \frac{\delta l}{\delta t} \right] = Q \sum_{n=1}^{K} \frac{\partial (\dot{w}/\rho)}{\partial s_n} \left[ q_n \frac{\delta l}{\delta t} \right] \]  \hspace{1cm} (3.42a)

n - direction
\[ \frac{d}{dt} \left[ \rho \frac{\delta l}{\delta t} \right] + \frac{1}{\rho \delta l^2} \frac{\partial u}{\partial n} \left[ p \frac{\delta l}{\delta t} \right] = Q \sum_{n=1}^{K} \frac{\partial (\dot{w}/\rho)}{\partial s_n} \left[ q_n \frac{\delta l}{\delta t} \right] \]  \hspace{1cm} (3.42b)

If because of the characteristics of the problem the gradient along the material line is zero \((p=0)\) and thus only gradient normal to the material line may exist, equations (3.42a,b) reduce to one equation which after rearranging becomes
\[ \frac{1}{\rho} \frac{d}{dt} \left[ \frac{q}{\delta l} \right] = Q \sum_{n=1}^{K} \frac{\partial (\dot{w}/\rho)}{\partial s_n} \left[ \frac{q_n}{q} \right] \]  \hspace{1cm} (3.43)

Since the scalar is spatially constant on material lines then the spacial difference across two such lines, and hence across material elements, is also spacially constant. An equation governing the evolution of this scalar variation \((\delta s)\) can be obtained by either differencing the scalar transport equation \((\text{eq.}(3.40))\) or integrating the gradient equation \((\text{eq.}(3.43))\) over the area of the element under the approximation that elements are thin enough in the direction normal to material lines so that
\[ \delta s = \int_{\delta n} \frac{\partial s}{\partial n} \, d n = \left( \frac{\partial s}{\partial n} \right)_{n=0} \delta n \Rightarrow \frac{\delta s}{\delta n} = \frac{q}{q_n} \]  \hspace{1cm} (3.44)

Clearly, this approximation improves as \(\delta n \to 0\). Hence, the equation for the scalar spacial variation across a material element is:
\[ \frac{1}{\delta s} \frac{d(\delta s)}{dt} = Q \sum_{n=1}^{K} \frac{\partial (\dot{w}/\rho)}{\partial s_n} \frac{\delta s_n}{\delta s} \]  \hspace{1cm} (3.45)

Recognizing that under these conditions \(\frac{q_n}{q} = \frac{\delta s_n}{\delta s}\) then the right hand sides of equations (3.43) and (3.45) are equal, which implies that their left hand sides are also equal. By rearranging the equality of the left hand sides one can obtain
\[ \frac{d}{dt} \left[ \rho \frac{\delta l}{\delta t} \frac{q}{\delta s} \right] = 0 \]  \hspace{1cm} (3.46)
which is a form without extra convective terms and which simply implies that along a material line

$$\frac{q}{\rho \delta t \delta s} = \text{constant}$$  \hspace{1cm} (3.47)

[NB/ The validity of this statement can more clearly be seen by using equation (3.44) to substitute for the scalar gradient which results in the evident conclusion that the mass of the element is conserved.]

The derivation of equation (3.47) and its numerical use to establish the gradient field, are essential parts of the reacting version of the TEM earlier proposed [24]. The enormously attractive simplicity of the scheme is evident. By defining the constant in equation (3.47) from initial conditions, obtaining $\delta l$ and $\vec{n}$ from the known topology of the material lines (Lagrangian scheme), and $\delta s$ from equation (3.45) the scalar gradient ($g = q \vec{n}$) for a convective-reactive process can be straightforwardly established.

However, the limitations of the scheme, already hinted to, are also severe. Most important amongst these is the limited applicability due to the unrealistic nature of the conditions imposed on material entering at the boundaries. As already noted, this makes the scheme inapplicable to spacially evolving flows like the one considered in this work. "Fresh" material line introduced at the inlet has a different reacting history than its immediate continuation downstream. Since the downstream material line has been experiencing combustion during the time of its presence in the flow domain, it is characterized by a different value of the scalars than the material line at the inlet. This implies that scalar-gradient along the material line must exist and thus the material line at the inlet should be initialized with such a gradient. Once this gradient exists then the above approach of eliminating the convective terms in the convection-reaction equation breaks down. The gradient in the material-line-based coordinates is now multicomponent and instead of equation (3.43), equations (3.42a,b) apply.
A similar problem, albeit to a lesser extent arises when diffusion is present. Small gradients set up by diffusion are enhanced by combustion thus resulting in significant gradients along the material line. Thus, for this case as well, the gradient will become multicomponent and the above simple scheme will break down necessitating the solution of equations (3.42a,b). These equations are non-linear, coupled and have non-constant coefficients. Furthermore one extra convective term is still present in equation (3.42b). For these reasons their solution is a very demanding task and is avoided in this work. Instead, a new scheme, using primitive (non-gradient) formulation is proposed to deal with the reacting scalar equations.

3.3.2.3. The Reacting Scalar Integration

For the finite speed reaction case, the product mass-fraction is chosen as the reacting scalar to be integrated for the complete description of the scalar field. A number of reasons led to this choice. First, in the absence of reaction, and hence of product, the integration of the product equation becomes unnecessary and the TREM simply reduces to the non-reacting flow TEM. This is not necessarily true for any other reacting scalar. Furthermore, it is noted that unlike the other reacting scalars the product is concentrated in the same regions as the scalar gradients (diffusion flame). Thus, the numerical savings of resolving only these regions of the flow domain, manifested in both the vorticity and gradient solutions, need not be lost. On the other hand, the advantages associated with the integration of the field solution in these latter cases, are, evidently, lost. Thus, special care must be taken to maintain high accuracy in the discretization and evolution of the product field.

The fact that for the formulation considered here the product mass-fraction is essential in the determination of the density (through the temperature), suggests another numerical problem as a result of the primitive variable approach: Since density gradients are required for the determination of the baroclinic term in the vorticity (circulation) equation (eq.(3.14)) then the product gradient also needs to be established. This can easily be seen
by combining the definition of the $\gamma$ Shvab-Zeldovich variable and the equation of state to obtain

$$\nabla p = \frac{\nabla \gamma + \frac{Q_0 \phi}{1+\phi} \nabla Y_p}{\gamma + \frac{Q_0 \phi}{1+\phi} Y_p}$$

(3.48)

Hence the product field solution will have to be differentiated, a process prone to numerical noise. On closer consideration though, it becomes clear that this problem does not severely handicap the scheme. This is because the baroclinic generation of vorticity is the only place in the scheme where the product gradient is used. Any numerical noise introduced into the vorticity field by this process is subsequently removed by the integration of the vorticity field.

It should also be pointed out that for non-reacting variable density flow, or for infinitely fast reacting flow the above problem does not exist since in these cases the density gradient can be established directly from the Shvab-Zeldovich variable gradients which are readily available.

3.3.3. The Scheme

In what follows the details of the numerical scheme for the most general case, the one characterized by a finite reaction rate, are described. For infinite reaction rates and for non-reacting flow, the integration of the product mass-fraction equation becomes redundant. For these latter cases, the parts of the scheme dealing with this integration are simply bypassed.

3.3.3.1. Discretization

The approach to discretization in the TREM is in general similar to that used in the VEM. This is particularly true of the gradients of the Shvab-Zeldovich variables. Thus, these gradients are initially discretized among, and later reconstructed by, a field of
transport elements which are characterized by a gradient strength \((g_i)\) and a finite area. The field of each element is defined by a radially symmetric core function, i.e.,

\[
g_j(\mathbf{x},t) = \sum_{i=1}^{N} g_{ji}(t) A_i(t) f_\delta(\mathbf{x} - \mathbf{\chi}_i) \tag{3.49}
\]

The conditions governing the accuracy, as well as the approach followed in the implementation of this discretization are identical to those governing the vorticity field presented in Section 3.2.3.1.

The discretization of the product mass-fraction field, while based on similar principles, exhibits some important differences. The discretization function is still the same, i.e.,

\[
Y_p(x,t) = \sum_{i=1}^{N} Y_{pi}(t) A_i(t) f_\delta(x - \chi_i) \tag{3.50}
\]

indicating that the product field is discretized among elements which are characterized by a product strength \((Y_{pi})\), an area and a core function. The deviation from the vorticity and gradient cases comes in the approach of implementing the discretization. Due to the absence of the subsequent integration of the field, the discretization errors which were tolerated in the vorticity and gradient cases cannot be tolerated here. Instead, for a highly accurate discretization, the set of equations described by the discretization function, eq.(3.50), is numerically inverted to yield the strengths.

The problem which arises by following such an approach is that the element product strength is not equal to the value of the product at the element center. Rather, this strength does not necessarily have a physical meaning (even though it can still be thought of as a crude approximation of the local product value) and should merely be treated as a weight factor of the interpolation-discretization function. Hence, it is not used in the numerical integration of the product equation. Rather, the integration is carried out using the actual local product value. Thus, the concept of the "product particle" is introduced. These particles coincide with the product element centers. They are convected by the local
velocity vector and they experience the combustion process. This implies that in order to obtain the product field, a discretization-interpolation (inversion of eq.(3.50)) must be carried out every step.

This inversion is economically possible because of the nature of the fast decaying core function, a second order Gaussian, which implies that only the closest neighbors of each element contribute to its product value. This is clarified in figure 3.4, where it is shown that only elements within a distance (cut-off distance) of three to four core radii from the element need be considered in the summation. This substantially improves the speed of the inversion which is performed via a Gauss-Seidel iteration. Since the values of the product do not significantly change within a single step, a good initial guess of the strength field is provided by the strengths of the previous step. This leads to fast convergence and hence further savings on the iteration time. The value of the cut-off distance to core radius ratio used in this work is $\sqrt{12}$. This value was arrived at by considering larger values and verifying that the difference in the product field solution was negligible.

An important feature of this inversion is that it enables a compatibility check between the numerical and physical parameters. If the chemical parameters specified result in product field features smaller than those which can be accommodated by the discretization function then this becomes evident via increases in the discretization error. This, in turn, implies that more particles/elements are required for compatibility of numerical and physical parameters and thus, for an accurate solution.

As previously explained the product gradient field, necessary in the calculation of the density gradient field, is obtained by differentiating the field solution. This yields

$$\nabla Y_p(x,t) = \sum_{i=1}^{N} Y_{pi}(t) A_i(t) \nabla f_\delta(x - \chi_i)$$  (3.51a)

with

$$\nabla f_\delta(x) = -2 \frac{(x,y)}{\delta^2} f_\delta(x)$$  (3.51b)
Such an expression for the scalar gradient field and the associated primitive scalar
discretization function (eq.(3.50)) were first introduced by Anderson [39] who, as already
noted, also introduced the gradient discretization function (eq.(3.49)).

Finally, it is pointed out that under the initialization conditions assumed in this work
the vorticity, Shvab-Zeldovich scalar-gradients and product mass-fractions occupy the
same spacial regions in the flow-domain. Thus, the same elements are used to carry all
three properties.

3.3.3.2. Evolution in Time

The time evolution of the reacting field is determined via integration of the Shvab-
Zeldovich scalar gradient and product mass-fraction equations under the appropriate
boundary conditions (see Section 3.4). This integration is carried out locally for each
element and in two fractional steps which are executed in parallel with the vorticity
integration steps. The first step includes all processes other than diffusion. The element
locations are updated by moving them with the local velocity vector as prescribed by
equation (3.18) which is also given here for completeness, i.e.

\[ \frac{d\chi_1}{dt} = u(\chi_1, t) \]  \hspace{1cm} (3.18)

The Shvab-Zeldovich scalar gradient strengths are updated according to discrete versions of
equations (3.37) and (3.35) i.e.

\[ \frac{q_{ij}(t)}{\rho(\chi_i, t) \delta l_i(t)} = \text{constant} \]  \hspace{1cm} (3.52a)

\[ g_{ij} = q_{ij} \hat{n}_1 \]  \hspace{1cm} (3.52b)

The constant in (3.52a) is specified by the initial conditions and \( \delta l_i(t) \), is established as
explained in Section 3.2.3.2. \( \hat{n}_1 \) is obtained as the unit vector normal to \( \delta l_i(t) \)

The product mass-fraction equation is integrated (under an Euler predictor-corrector
scheme) for the product particles located at the element centers, i.e.
\[ \frac{dY_p(\chi_{i}, t)}{dt} = (1+\phi) \frac{\dot{w}(\chi_{i}, t)}{} \]

(3.53)

to yield the product values there, prior to diffusion, \( Y_p^{*}(\chi_{i}, t) \). (In what follows * indicate intermediate solutions.) These values are used to rediscretize the product field and obtain the element product strengths as explained in the previous section, i.e.

\[ \sum_{i=1}^{N} Y_{pi}(t) A_{i}(t) f_{g}(l x - \chi_{i}) = Y_p^{*}(\chi_{i}, t) \]

(3.54)

To check the discretization error which by construction is small, and to be able to minimize its effects, the product particle values are reconstructed from the obtained strengths yielding \( Y_p^{**}(\chi_{i}, t) \). Thus, \( |Y_p^{**}(\chi_{i}, t) - Y_p^{*}(\chi_{i}, t)| \) is the absolute value of pointwise discretization error.

Subsequently, the diffusion step is carried out. It is implemented via the core expansion scheme, i.e.

\[ \delta^2(t+\Delta t) = \delta^2(t) + \frac{4\Delta t}{Pe} \]

(3.20)

for both the Shvab-Zeldovich gradients and the product mass-fraction. For the gradients this signifies the end of the integration. For the product mass-fraction, one more manipulation is executed to remove (for the most part) the effect of the discretization error.

Clearly, the solution after the diffusion step, \( Y_p^{**D}(\chi_{i}, t) \), includes this error. By subtracting the discretization error from this solution a new, corrected, solution is obtained

\[ Y_p(\chi_{i}, t) = Y_p^{*}(\chi_{i}, t) + \Delta Y_p^{**D}(\chi_{i}, t) \]

(3.55a)

where

\[ \Delta Y_p^{**D}(\chi_{i}, t) = Y_p^{**D}(\chi_{i}, t) - Y_p^{**}(\chi_{i}, t) \]

(3.55b)

which includes discretization error effects only in the change of the product particle field due to diffusion \( \Delta Y_p^{**D}(\chi_{i}, t) \). Since the physical problem definition specifies the diffusion to be small, this approach allows even significant discretization errors to be tolerated. In this work, however, this effect was not exploited and the average discretization error was kept smaller than 1%. The reason for this is that even though the discretization error is
subtracted from the product particle solution \( Y_p(\chi, t) \) it is not removed from the product field solution \( Y_p(x, t) \) since it is still included in the product strengths. Thus, while the error is not fed back into the Lagrangian calculations (i.e. the integration of the product equation) it is present in any instantaneous product field spacial evaluation.

### 3.3.3.3. Scalar Field Reconstruction

The gradient related component of the Shvab-Zeldovich variable solutions is obtained by a desingularized, discrete version of equation (3.31), arrived at by using the representation of the gradient field given by equation (3.49), i.e.

\[
s_{gj}(x, t) = \sum_{i=1}^{N} g_{ij}(t) \ A_i(t) \cdot \nabla G_\delta(x - \chi_i(t))
\]  

(3.56)

This expression is a manifestation of the solution of the Poisson equation in an unbounded domain (see Section 3.3.1). Similarly to the VEM, boundaries confining the flow are implemented via a system of images (see Section 3.5). The solution is completed by adding the "potential" part to satisfy the boundary conditions i.e.

\[
s_j(x, t) = s_{gj}(x, t) + s_{pj}(t)
\]  

(3.57)

The product field solution is, as already explained, obtained from the corresponding discretization function (eq.(3.50)). This completes the scalar field calculations since equations (3.56) and (3.57) can be used to construct all the primitive scalars as described in the previous chapter (i.e. eqs.(2.9a,b) and (2.10))

### 3.4. Geometry, Boundary and Initial Conditions

#### 3.4.1. Geometry

The geometry of the computational domain is shown in figure 3.5. (The figure also displays the main boundary and initial conditions.) The two fluid streams, denoted as (1)-top and (2)-bottom, which set up the shear layer flow are constrained in a rectangular
channel of length \(X_{\text{max}}\) and height \(H\). This latter dimension is used as the non-dimensionalizing length scale in the numerical calculations. The inlet of the computational domain is located slightly downstream of a thin splitter plate. This plate, which initially separates the two fluids, is situated half-way between the two walls.

3.4.2. Boundary Conditions

These consist of all the conditions specified at the domain boundaries including those at the inlet. The inlet conditions related to quantities evolving in a Lagrangian frame of reference are, in a strict mathematical sense, initial conditions, but here they will be termed as boundary conditions. This is to distinguish them from the initial conditions considered in the next section which are the field conditions specified at time zero.

3.4.2.1. Flowfield

The formulation presented in this work requires flow-related boundary conditions for all three components of the velocity (vortical, expansion, "potential"). The vorticity boundary conditions are deduced from those of the rotational component of the velocity field (and vice versa). Evidently, the velocity boundary conditions are explicitly known for the total velocity. Arguments based on the physical characteristics of each component are used to deduce the component conditions from the total velocity conditions.

The walls of the channel are impermeable i.e.

\[
\mathbf{u}(x,y_w,t) \cdot \hat{n}_w = 0
\]  

(3.58)

where \(y_w = 0\) or \(1\) and \(\hat{n}_w\) is the unit vector normal to the wall. For the three velocity components, the impermeability of the walls is implemented by enforcing a condition of the form of equation (3.58) for each component. The vortical velocity boundary condition implicitly provides the condition for the vorticity. In a strict sense the fact that the velocity normal to the walls is zero implies that no elements should cross them. The discrete nature of the numerical integration, however, might lead to some elements slightly crossing the
walls. To avoid this problem, elements which experience this effect are simply reflected back into the domain.

The channel walls are also assumed to be frictionless. The consequence of this assumption is that the formation of boundary layers on them is avoided. This is done to reduce computational cost and is justified by the fact that at high Reynolds-Peclet numbers these layers are thin, with small displacement thicknesses and thus do not significantly interfere with the shear layer flow. (This assumption was validated in ref.[50] where the uniform density shear layer with and without the wall boundary layers was studied.)

At the inlet of the domain a velocity profile is specified. For all calculations carried out in this work (i.e. for both non-reacting and reacting shear layers) this profile is chosen to be an errorfunction i.e.

\[
    u(0,y,t) = \left(\frac{U_1 + U_2}{2}\right) + \left(\frac{U_1 - U_2}{2}\right) \frac{y}{\sigma} 
\]

(3.59)

where \( \sigma \) is the errorfunction standard deviation. This profile represents the experimentally observed downstream evolution of the wake profile present at the trailing edge of the splitter plate. (This latter profile is a manifestation of the merging at the trailing edge of the boundary layers growing on each side of the plate.) The use of a wake profile at the inlet is avoided due to numerical difficulties associated with its discretization and the high cost associated with capturing the region of strong turbulence downstream of the splitter plate which transforms the mean profile from a wake to an errorfunction. Evidently, the use of the errorfunction removes some of the information inherent in the flow evolution. One important example of this is the fact that the wake profile, with is two inflection points, experiences two instability modes: the errorfunction and the wake modes. As the name implies, the errorfunction mode is the same as that of the errorfunction profile which experiences only one instability mode (one inflection point). Numerical calculations of the initial evolution of the flow instability [51] indicate that under most conditions the errorfunction mode prevails. This is also supported by experimental results which suggest
that the errorfunction related features are the most dominant in the flow. This provides the main justification for using the errorfunction as the inlet profile. Finally it should be clarified that both the wake and errorfunction profiles are in fact the mean profiles experienced by the flow. Nevertheless, here they are used as the instantaneous ones. This introduces a further unavoidable approximation into the numerical simulation of the flow.

The vorticity inlet profile is obtained from the velocity profile \((\omega=\nabla \times \mathbf{u})\) and is a Gaussian, i.e.

\[
\omega(0,y,t) = -\frac{U_1-U_2}{\sqrt{\pi} \sigma} \exp\left(-\frac{(y-0.5)^2}{\sigma^2}\right)
\]  \hspace{1cm} (3.60)

The implementation of this condition is carried out by introducing at the inlet, columns (note that the profile is one dimensional) consisting of vortex elements of square area which discretize the above profile. The vortical velocity component condition is obtained by integration of the vorticity profile and is, hence, an errorfunction differing by a constant from the total velocity profile (eq.(3.59)). This constant is the "potential" component and is related to the volume of fluid entering the domain (note that the vortical component results at a zero net volume across the inlet). This in turn implies that the expansion component has been assumed to be zero across the inlet. In physical terms this implies that the expanding field is not allowed to cause reverse flow upstream. This is a physically motivated assumption since in reality reverse flow is usually undesirable and is prohibited by controlling the inlet pressure.

The channel exit boundary conditions are not explicitly known and need to be assumed. The arbitrariness of the choice of some of these conditions raises major questions on the validity of the obtained solutions. The equations governing the flowfield evolution are elliptic and thus effects induced by the exit boundary conditions are felt throughout the domain. On the other hand, the strongly streamwise-convective nature of the flow implies that the upstream propagation of these effects is resisted. Thus, the exit boundary condition problem can, for the most part, be bypassed by altering the length of
the domain and observing the upstream changes in the flowfield. The part of the solution which seems to be insensitive to the location of the exit boundary can be assumed to be practically free of the limitations of the assumed exit boundary conditions. This approach was used in this work to determine that for all practical purposes the effects of the exit boundary conditions can be neglected at a distance approximately one channel width upstream from the exit boundary.

A condition of vanishing vorticity is imposed at the exit. This is implemented by deleting the vortex elements once they cross the exit boundary. Integration of the local vorticity field yields the vortical velocity boundary condition. Expansion elements are also deleted at the exit and the resulting local distribution yields the expansion velocity condition. The "potential" velocity component condition is assumed to be the same as that of the inlet; i.e. the "potential" velocity is uniform at the exit.

3.4.2.2. Scalar-field

The scalar field boundary conditions are in many ways related to those of the velocity. Conditions are, in the most general case, required for the Shvab-Zeldovich variables and the product mass-fraction.

The walls are assumed impermeable and adiabatic, i.e.

\[ g_j(x, y_w, t) \cdot \hat{n}_w = 0 \]  (3.61)

where \( g_j \) the gradient of any scalar. The accidental crossing of the walls by transport elements is prohibited in a similar fashion to that of the vortex elements (note that in this work the same elements are used for all transported properties).

The inlet boundary conditions are obtained by specifying inlet scalar profiles. These profiles are not given here since they differ for the different cases considered (i.e. non-reacting, reacting). They will be presented as each individual case is considered. At this stage it suffices to point out that these profiles are of the erf or Gaussian type and they have the same thickness (\( \sigma \)) as that of the velocity profile.
At the exit, and in analogy to the treatment of the flowfield, boundary conditions of vanishing Shvab-Zeldovich variable gradient and product mass fraction are implemented by deleting the corresponding elements.

Finally it is reminded (see Chapter Two, Section 2.2) that integration of the Shvab-Zeldovich gradient fields yields the corresponding scalar fields within a constant \( s_p \). This constant is obtained by matching the scalar solution at a point with the known value there. This in general is done on a boundary where the probability of knowing the value of the scalar mainly exists. To improve the accuracy of this approach, in this work the constant is determined at two locations and in the case that a small difference between the two established values exits, their average is used. These locations are chosen along the top and bottom walls and relatively close to the inlet so that the value of the scalar there can be assumed to be equal to the inlet wall -inlet free stream- value. Specifically the locations are defined according to \( x_p = \left( \frac{2X_{\text{max}}}{3} , y_w \right) \).

### 3.4.3. Initial Conditions

Initial conditions as earlier defined, are required for the vorticity the Shvab-Zeldovich variable gradients and product mass-fraction; i.e. the integrated quantities whose equations exhibit transient behavior.

The simplest and most intuitive initialization of the fields of these properties is to assume that they are all null at time zero and that at subsequent times they are set up by the elements introduced at the inlet, the characteristics of which are determined by the inlet conditions. Unfortunately, numerically this is not a very efficient approach as it leads to an initial over-accumulation of elements in the slower of the two streams. Substantial computational effort needs to be expended to convect these elements all the way to the domain exit. Since what is of greatest interest is the quasi-stationary behavior of the flow which follows this initial transient period, alternative, computationally less expensive initialization approaches can be used.
The approach used in this work is to assume that initially the shear-mixing layer is flat throughout the domain. In other words, the inlet profiles are assumed to be valid along the whole length of the domain. Hence a series of columns of square elements are stacked next to one another throughout the domain setting up what appears to be a square mesh and giving rise to the concept of layers-rows of elements (see figure 3.5). The destabilization of the layer (shear layer roll-up) is obtained by either perturbing the flow at the inlet or via random perturbations, the origins of which can be traced to the discrete nature and numerical approximations involved in the numerical scheme. Such perturbations arise, for example, from the implementation of the exit boundary condition.

3.5. The Schwartz–Christoffel Domain Transformation

3.5.1. The "Potential" Velocity Solution

The initial motivation for the use of the Schwartz–Christoffel transformation [52] is its ability to provide analytical, grid-free solutions for the "potential" velocity field. The physical domain (which can be considered as a complex domain \(z=x+iy\), where \(i=\sqrt{-1}\)) is conformally mapped into an upper half-plane domain \((\xi=\zeta+i\eta)\) (see figure 3.6a). The details of the derivation of the mapping function are given in ref.[50]. Here only its most important features are given.

The function relating the two complex domains is given by:

\[
\frac{d\xi}{dz} = \frac{\pi}{H} \left( \frac{\xi - 1}{\xi} \right)
\]

(3.62)

which upon integration yields the mapping function

\[
\xi = \pm \sqrt{\exp(\frac{2\pi z}{H}) + 1}
\]

(3.63a)

or

\[
z = \frac{H}{2\pi} \ln|\xi^2 - 1|
\]

(3.63b)

where the "+" sign in equation (3.63a) is used when \(y<0.5\) and the "-" when \(y>0.5\).
Under this mapping the two fluid streams in the \( z \) domain are represented as point volume sources located at \((0, -1)\) and \((0, 1)\) in the \( \xi \) domain (see fig. 3.6a). Their strengths are derived from the inlet boundary conditions of the \( z \) domain and are:

\[
S_1 = \frac{U_1 H}{2} \quad S_2 = \frac{U_2 H}{2}
\]

(3.64a,b)

The velocity field resulting from these sources and which is also subject to the rest of the boundary conditions given earlier, is obtained by considering conservation of fluid volume radially outward from each source and by employing the concept of the complex velocity potential, \( w \), i.e.

\[
\frac{dw_p(\xi)}{d\xi} = \frac{H}{2\pi} \left( \frac{U_1}{\xi + 1} + \frac{U_2}{\xi - 1} \right)
\]

(3.65a)

\[
\overline{u}_p(z) = u_p - iv_p = \frac{dw_p(z)}{dz} = \frac{dw_p(\xi)}{d\xi} \frac{d\xi}{dz}
\]

(3.65b)

where the overbar here denotes a complex conjugate. Hence, an analytic solution for the "potential" velocity has been established.

### 3.5.2. Determination of the Total Velocity Field

But the conformal mapping of the domain to an upper half plane (\( \xi \)) domain entails important advantages beyond the analytical determination of the "potential" velocity field. These result by executing the summations over the fields of the elements (i.e. for the velocity and scalar fields) in this domain rather than in the original \((z)\) domain. The reason for this, is that the implementation of the wall boundary conditions is significantly simplified in the \( \xi \) domain.

In the VEM the impermeability of walls is imposed by using a system of element images. In this approach a mirror image of an element is created behind the wall to counteract the velocity induced by the original element normal to the wall. Thus, for the vorticity, the image element is assigned a strength of equal magnitude but opposite sign to that of the original element. For the expansion, on the other hand, the image strength is
equal in both magnitude and sign to that of the original element. In the $\xi$ domain, the
presence of a single plane enables a single image for each element to enforce the wall
boundary conditions. This is shown in figure 3.6b. In the $z$ domain, on the other hand,
where two planes are present, an infinite series of images for each element, located both
above and below the walls are required to implement these conditions.

The mapping of the locations of the vortex and expansion elements into the $\xi$
domain is achieved using the mapping function (eq.(3.63a)). Their cores are mapped using
a more general expression which maps areas between the two domains, i.e.

$$A(z) = A(\xi) \left| \frac{d\xi}{dz} \right|^2$$  \hspace{1cm} (3.66)

Their circulations and area-weighted material density derivatives remain unchanged.

Hence, the three components of the velocity field (vortical, expansion, "potential"),
all represented by derivatives of the corresponding complex velocity potentials are obtained
in the $\xi$ domain and they are summed to yield the total potential derivative there.
Transformation back to the $z$ domain is executed in similarity to the "potential" velocity
case with the added complexity of subtracting the element self-induced velocity [53], a by-
product of the domain mapping, i.e.

$$\bar{u}(z) = u - iv = \frac{dw(z)}{dz} = \frac{dw(\xi)}{d\xi} \frac{d\xi}{dz} + i \frac{\Gamma_j}{4\pi} \frac{d^2\xi}{dz^2}$$  \hspace{1cm} (3.67)

where the $j$ subscript denotes an element number. The self-induced velocity is introduced
in the above expression only in the case where the velocity of an element is being
calculated. For a velocity calculation at any other location in the domain this term is
eliminated.

3.5.3. Determination of the Scalar Fields

The simplification of the element image system in the $\xi$ domain also motivates the
evaluation of the scalar fields there. For the Shvab-Zeldovich gradient fields the element
images are given strengths of equal magnitude and opposite sign to that of the corresponding original elements. This eliminates scalar fluxes normal to the wall. For the same reason the product element images are given strengths of both equal magnitude and sign to the original elements. (It should be noted at this point that unless the flow significantly approaches the wall, a condition not encountered in this work, the effect of the product images is negligible and their use can be avoided.)

The location and core mapping of the gradient and product elements to the \( \xi \) domain is carried out in a similar fashion to that of the vorticity and expansion elements (it should be remembered that in this work the same elements are used to carry both sets of properties). The area-weighted product strength remains unchanged by the mapping. The gradient, on the other hand, with is vectorial nature is mapped according to

\[
\overline{g}(\xi) = \frac{\overline{g}(z)}{d\xi/dz} \quad (3.68)
\]

where the overbar denotes a complex conjugate. This expression implies that the gradient is in fact used in an analogous sense to the derivative of the complex velocity potential. The area weighted gradient is obtained by combining equation (3.68) with equation (3.66).

The summation over the product element fields totally determines the product field. For the Shvab-Zeldovich variable fields, on the other hand, where the summation represents an integration over the gradient fields a "potential" part \( s_p \), related to the boundary conditions, needs to be added to the obtained solution \( s_g \). While, as earlier noted, in the \( z \) domain this is merely an integration constant, in the \( \xi \) domain it exhibits additional components which arise due to the mapping. This can be seen by following an approach similar to that used in the determination of the "potential" velocity field. The flux of material introduced by each source (stream) is conserved radially outward from the source [50]. Integration of the resulting expression yields

\[
s_p(\xi) = C_0 + C_1 \ln|\xi| + C_2 \ln|\xi-1| \quad (3.69)
\]
where $C$'s are constants. $C_0$ is in fact a constant related to the $z$ domain integration constant and is obtained by matching the total scalar solution ($s_g + s_p$) to the known value of the scalar on the wall, as described in Section 3.4.2.2. $C_1$ and $C_2$ and the associated terms are the by-products of the mapping. The two constants are obtained by matching the total solution at two points close to the domain inlet (i.e. where the contribution of these terms is highest). The points chosen in this work are located on the top and bottom wall at the inlet of the $z$ domain. Hence, upon determination of all three constants the Shvab-Zeldovich variable field is established and can then be combined with the product field to completely determine the reacting field.
Core function: \[ f_\delta(r) = \frac{1}{\pi \delta^2} \exp\left(-\frac{r^2}{\delta^2}\right) \]

Figure 3.1 Schematic distribution of the vorticity and vortical velocity for vortex elements with second order Gaussian core function.

Figure 3.2 Schematic representation of the element injection scheme at regions of high strain.
Figure 3.3 Intensification of the gradient on material-isoscalar lines due to pure stretch

Figure 3.4 Schematic illustration of the inversion of the product field discretization function.
Figure 3.5  The geometry of the computational domain together with the initial element configuration and some of the boundary conditions.

Figure 3.6  Illustration of the basic features of the Schwarz-Christoffel conformal mapping.
4. THE VARIABLE DENSITY NON-REACTING SHEAR LAYER

4.1. Introduction

Spacially-developing, post-transitional, variable-density shear layers arise in a large number of mixing processes. They are created by merging, downstream of a splitter plate or a bluff-body, of two streams of unequal velocity and density (see figure 1.1a). Experimental [30,54,55] and numerical [13,19,20] evidence suggests that the flowfield resulting from this merging is essentially two dimensional at its early stages and can be described in terms of large vortical structures (eddies). These structures form as a result of the inherent instability of the vorticity layer between the two streams and represent the primary mechanism of mixing. The development of the layer follows the amplification of perturbations, naturally present in experimental devices or numerical simulations, or of externally imposed forcing signals. These mechanisms trigger the Kelvin-Helmholtz instability which, in its non-linear stages, leads to layer rollup and the formation of concentrated vortices. Further development of the layer is in large part dominated by the mutual interactions of these vortices. These interactions involve pairing mechanisms, a manifestation of the growth of subharmonic perturbations, in which eddies merge to form larger structures.

The effects of density variation in shear layers have been the focus of intense experimental and numerical studies. Early experimental results have shown that density variation plays an important part in determining the growth of the layer, the speed of its eddies and the entrainment and mixing patterns which these eddies induce [29-32]. Stability analysis of the flow [51,56-58] has been able to predict the modification of the early stages of the instability of the vorticity layer by the local variable density field. Two and three-dimensional numerical simulations have been carried out under the temporal evolution idealization and have provided solutions which extend to the non-linear range and which capture some of the essential flow features [26,59]. As explained in Chapter One, temporal layers represent a mathematical idealization of the flow and cannot be used to
exactly reproduce it. Hence, results obtained from such simulations lack quantitative predictability and can only be utilized in a qualitative description of the flowfield.

In this work, a numerical simulation of the post-transitional spacial, variable density shear layer is carried out. In contrast to the temporal model the spacial evolution model attempts to exactly reproduce the flow and is, hence, endowed with quantitative prediction capability. The effects of the variable density field on the flowfield are investigated and are compared with experiments. Explanations are sought via consideration of the vorticity field. For this field the effects of the variable density field are manifested only via the generation of baroclinic vorticity. Thus, differences between the behavior of the uniform and variable density flow must be attributed to the presence of this process. (As earlier noted, a deeper understanding of the mechanism of baroclinic vorticity generation is beneficial also for the study of combusting layers where it is also present.)

The sensitivity of the shear layer to its initial conditions and to the perturbations in the flow field have raised the possibility of manipulating its development by means of external forcing. In uniform-density layers, experimental (e.g. [60]) and numerical (e.g. [20]) results indicate that the spreading of the layer is significantly enhanced by forcing at the subharmonic mode of the instability, which promotes interactions among the vortices. A strong monochromatic fundamental forcing signal, on the other hand, suppresses these interactions and promotes single-eddy growth. This results in reduced spreading of the layer. These substantial effects of external forcing on the growth of the uniform density layer strongly motivate their investigation in the case where a variable density field is present. In this work this is achieved by simultaneously exciting both the fundamental and subharmonic frequencies of the instability mode.

4.2. Formulation and Numerical Scheme

The equations governing the evolution of the variable density non-reacting shear layer can be obtained from the equations of the reacting shear layer presented in Chapter
Two by simply eliminating the presence of reaction. Under this condition, the evolution of the species mass-fractions is not of particular interest and the only scalars considered here are the temperature and density. One extra assumption is imposed which further restricts the equations: The flow is assumed to be free of diffusion effects. The implications of this assumption are that the flow is inviscid and incompressible.

Under this formulation the variable density field is a consequence of the temperature field via the connection of the two properties by the equation of state and the assumptions of constant thermodynamic pressure and equal molar masses for the free-stream fluids. It should be noted though that in many mixing processes this is not the case; the two fluid streams are at the same temperature and the presence of the variable density field is a result of their different molar masses. The formulation considered here, does not necessarily exclude this case. This can be achieved by using the initial density field to initialize the temperature field, which then, for all practical purposes, becomes a dummy variable and can also be considered as the inverse of the mean molar mass. Pursuing the same argument further, it becomes evident that the scalar field formulation presented in Chapter Two can be avoided altogether and solutions for the density field can be obtained by using the density directly. This in fact was the approach used in obtaining the results presented here.

Hence, the governing equations for the variable density, non-reacting inviscid and incompressible shear layer become:

\[
\begin{align*}
\text{Incompressibility} & \quad \frac{dp}{dt} = 0 \\
\text{Continuity} & \quad \nabla \cdot \mathbf{u} = 0 \\
\text{Momentum} & \quad \frac{d\mathbf{u}}{dt} = -\frac{\nabla p}{\rho}
\end{align*}
\]

(4.1) \quad (4.2) \quad (4.3)

where all symbols as earlier defined.
As before, the equations of motion (eq.(4.2)-(4.3)) are recast into a vorticity-streamfunction formulation. The velocity field is reconstructed via the Helmholtz decomposition by recognizing that in this case the expansion component is absent, i.e.

\[ u = u_\omega + u_p \]  
\[ u_\omega = \nabla x (\psi \hat{k}) \]  
\[ u_p = \nabla \phi_p \]  
\[ \nabla^2 \psi = - \omega \]  
\[ \nabla^2 \phi_p = 0 \]

where symbols as earlier defined. For the scalar field the incompressibility condition (eq. (4.1)) is recast into gradient form:

\[ \frac{d\omega_k}{dt} = \frac{\nabla \rho \times \nabla p}{\rho^2} \]  
\[ g = g + \nabla \nabla u + g \times (\omega \hat{k}) = 0 \]  
\[ \rho = \rho_g + \rho_p \]

where \( g \) is the density gradient (\( g = \nabla \rho \)). \( \rho_g \) is the part of the density field related to the density gradient and \( \rho_p \) the part added to satisfy the boundary conditions. If instead of this density based formulation, the one presented in Chapter Two is used the same type of equation is still solved. This is because the temperature and, hence, the \( \gamma \) Shvab-Zeldovich variable (no product!) obey the same equation as the density (eq.(4.1)).

The numerical schemes described in Chapter Three are used to obtain the solutions of these equations under the relevant boundary conditions. The VEM is used to solve the flowfield. The parts of the scheme dealing with the expansion velocity field are simply not implemented. The TREM, which in this non-reacting case reduces to the TEM, is used to deal with the scalar field.

### 4.3. Geometry, Boundary and Initial Conditions

The flow geometry considered here is the same as that discussed in Chapter Three
(see figure 3.5) i.e. the shear layer flow is set up inside a two dimensional channel of height $H$ and length $X_{\text{max}}$ where the two parallel fluid streams (1-top, 2-bottom) mix downstream of a thin splitter plate. The boundary and initial conditions of the flow are given in the same chapter (Section 3.4). The only boundary conditions not specified there, were those of the scalar field at the inlet of the domain. Hence, these conditions are given here in the form of the density and related density-gradient profiles at the inlet. The velocity-vorticity profiles at the inlet are also repeated for completeness:

Velocity

$$U(x=0,y,t) = \frac{U_1 + U_2}{2} + \frac{U_1 - U_2}{2} \text{erf} \left( \frac{y-0.5}{\sigma} \right)$$  \hspace{1cm} (4.10)

Vorticity

$$\omega(x=0,y,t) = -\frac{U_1-U_2}{\sqrt{\pi} \sigma} \exp \left( -\frac{(y-0.5)^2}{\sigma^2} \right)$$  \hspace{1cm} (4.11)

Density

$$\rho(x=0,y,t) = \frac{\rho_1 + \rho_2}{2} + \frac{\rho_1 - \rho_2}{2} \text{erf} \left( \frac{y-0.5}{\sigma} \right)$$  \hspace{1cm} (4.12)

Density gradient

$$\nabla \rho(0,y,t) = (0, \frac{\partial \rho}{\partial y}(0,y,t))$$  \hspace{1cm} (4.13a)

with

$$\frac{\partial \rho}{\partial y}(x=0,y,t) = \frac{\rho_1-\rho_2}{\sqrt{\pi} \sigma} \exp \left( -\frac{(y-0.5)^2}{\sigma^2} \right)$$  \hspace{1cm} (4.13b)

where erf denotes the error function and exp the exponential function. Distances in the above profiles as well as in the numerical simulations are non-dimensionalized with the channel height, $H$. $\sigma$ denotes the standard deviation of the Gaussian profile which describes both the initial vorticity and density-gradient distributions. The thickness of the vorticity layer is defined as $d=2\sigma$ and is scaled so that the height of the channel ($H$) equals twice the wavelength of the most unstable fundamental mode of the vorticity distribution of the uniform density layer ($\lambda_{uw}$). This scaling enables paired eddies (the manifestation of the merging of two non-linear waves into a larger structure), which are the largest structures anticipated within the computational domain, to fit into the channel and not be obstructed by the walls. As will later be shown (Section 4.4), the size of this scaling wavelength is not
particularly sensitive to the presence of the different densities of the free streams. Hence, its uniform density value is used to scale all cases simulated in this work. For the profiles considered here, this wavelength is equal to $\lambda_w=12.8\sigma$, yielding a value of $d = 0.08$.

The velocity and density scaling is carried out via the values of these properties for the top stream, i.e. $U_1, \rho_1$. The velocity and length scales are used to deduce a time scale. This scaling approach points to the importance of three non-dimensional groups in the analysis of the flow: The

(a) velocity ratio, (b) density ratio, and (c) momentum ratio.

$$
r = \frac{U_2}{U_1} \quad \quad \quad s = \frac{\rho_2}{\rho_1} \quad \quad \quad m = sr^2 = \frac{\rho_2}{\rho_1} \left( \frac{U_2}{U_1} \right)^2 \quad (4.14abc)
$$

Evidently, only two of these groups are independent. Commonly, the first two are used, but in this study the momentum ratio is also included because of its important physical significance to the flow. It should also be noted that the top stream is assumed to have higher speed than the bottom stream, so that $r < 1$, while $s$ and $m$ are allowed to assume any non-negative value.

The vorticity layer is initially discretized by distributing vortex-transport elements over seven material layers (lines) lying within the support of vorticity, as described in Chapter Three. The elements are of square area of side $h=0.0234$. Hence a square Lagrangian mesh is defined as the initial condition (see fig. 3.5). Via the assumption that the inlet conditions persist throughout the domain the element discrete vorticity and density gradient values are readily obtained from equations (4.11) and (4.13) respectively. The value of the core radius ($\delta$) is found by the procedure described in Chapter Three which allows the variation of this quantity for the minimization of the discretization error. For the specific conditions used here, this procedure yields $\delta=0.0273$. Evidently, such a value of the core radius ensures core overlap and is in agreement with the accuracy and convergence requirements of the scheme (i.e. $\delta>h$).
Finally, it is noted that in some of the numerical simulations the boundary condition at the inlet is modified by the introduction of a perturbation which forces the early destabilization of the flow (forced layer). In the absence of this externally specified perturbation the evolution of the layer reflects the amplification of numerically-excited instability waves. Such a process yields the "natural"-unforced behavior of the layer, since, the numerical error may be treated as a white noise of very weak amplitude [20]. When the inlet perturbation is imposed, it is governed by a forcing signal which is expressed in terms of two in-phase sinusoidal waves whose frequencies are those of the most unstable Kelvin-Helmholtz mode and its first subharmonic. These frequencies are obtained from the linear stability analysis of the flow, discussed in the next section. The amplitude assumed for both frequencies is $A_f=A_s=0.015 (=0.03\lambda_w)$. The details of the forcing signal are shown in figure 4.1. Implementation of the forcing is manifested by displacing the vortex elements at $x=0$ about their mean locations according to the forcing signal.

4.4. Linear Stability Analysis

As a first step in the analysis of the flow, and prior to the description of the numerical simulation results, its linear stability characteristics are analyzed. Such an analysis can provide information about the effect of the presence of the variable density field on the initial stages of the instability and can be used as a validating mechanism for the simulation results.

The analysis, the features of which are considered standard [61] and are, hence, not presented in detail here, is carried out for a flow governed by the equations presented in Section 4.2 (eqs.(4.1)-(4.3)). The linearization of these equations starts by splitting the dependent variables ($\phi$), into base ($\Phi_{\text{Base}}$) and perturbation ($\tilde{\phi}$) components. i.e.

$$\phi(x,y,t) = \Phi_{\text{Base}}(x,y,t) + \tilde{\phi}(x,y,t)$$  \hspace{1cm} (4.15)
A base flow is assumed which is described by the velocity and density profiles of the previous section (i.e. errorfunctions, but in a frame of reference shifted to the centerline of their variation region) and by a constant thermodynamic pressure, i.e.

\[ u = (U(y),0) \quad \rho = \rho(y) \quad p = p_0 \]

and is used to define the base values of the properties. The velocity ratio for this flow is taken as \( r = 0.5 \) and the density ratio is allowed to vary so that its effects on the flow instability can be determined.

The perturbation components are assumed to exhibit the form of propagating waves,

\[ \phi(x,y,t) = \bar{\phi}(y) \exp(ia(x-ct)) = \bar{\phi}(y) \exp(i(ax-wt)) \quad (4.16) \]

where \( a, c \) and \( w (=ac) \) are the wave number, speed and frequency respectively. For a spacial shear layer \( a \) and \( c \) are complex and \( w \) is real. Quantities under overbars denote the variation of the perturbation in the \( y \) (cross-stream) direction and \( i = \sqrt{-1} \).

Equations (4.15) and (4.16) are substituted into the governing equations and are used to linearize them by neglecting, as small, terms involving the products of the perturbations. i.e.

Compressibility

\[ i(aU-w) \bar{\rho} + \frac{d\rho}{dy} \bar{v} = 0 \quad (4.17) \]

Continuity

\[ ia \bar{u} + \frac{d\bar{v}}{dy} = 0 \quad (4.18) \]

\( u \)-Momentum

\[ i\rho(aU-w) \bar{u} + \rho \frac{dU}{dy} \bar{v} + i\rho \bar{p} = 0 \quad (4.19) \]

\( v \)-Momentum

\[ i\rho(aU-w) \bar{v} + \bar{p} = 0 \quad (4.20) \]

By employing a process of elimination, an equation governing the evolution of one cross-stream perturbation variation can be obtained. In this work this perturbation is chosen to be the cross-stream velocity \( (\bar{v}) \). The resulting equation is a modified Rayleigh equation for stratified flow, i.e.
\[
\frac{d^2\tilde{v}}{dy^2} + \left[ \frac{1}{\rho} \frac{d}{dy} \left( \frac{d\Pi}{dy} \right) + \frac{a U}{(aU-w)} \left( \frac{d^2U}{dy^2} + \frac{1}{\rho} \frac{d\Pi}{dy} \right) + a^2 \right] \tilde{v} = 0
\] (4.21)

and its solution, which is strongly dependent on boundary conditions, poses an eigenvalue problem due to the presence of the wave parameters \(a\) and \(w\).

The boundary conditions are obtained by considering that far away from the base flow variation region the base derivatives are zero. Hence the equation reduces to

\[
y \to \pm \infty \quad \Rightarrow \quad \frac{d^2\tilde{v}}{dy^2} - a^2 \tilde{v} = 0
\] (4.22)

which for a bounded solution (i.e. avoiding positive exponential growth) dictates that

\[
y \to + \infty \quad \Rightarrow \quad \frac{d\tilde{v}}{dy} - a \tilde{v} = 0
\] (4.23a)

\[
y \to - \infty \quad \Rightarrow \quad \frac{d\tilde{v}}{dy} + a \tilde{v} = 0
\] (4.23b)

The solution of equation (4.21) presented here treats the wavenumber \(a\) as the eigenvalue for an externally specified frequency. It is initiated by assuming a starting value for the wavenumber and a value for \(\tilde{v}\) below and far away from the base flow variation region (i.e. \(\tilde{v}(y_0) = \tilde{v}_0\)) so that equation (4.23b) can be applied to yield the local derivative \(\frac{d\tilde{v}}{dy}(y_0)\). Knowledge of both the value and the derivative at \(-y_0\) enables the initiation of a shooting numerical procedure which integrates equation (4.21) across the base flow variation region and checks at a point above the region symmetrical to the starting point (i.e. at \(+y_0\)) if the other boundary condition is observed. Information from the upper boundary condition is used to "improve" the value of the wavenumber and the procedure is repeated. This is done iteratively until convergence of the wavenumber value is achieved.

A central-difference scheme is used to discretize the equation on an equispaced one dimensional mesh, a Runge-Kutta fourth order integration scheme to perform the numerical integration and a Newton-Raphson shooting method to carry out the iterative shooting. Convergence is found to be strongly dependent on a good starting guess for the wavenumber.
Results from the above analysis are plotted in figure 4.2ab, which shows the wave spacial amplification rate (-Imag(a)) and the wave phase speed (Real(c)) versus the wave frequency, for density ratios $s = 0.25, 0.333, 0.5, 1, 2, 3, 4$ (these values of the density ratio also used in the numerical simulations). The figure clearly shows that the most unstable mode (frequency with maximum growth rate) of the Kelvin-Helmholtz instability of the variable-density layer exhibits a very weak dependence on the value of the density ratio and experiences a minimum for the uniform density case. The associated growth rate is also seen to be only weekly dependent on the density ratio increasing with increasing values of this parameter. In contrast, the phase speed of the most unstable waves is highly sensitive to the value of the density ratio. Its value sharply decreases with increasing value of $s$. Thus, the results of the linear stability analysis dictate that as the density of the slower stream increases ($s$ increases) the wave growth rate increases and the wave speed decreases. Experimental results, as well as the results of the numerical simulations presented in this work, indicate that this type of behavior persists into the non-linear stages of the flow.

4.5. Numerical Results

In order to investigate the effect of density variation on the evolution of spacially-developing vorticity layers, numerical results are obtained for layers with two inlet velocity ratios, $r = 0.5$ and $0.625$, and for a wide variety of density ratios. The computations are initialized by assuming that unperturbed vorticity and density layers extend horizontally throughout the domain. In all computations, the time step $\Delta t = 0.1$, and the computations are carried out long enough to observe several "cycles" of the evolution of the Kelvin-Helmholtz instability. The transient period may be estimated by $t < 9$, i.e. by the time period required for the initial computational elements to exit the computational domain. Calculations for both unforced and forced layers are carried out and their results are presented in sequence.
4.5.1. The Unforced Layer

The dynamics of the vorticity field in confined variable-density shear layers are investigated by computing the development of the flow field for layers characterized by fixed velocity ratio $r = 0.5$, and computational domain length $X_{\text{max}} = 6$, and varying density ratios. Cases with $s = 0.333, 0.5, 1, 2$ and $3$ are considered, i.e. the density of the slower stream is incrementally increased from a small fraction of the fast-stream density to eventually exceed the latter. The structure of these layers is first examined in figure 4.3 by illustrating the location of the transport elements at $t = 10.5$, a time at which a periodic shedding of large scale vortical structures is established. The figure is generated by plotting both the location of the elements and their velocity vector relative to the average flow.

Examination of the flow realizations of figure 4.3 reveals that, for all values of the density ratio, the development of the layer can be divided into several stages. For short distances downstream of the splitter plate, the vorticity layer remains flat, and the flow field appears to be steady. Immediately following this region, the layer rolls into coherent eddies which propagate downstream. These vorticity structures form as a result of the growth of numerically introduced perturbations which excite the Kelvin-Helmholtz instability mode of the vorticity layer [62,63]. These instability waves cause a sinusoidal deformation of the layer, such that the peaks and the valleys of the waves protrude into the top and bottom streams respectively. The growth of the waves involves an energy migration from the mean flow into the perturbation [20]. In its non-linear stages, this mechanism leads to the saturation of this "fundamental" mode of instability and to the wave-breaking of the perturbation and the reorganization of the vorticity field into coherent eddies where most of the vorticity is concentrated. Neighboring eddies are joined by thin braids, which are constantly strained by the flowfield induced by the former. Further downstream, especially for $s > 1$, the evolution of the vorticity field is dominated by the mutual interaction of neighboring eddies. This interaction occurs as eddies which are
displaced toward the faster top stream acquire a higher streamwise velocity than their
downstream neighbor, a mechanism which eventually results in the merging or pairing of
these structures. Pairing mechanisms, which are a manifestation of the amplification of
subharmonic instability modes, are responsible for the generation of vorticity structures of
larger streamwise and cross-stream extent, and thus are prime contributors to the overall
growth of the layer.

The dynamics and organization of the eddies in the second half of the domain are
strongly dependent on the value of the density ratio, and significant differences exist
between eddy interactions for $s < 1$ and $s > 1$. The cases of figure 4.3 can be differentiated
by the shape of the eddies, their organization within the layer, and the net deformation of
the computational mesh. These differences are summarized in the following. With
increasing density ratio, the layer starts to roll earlier and closer to the tip of the splitter
plate. This is accompanied with the increase in the number of transport elements used to
discretize the layer, and hence with higher rate of deformation of the material layers within
the same computational domain. The shape of the eddies is also affected by increasing the
density difference between the two streams. The eddies deform more as $s$ increases and
acquire a more elliptical shape for $s > 1$. These elliptical-shape eddies are not symmetric
with respect to both streams. Early pairing is observed for $s > 1$, accompanied with faster
growth rate.

In order to quantify the effect of the density ratio on the flowfield, the spacial
growth rate of the layer and the volumetric entrainment ratio from the free streams are used
as measures of the mean flow properties, and the streamwise convective speed of the
eddies is used to characterize the flow unsteady dynamics. These quantities are also
compared with available experimental and analytical evidence, and are thus used to validate
the computations.
The bulk of the available experimental and analytical data describing the behavior of the layer growth rate ($\delta'$), entrainment ratio ($E_v$) and speeds of eddies ($r_e$) were summarized by Dimotakis [64 or 65] into the following empirical formulas:

\[
  r_e = \frac{U_e}{U_1} = \frac{1 + r s^{1/2}}{1 + s^{1/2}}
\]

(4.24)

\[
  E_v = \frac{V_{e1}}{V_{e2}} = s^{1/2} \left( 1 + 0.68 \left( \frac{1 - r}{1 + r} \right) \right)
\]

(4.25)

\[
  \delta' = C_\delta \frac{(1 - r)(1 + s^{1/2})}{2(1 + r s^{1/2})} \left( 1 - \frac{1 - s^{1/2}}{1 + s^{1/2}} \right) \left( 1 + 2.9 \left( \frac{1 + r}{1 - r} \right) \right)
\]

(4.26)

where the entrainment ratio is defined as $E_v = \frac{\text{Volume entrained from fluid (1)}}{\text{Volume entrained from fluid (2)}}$ and the growth-rate as $\delta' = \frac{\delta(x)}{x-x_0}$ with $\delta$ being the layer thickness, assumed to be growing linearly, and $x_0$ the layer virtual origin [30]. $C_\delta$ is an empirically determined constant dependent on initial conditions. The high sensitivity of the layer to its initial conditions results in a large range of values for this constant i.e. $0.25 < C_\delta < 0.45$ [65].

Figure 4.4 shows the spacial growth rate of the thickness of the layer for different values of density ratio, plotted against the empirically deduced formula suggested by Dimotakis with coefficient $C_\delta = 0.31$. The mean density profile is used to define the thickness of the layer, which is assumed to be confined within a region bounded by the lines where the mean density first deviates from the free stream values by 1% of the density difference. These lines are obtained by a least-squares fit of the 1% points specified by the profiles at different stations downstream. (For uniform-density flow, a passive scalar having similar inlet profile to that of the density is used). The figure exhibits a favorable agreement between the numerical solution and the experimental curve fit, and indicates that, at fixed velocity ratio, the growth rate of the layer increases with increasing the density of the low speed stream. A better agreement is obtained when the experimental curve fit is corrected by using the local mean streamwise velocity ratio, deduced from the mean flow
profiles by averaging the local velocity ratio over several streamwise sections. This correction, which was suggested in the initial presentation of the above empirical formulas, is necessary since the velocity drop across the layer may vary in the streamwise direction due to confinement.

An equally favorable agreement is obtained for the volumetric entrainment ratio, which characterizes the composition of the eddies (see figure 4.5a). As previously mentioned and experimentally observed, this ratio increases with increasing density of the low-speed stream. It should be noted, however, that this ratio is higher than unity for uniform-density layers, since the latter naturally tend to entrain more from the high-speed stream [65]. In this latter case, this deviation is due to the asymmetry of the flow conditions upstream and downstream of the vortices, which originates due to the spacial spreading of the layer. Thus, at fixed velocity ratio, variation of the free stream density ratio modulates the entrainment patterns in such a way as to favor volumetric entrainment from the low-density stream.

Finally, the computed results are compared in figure 4.5b with experimental data on the propagation velocity of the eddies. The results are best interpreted by considering the variation of the convective speed of the eddies as it deviates from unity. In the uniform-density case, both the numerical simulation and experimental data show that the eddies move with the mean flow velocity. As the density ratio varies, the eddies acquire an additional convective component. This additional component is of the same sign as the relative velocity of the high-density stream, so that, for density ratios smaller (larger) than unity, the convective speed of the eddies becomes larger (smaller) than the mean flow velocity. As for the estimates of the spreading rate and the volumetric entrainment ratio, the computed values of the eddies convective speed exhibit excellent agreement with experimental data.

The dependence of the motion of the vortices on the density ratio may be examined using two different approaches. The first approach, suggested by Dimotakis [64] (and
which leads to eq.(4.24)), uses a pressure argument to estimate the convective speed of the eddies. It is based on the argument that, in a reference frame moving with the eddy, stagnation points must exist along the braids joining neighboring eddies. Equating the total pressure for streamlines originating in the free streams and meeting at the stagnation points yields an estimate of the eddy convective speed. This estimate shows good agreement with experimental data, and indicates that the convective speed of the eddies changes in such a way as to balance the pressure forces at the stagnation points. It is interesting to note that the phase speed of the most unstable mode calculated in the linear stability analysis (see Section 4.4) coincides with the convective speed of the eddies determined using the above argument. Thus, both the linear growth of the instability waves and the large non-linear eddies are characterized by the same speed. A similar behavior has been observed in the numerical simulation of temporally developing layers [26], in which the transition of the unstable mode to non-linear regimes is not accompanied by a noticeable change in its phase speed.

An alternative approach in explaining the above described behavior of the flow can be achieved by considering the dynamic effects of baroclinic vorticity generation. The reason for this is that baroclinic vorticity generation is the only extra mechanism of flowfield modification distinguishing the variable and uniform density cases. This approach in the analysis of variable density flows was also followed by Krishnan [26] in his study of the variable density temporal shear layer which showed that baroclinic torques lead to the intensification of the vorticity in regions displaced towards the low-density stream, and to its reduction at those points moving towards the high-density stream. This effect was also encountered in this work and is illustrated in figure 4.6 which shows the vorticity distribution within the fundamental eddy and the associated streamline pattern for layers with $s = 0.25, 1, \text{ and } 3$. As expected, the results indicate that for $s < 1$, the baroclinic vorticity generation leads to the intensification of vorticity in the bottom part of the eddy, while vorticity generation of the opposite sign takes place in the top part. This
trend is reversed for $s > 1$, i.e. when the density of the bottom low-speed stream exceeds that of the top stream. This vorticity generation mechanism leads to the formation of zones of opposite signs of vorticity, so that, for high density variation, the eddy becomes composed of two counter-rotating vortices (see following sections). The case $s = 1$ is included to verify that the asymmetry of the vorticity within the eddy persists in the uniform-density case, contrary to results of temporal calculations [26]. This form of asymmetry, which is experimentally observed, is due to the spacial growth of the layer and should be distinguished from the previous effect. It should also be noted that, as shown in the streamline plots, the vertical location of the center of the eddy varies according to the density ratio. The center of the eddy moves upward as the density of the low speed stream increases. This motion influences the orientation of the vorticity layer, which, as shown in figure 4.3, follows a similar trend.

This asymmetric vorticity generation can be explained and subsequently be used to deduce many of the flow features, by considering a simple kinematical argument for the interaction of the baroclinic vorticity generation term with the destabilization of the initial vorticity layer. This is schematically illustrated in figure 4.7 which considers a case where the fast stream is the denser. The vectorial nature of the baroclinic term is seen to yield positive vorticity in the top denser stream and negative vorticity in the slow less-dense stream, in agreement with previous evidence. Thus, the vorticity field of the rolled structure (eddy) can be viewed as a dipole of vortices of opposite signs. The generated vorticity lying on the low-density side has the same sign of vorticity as that of the initial layer. The dipole induces an additional streamwise velocity component to the motion of the eddy, $U_e$, which has the same sign as the relative velocity of the high-density free stream. The velocity field induced by the dipole leads to the distortion of the entrainment currents in such a way as to favor higher entrainment rates from the low-density stream. Incompressibility and continuity thereby imply that the eddy will tend to move towards this
stream. All these features are in agreement with the numerical evidence noted earlier (see figure 4.6).

4.5.2 The Forced Layer

In this section, the dynamics of the mixing layer under high amplitude forcing are examined. The evolution of variable-density layers characterized by the same velocity used in the previous section, \( r = 0.5 \), and density ratios \( s = 0.25, 0.5, 1, 2, \) and \( 3 \), is computed. The corresponding momentum ratios are \( m = 0.0625, 0.125, 0.25, 0.5, \) and \( 0.75 \), respectively. In these computations, a domain length \( X_{\text{max}} = 5 \) is selected in order to limit the computational effort. The shorter domain length is not expected to limit the complexity of the phenomena numerically visualized, since, due to high amplitude forcing, the initial rollup of the layer occurs closer to the splitter plate. Thus, several pairing events can still be observed within the domain. The same analysis tools developed in the previous section are used, and attention is focused on the effect of forcing on the evolution of the density and vorticity fields.

Figure 4.8 shows the instantaneous realization of the flow at \( t = 18.5 \) for all the cases considered. The large scale features of the flow field as perceived in this representation, show the same stages of development as in the unforced layer computations. In this case, the development of the layer at short distances downstream of the splitter plate is dominated by the external forcing. The layer amplifies the forcing frequency which coincides with its most unstable fundamental mode, so that a regular shedding of eddies is achieved. Comparison of the various frames of figure 4.8 shows that, in agreement with the unforced layer results the rollup of the layer occurs earlier as the density ratio is increased. But the growth of the eddies downstream appears to follow a trend opposite to that of the unforced cases, decreasing with increasing density ratio.

A quantitative examination of the dependence of the asymmetric entrainment patterns and of the convective velocity of the eddies on the density ratio is shown in figure 4.9ab. The figure also shows the empirically fitted curves for a fixed velocity ratio \( r = 0.5 \).
and a wide range of density ratios. Both plots in the figure exhibit the same trend established in the unforced layer computations at fixed inlet velocity ratio, namely an increase (decrease) of the entrainment ratio (eddy convective speed) with increasing density ratio. This is not surprising since, due to the similarity of the velocity and acceleration fields, the baroclinic generation of vorticity is expected to induce similar trends. Moreover, the computed results exhibit good agreement with the experimental data obtained with no external forcing, and hence with the results of the unforced layer computations. Thus, neither the eddy convective speed nor the entrainment patterns are significantly affected by the application of strong external forcing.

On the other hand, and as already pointed out, the development of the flowfield following the early rollup of the layer, differs significantly from the previous case. Figure 4.8 shows that for small density ratios, the vorticity field at large streamwise coordinates is characterized by large, well separated eddies. The formation of the large eddies results from the amplification of subharmonic modes which lead to the merging of neighboring eddies. These pairing interactions appear to be suppressed at high density ratio, and the vorticity field is described by an almost periodic array of vortices whose size almost equals that of the fundamental perturbation. Also note that, while the initial rollup of the layer and the formation of coherent eddies occur closer to the splitter plate as the density ratio increases, pairing interactions among neighboring eddies are significantly delayed.

A similar observation holds regarding the mean flow and density fields, so that, unlike the entrainment ratio and eddy convective speed, the behavior of the spreading rate is significantly altered from that of the unforced layer computations. This is shown in figure 4.10 where the computed spreading rates for various density ratios are plotted against the experimentally fitted curve of Dimotakis (eq.(4.26)). With the imposed high amplitude forcing, the results show that for low values of density ratio (high-density fast stream), the spreading rate of the layer is greatly increased over its unforced counterpart. Conversely,
the spacial growth of the layer is significantly reduced as the slow stream becomes increasingly heavier, that is for s>1.

This result is further investigated by considering one more set of numerical results, namely variable-density layers with velocity ratio \( r = 0.625 \), and density ratios \( s = 0.427, 0.64, 1.28, 2.56, 5.10, 10.2 \) and 15.4. These values are chosen so that the unexpected behavior of the spreading rate curve can be examined in a wider range of density ratios, and also to investigate the effect of the momentum ratio which is suspected to be particularly important for the forced layer case. (It should be noted that for the previous set of forced results this ratio was always smaller than unity -see figure 4.10- thus not allowing a complete analysis of its effects.) The corresponding momentum ratios are \( m = 0.166, 0.25, 0.5, 1, 2.4 \) and 6. The time step is decreased to \( \Delta t = 0.05 \), while the remaining numerical parameters are not altered. The same external forcing function is applied on the inlet vorticity distribution, and the computations are carried over several cycles of shedding of shear layer eddies. The results are analyzed in terms of instantaneous flow realizations, eddy convective speed, entrainment ratio and layer spreading rate. It is noted however that, as in all the previous cases, the entrainment ratio and the convective speed of the eddies are found to be in very good agreement with the experimentally fitted curves, and consistent with the results of the unforced case, so that further discussion of this behavior is omitted. Results are first interpreted in terms of the instantaneous realization of the flowfield, shown at \( t=18.5 \) in figure 4.11 for three characteristic cases from the above mentioned set of results.

Figure 4.11 acts to further clarify that in contrast to the unforced layer behavior, the forced layer growth is not monotonically varying with the density ratio. In agreement to the previous forced results (note the momentum ratio range) initial increases of the density ratio from the \( s=0.427 \) to 2.56 lead to what appears to be smaller layer growth (assessed by the smaller protrusions of eddies in the free-streams) and the inhibition of the eddy pairing interaction. But further increases to \( s=15.4 \) result in increases in the layer growth via new
types of eddy interactions (see following paragraphs). The fact that this type of behavior correlates with the variation of the momentum ratio, which experiences a value equal to unity for the case with the smallest growth, makes evident the paramount importance of this parameter. This ratio which is indicative of the lateral forces acting on the shear layer region also governs the layer orientation. This can clearly be seen in figure 4.11. At small momentum ratio, the layer is tilted towards the bottom, lower momentum, stream. With increasing the momentum of the low speed stream, the centerline of the layer is gradually displaced upwards. For the intermediate, unit momentum ratio case, the layer does not appear to favor either free stream and its centerline almost coincides with the axis of the splitter plate. As the momentum of the slower stream is further increased, the layer is clearly pushed into the upper, faster, but lower momentum, stream.

To clarify the point that the momentum ratio related growth behavior is characteristic only of forced layers, the cases of figure 4.11 are repeated without forcing and presented in figure 4.12. The previously verified monotonical increase of the layer growth with the density ratio is evident and no correlation with the momentum ratio appears to be present.

Returning to figure 4.11 it is noted that for small momentum and, hence, density ratio \( m=0.166, s=0.427 \), eddy interactions are by pairings which involve large displacement of consecutive eddies about the centerline of the layer. In this type of interaction (see figure 4.13 for details of eddy interactions), the leading eddy is larger than its upstream partner. The leading eddy is displaced toward the slower bottom stream, while its upstream neighbor moves vertically towards the faster top stream. The merging of the eddies thus leads to the formation of a single composite structure of larger streamwise and cross-stream extent. This type of vorticity reorganization is representative of forced layers of momentum ratios smaller than unity (see also the previous set of results with \( r=0.5 \)).
As the momentum ratio approaches unity (s=2.56), however, this mechanism is significantly altered. In this case, merging eddies approach each other without a noticeable cross-stream displacement, and contrary to the above case, the leading eddy has smaller size than its upstream pairing partner. As the separation distances between the merging eddies decrease, the braid region separating neighboring eddies is squeezed between their cores, and finally disappears at the end of the interaction period. The vorticity of the two eddies is reorganized by a predominantly streamwise fluid motion that includes a very weak rotating component. This process, which resembles tearing and merging of various sub-regions of interacting eddies, results in the formation of a composite structure of larger streamwise extent but whose cross-stream extent is only slightly larger than that of the original eddies. It should be noted that this type of eddy interactions were also seen in the r=0.5 set of forced results presented earlier, as the momentum ratio tended to unity.

When the momentum ratio becomes significantly larger than unity (m=6, s=15.4) the dynamics of the interaction among eddies are also distinguished from the two previous cases. In this case, due to the very high value of the density ratio, baroclinic vorticity generation leads to pronounced intensification of the vorticity at the outer edges of the eddy curved towards the faster high-density stream, and to the creation of zones of vorticity of the opposite sign around the bottom edges. While this process does not result in a net variation of the circulation of the eddy, it leads to the division of the eddy into two strong counter-rotating vortices. Vortices of the same sign as the original vorticity of the layer have higher circulation. These vortices play an important role in eddy interactions which are described in the following. At the beginning of the interaction among neighboring eddies, the "trailing" eddy is displaced upwards towards the faster stream, while its downstream eddy is displaced downwards towards the low-speed stream. As the eddies approach one another, they are deformed according to the sign of the vortices contained therein. Vortices having the same sign of vorticity as that of the unperturbed vorticity layer approach one another, while the counter-rotating vortex of the leading eddy is ejected
upwards towards the faster stream. The counter-rotating vortex of the trailing eddy is left behind and lies on the side of the low-speed stream. At its early stages, the composite structure is composed of two pairs of counter-rotating vortices. The stronger vortices then merge to form a single structure, which entrains the vorticity of top counter-rotating vortex. The bottom counter-rotating vortex is highly deformed and appears as an elliptical vortex trailing the bottom of the composite eddy. (See figure 4.13). This interaction yields a complicated eddy which has larger streamwise and cross-stream extent than the original eddies.

The above described instantaneous flowfield behavior which relates the forced layer growth to the free stream momentum ratio implies that the growth rate based on the flow mean characteristics is also controlled by this parameter. This is shown in figure 4.14 where the growth rate is plotted versus both the density and momentum ratio. The unforced behavior is also included by plotting the empirical growth rate formula. As anticipated, the forced layer growth rate increases on both sides of the unity momentum ratio value, the increase being more significant for values greater than unity. Comparison with the unforced case shows that the growth rate of the variable density layer may be enhanced via external forcing only if the layer momentum ratio is substantially different from unity. For momentum ratios close to unity, the growth rate is considerably reduced. It should be noted that this latter trend is in agreement with the results of the $r = 0.5$ cases shown in figure 4.10.

The above noted dependency of the forced layer growth rate on the momentum ratio can be qualitatively explained by relating it to the layer orientation discussed earlier. As the momentum ratio pushes the layer into one of the two free streams it also exposes it to more entrainment from that stream. Thus minimum entrainment, and hence layer growth, is to be expected when the layer does not significantly intrude into the free streams i.e. the momentum unity case. Furthermore, more entrainment should be expected if the layer is
pushed into the fast stream (m>1) than in the slow stream (m<1). This explains the asymmetry in the layer growth rate about the unity momentum ratio case.

In an attempt to better understand this behavior, a simple explanatory analytical model capable of predicting the nature of the relationship between the momentum ratio, layer orientation and growth rate is developed. In this model, an eddy-like structure of circular geometry is assumed to exist. In an effort to model the existence of the externally imposed perturbation on the actual flow, the structure is given a finite but very small initial size, equal for all cases investigated. Subsequently it is convected downstream and it is allowed to grow by entrainment from the free streams. Its convective velocity and entrainment ratio are assumed to obey the empirical formulas of Dimotakis (eqs.(4.24) and (4.25)). It should be remembered that these formulas were found to be valid for all cases studied, both forced and unforced. Finally, and in order to satisfy the incompressible nature of the flow, the structure is given a cross-stream velocity which is determined by the amount of fluid it entrains from the two streams. In other words it is forced to move into the stream from which it entrains most.

The model configuration is shown in figure 4.15 which defines the geometry related symbols and it points to the fact that the structure is considered in a frame of reference moving with its convective speed. The implementation of the model is as follows: The structure convective speed and entrainment ratio are determined from the empirical formulas for the particular case of velocity and density ratio considered. The ratio of the distance of the center of the structure from the splitter plate axis (y_{cl}) to the structure radius (i.e. \( \frac{y_{cl}}{R} \)), is determined by relating the entrainment ratio to the ratio of the area of the structure above (A_T) and below (A_B) this axis, and by using the information provided by the circular geometry. i.e.

\[
E_v = \frac{A_T}{A_B} = \frac{\pi}{\cos^{-1}\left(\frac{y_{cl}}{R}\right)} - \frac{y_{cl}}{R} \sqrt{1\left(\frac{y_{cl}}{R}\right)^2} - 1
\]  

(4.27)
Due to the implicit nature of this expression for \( \frac{Y_{el}}{R} \), a Newton-Raphson scheme is used in its solution. The reasoning behind equation (4.27) is that, neglecting the initial volume of the structure (which by creation is small), then its downstream volume is only a manifestation of entrainment from the free streams. Since this is carried out under the specific entrainment ratio prescribed, the ratio of volume of the two fluids inside the structure should be equal to this entrainment ratio. Incompressibility then requires the structure to locate itself in such a way that the volume (area in 2-D) is preserved yielding the situation visualized in figure 4.15 and expressed in equation (4.27). The growth rate of the structure can then be obtained by considering its temporal growth rate \( \frac{d\delta}{dt} \) in the moving frame of reference and using

\[
\frac{d\delta}{dx} = \frac{1}{U_c} \frac{d\delta}{dt}
\]  

(4.28)

The temporal growth rate of the structure is related to the volume flowrate entering it, i.e. to the sum of the flowrates from the two streams. These, in turn, are assumed to be proportional to the extend by which the structure protrudes into each stream. (This type of assumption governing entrainment was first suggested in ref.[64] were it was used in the derivation of equation (4.25).) The resulting temporal growth rate is combined with equation (4.28) to yield

\[
\delta' = \frac{d\delta}{dx} = \frac{C}{\pi r_c} \left[ (1-r_c)(1+\frac{Y_{el}}{R}) + (r_c-r)(1-\frac{Y_{el}}{R}) \right]
\]  

(4.29)

where \( C \) is a constant. The presence of this constant, which is introduced via the entrainment assumption and requires empirical definition, implies that at this stage, the developed model cannot be used for quantitative predictions. It can, however, be used to determine trends in the behavior of the growth rate (if \( C \) is given an arbitrary value e.g \( C=1 \)) which is what is required in this study. The locus of the center of the structure (the layer centerline) can straightforwardly be obtained from the above quantities by recognizing that
\[ \delta(x) = \delta(x_o) + (x-x_o)\delta' \]  
\[ R(x) = \frac{\delta(x)}{2} \]  
\[ y_{cl}(x) = R(x) \left( \frac{y_{cl}}{R} \right) \]  

where \( x_o \) is the initial location of the structure.

Results from the model are shown in figure 4.16. In part (a) the growth rate versus the density and momentum ratios is displayed. The substantial qualitative similarity of this result with that of figure 4.14, exemplifies the controlling nature of the physical arguments used in the model. The growth rate experiences a minimum around momentum ratio unity and the increase in growth away from this region is more significant for large momentum ratios. The slight shifting of the minimum growth rate to lower momentum ratios can be attributed to the oversimplifying nature of some of the model assumptions, particularly that of the circular eddy geometry. In part (b) the layer centerline (orientation) is shown. In agreement to what was seen and discussed earlier the layer centerline shifts from the slow stream (\( y<0 \)) to the faster stream as the momentum ratio increases. The arrow at \( x=6 \) indicates the centerline location for the case which experiences the minimum growth rate in figure 4.16a. It is clearly seen that the minimum growth takes place close to the splitter plate axis (shown by the dotted line) which is in agreement with earlier discussions.

Thus the dependence of the forced layer growth rate on the momentum ratio has been explained and justified. The problem which then arises, it to explain why the unforced flow does not exhibit a similar behavior. Evidently, the answer to this question would have to deal with the introduction and initial evolution of the destabilization perturbation of the flow. Hence, it is here suggested that the momentum ratio related growth rate behavior is exhibited when a perturbation of fixed size is introduced at the same location in the flow for the different cases investigated. Under this approach the natural instability characteristics of the layer are bypassed. If the layer is not forced, on the other hand, these characteristics (which were presented in Section 4.4) determine the size and
location of the destabilizing perturbation. This leads to different initialization of the flow for different density ratios thus confusing the momentum ratio argument.

4.6. Conclusions

The Vortex and Transport Element Methods have been applied to study the effect of density variation and externally imposed forcing on the development of inviscid vorticity layers.

Computed results indicate that, in the absence of external forcing, density variation affects the development of the Kelvin-Helmholtz instability of the vorticity layer, both in its linear and non-linear stages. At fixed velocity ratio, the layer spreading rate and entrainment ratio increase with increasing density of the low speed stream. The phase speed of the (linear) Kelvin-Helmholtz wave, and the convective speed of the non-linear eddies which form following its maturation, decrease with increasing low speed stream density. For the inlet density and vorticity profiles considered, the eddy convective speed and phase speed of the linear instability waves almost coincide. The computed results are found to be in good agreement with experimentally obtained data and are explained in terms of the effect of baroclinic vorticity generation.

External, high-amplitude, in-phase forcing at the fundamental and subharmonic frequencies strongly influences the layer growth behavior while leaving the entrainment ratio and eddy convective speed behavior unchanged. For short downstream distances, external forcing leads to an earlier growth and maturation of the Kelvin-Helmholtz waves. The dynamics of the vortex interaction downstream of the rollup of the layer changes according to the momentum ratio. These interactions have strong effect on the orientation of the layer, whose centerline tilts towards the low-speed stream at low momentum ratio and gradually shifts upwards as the momentum ratio increases. Pairing of the eddies yields composite structures whose shape and size differ according to baroclinic vorticity generation. These mechanisms occur in such a way as to enhance the spreading rate of the
layer at low or high momentum ratios, and to substantially decrease the latter when the
momentum ratio is near unity. The layer orientation is related to its growth behavior and an
analytical model is derived based on this and other basic principles which explains the
numerically encountered behavior. It is proposed that the fact that the unforced layer does
not exhibit a similar behavior is a manifestation of the initial instability characteristics of the
flow which are bypassed in the forced layer case.
The forcing function

\[ f(t) = A_f \sin(2\pi f_t t) + A_s \sin(2\pi f_s t), \quad A_s = A_f, \quad f_s = \frac{f_t}{2} \]

Figure 4.1 The forcing function used to destabilize the flow and to promote eddy interactions. It represents the cross-stream distance by which elements are displaced at the inlet.
Figure 4.2 The spatial amplification rate (a) and wave phase speed (b) predicted by the two-dimensional linear stability theory. The curves are generated for a velocity ratio $r=0.5$ and various density ratios (indicated).
Figure 4.3. Geometry of the unforced layer with velocity ratio \( r = 0.5 \). The layer is represented by plotting the location of the vortex elements and their instantaneous relative velocity vectors with respect to the mean streamwise flow speed. The plots are generated at \( t = 10.5 \) for various density ratios (indicated) increasing from the top. The length of the computational domain \( X_{\text{max}} = 6 \).
Figure 4.4 The spatial growth rate of unforced variable density layers with velocity ratio $r=0.5$. The solid line represents the empirical formula suggested by Dimotakis for constant $r$. The numerical results are denoted by stars (*), while open circles (o) denote the suggested correction to the empirical formula based on the average $r$. 
Figure 4.5 The volumetric entrainment ratio (a), and eddy convective speed (b), for unforced variable density layers with velocity ratio $r=0.5$. The solid line represents the empirical formula suggested by Dimotakis for constant $r$. The numerical results are denoted by stars (*), while open circles (o) denote the correction to the empirical formula based on the average $r$. 
(a) The vorticity distribution within the fundamental eddy for $r=0.5$ and various density ratios. Solid (dashed) lines indicate negative (positive) vorticity. The domain represented is a square of side half the channel height ($H$) and the dividing horizontal line represents the position of the channel centerline.

(b) Streamline pattern for the fundamental eddy in the vorticity layer for $r=0.5$ and various density ratios. The domain represented is a square of side half the channel height ($H$) and the horizontal line indicates the position of the channel centerline. Plots are generated at the same streamwise coordinate position.

Figure 4.6
$$\dot{\omega}_b = a \times \frac{\nabla \rho}{\rho}$$

Figure 4.7 Schematic illustration of the effect of vorticity generation for the $s<1$ case. $\omega_0$ denotes the initial vorticity of the layer and $\omega_b$ the vorticity generated by the baroclinic torque. $\nabla \rho$ is the density gradient, $a$ the material acceleration and $U_c$ the eddy induced speed due to the presence of $\omega_b$. 
Figure 4.8 The location of the vortex elements and their instantaneous relative velocity vector with respect to the mean streamwise flow speed for forced vorticity layers, with velocity ratio $r=0.5$ and various density-momentum ratios (indicated) increasing from the top. The plots are generated at $t=18.5$ and the length of the computational domain $X_{max}=5$. The arrows indicate the streamwise location of the formation of the first eddy following the rollup of the instability.
Figure 4.9 The volumetric entrainment ratio (a), and eddy convective speed (b), for forced variable density layers with velocity ratio $\tau=0.5$. The solid line represents the empirical formula suggested by Dimotakis for constant $\tau$. The numerical results are denoted by stars (*), while open circles (o) denote the correction to the empirical formula based on the average $\tau$. 
Figure 4.10 The spatial growth rate of forced variable density layers with velocity ratio $r=0.5$. The solid line represents the empirical formula suggested by Dimotakis for constant velocity ratio, $r$. The numerical results are denoted by stars (*), while open circles (o) denote the suggested correction to the empirical formula based on the average $r$. The dashed line indicates the trend suggested by the numerical results.
Figure 4.11 The location of the vortex elements and their instantaneous relative velocity vector with respect to the mean streamwise flow speed for forced vorticity layers with velocity ratio \( r = 0.625 \) and various density-momentum ratios (indicated) increasing from the top. The plots are generated at \( t = 18.5 \) and the length of the computational domain \( X_{\text{max}} = 5 \).
Figure 4.12 The location of the vortex elements and their instantaneous relative velocity vector with respect to the mean streamwise flow speed, for vorticity layers with the same velocity, density-momentum ratios to those of figure 4.11 but without external forcing. The plots are generated at t=8.5 and the length of the computational domain X_{max}=6.
Figure 4.13. Sequences of typical vortical structure interactions for the forced vorticity layers of figure 4.11 (r=0.625, s=0.427, 2.56, 15.4 arranged from top). The times and streamwise locations ($x_o$) of the interactions are indicated.
Figure 4.14 The spatial growth rate of forced variable density layers with velocity ratio $r=0.625$. The solid line represents the empirical formula suggested by Dimotakis for constant $r$. The numerical results are denoted by stars (*), while open circles (o) denote the suggested correction to the empirical formula based on the average $r$. The dashed line indicates the trend suggested by the numerical results.
Figure 4.15 The geometric and flow configuration on which the model predicting the forced layer growth behavior is based. The square box indicates the moving frame of reference and the circle models the coherent flow structures. Symbols are as defined in the text.
Figure 4.16 Results of the simple analytical model for the forced layer spacial growth rate (a), and for the corresponding layer centerline (b). In (a) (*) indicate the model results and the dashed line the trend suggested by them. In (b) the horizontal arrow at x=6 indicates the centerline location for the case which experiences the minimum growth rate in (a).
5. THE EXOTHERMICALLY REACTING SHEAR LAYER

5.1. Introduction

Post-transitional exothermically reacting shear layers are commonly present in many combustion systems. The flow, which is a manifestation of the growth of the instability of the shear region between two reacting fluids at different velocities represents an important mechanism by which reactants mix and burn, in such systems. Experimental [e.g. 6] studies indicate that the vortical structures which dominate non-reacting shear layers (see Chapter Three) persist in their reacting counterparts despite the substantial effects of the combusting field on the flowfield. These structures are found to coincide with the region where product exists, thus exemplifying their fundamental importance to the combustion process. Combustion, in turn, strongly influences their evolution and interactions via the release of chemical energy and the resulting variable density field.

The effects of the combustion heat release and of the related variable density field on the flowfield have been the subject of significant interest recently. As was seen in the previous chapter, even in the absence of reaction the presence of a variable density field substantially alters the properties of the flow, modifying the growth of the mixing region the entrainment from the free streams and the unsteady evolution of the eddies. Experimental studies [4-6] have indicated that in the presence of an exothermically combusting field the shear layer growth is reduced, resulting in diminished efficiency of mixing and burning. This was initially a rather surprising finding since combustion was anticipated to increase the size of the mixing region via volumetric expansion. Numerical studies [16,17,25] of temporally evolving reacting shear layers, have, to some extend, been able to reproduce this behavior. But the substantial limitations of the temporal layer model, discussed in Chapter One, fundamentally limit the generality of its results and of its predictive capability, particularly for reacting flows. Spatially evolving shear layer numerical studies [22,23], which attempt a much more physical description of the flow, have, on the other hand, been restricted to cases where the effects of combustion on the
flowfield are negligible (low combustion heat release). Such studies have been used to discern the structure of the reaction zone and the effects of the reaction speed (Damkohler number) on the relative location of the reaction zone with respect to the large structures. It was concluded that at small Damkohler number, the reaction is most intense near the center of the large eddy, while as the Damkohler number increases, the reaction zone moves outwards towards the outer edges of the eddies. It was also found that, under conditions of unity stoichiometry, a strong similarity exists between the products concentration field and the vorticity field.

In this work a numerical simulation of the spacial shear layer at significant combustion heat release is carried out. The dynamical effects of the heat release on the flow are studied in detail with the aim of determining the mechanism(s) by which the resulting variable density field reduces the growth of the shear layer. In particular, the mechanisms of volumetric expansion and baroclinic vorticity generation are closely investigated to establish their effect on the flowfield. Of prime importance is to determine whether the reduced growth is a result of a delay in the flow instability or of an actual reduction of the size of the vortical structures, or both. As was seen in the previous chapter, high amplitude external forcing can be used to bypass the natural stability characteristics of the layer and to alter its growth behavior. Thus, the stabilizing effects of the combustion heat release on the flow, as well as the latter's diminished downstream growth are susceptible to manipulation by such forcing. Hence, in this work the spacial shear layer is studied under both unforced and forced destabilizing conditions.

The VEM and the TREM are used in the simulations. The details of the formulation and numerical schemes were presented in Chapters Two and Three.

5.2. Geometry, Boundary and Initial Conditions

The geometry considered for the reacting shear layer is the same as that presented in Chapter Three and used in Chapter Four; i.e. the shear layer evolves in a two dimensional
channel of height $H$ and length $X_{\text{max}}$, between two parallel streams (1-top, 2-bottom) which mix downstream of a thin splitter plate (see figure 3.5). The same is true for the boundary conditions except for those of the scalar field at the inlet. These latter conditions were not specified in Chapter Three and are, hence, given here. They are required for the two Shvab-Zeldovich (S-Z) variables ($\lambda = Y_1 - \phi Y_2$, $\gamma = T + \frac{Q_0 \phi}{1 + \phi} Y_p$) and, in the case of finite speed of reaction, for the product mass-fraction as well (variables integrated by the numerical scheme). They are summarized below, together with the velocity-vorticity inlet profiles which are provided for completeness.

Velocity

$$U(x=0,y,t) = \frac{U_1 + U_2}{2} + \frac{U_1 - U_2}{2} \text{erf}\left(\frac{y-0.5}{\sigma}\right)$$

(5.1)

Vorticity

$$\omega(x=0,y,t) = \frac{U_1 - U_2}{\sqrt{\pi} \sigma} \exp\left(-\frac{(y-0.5)^2}{\sigma^2}\right)$$

(5.2)

S-Z variables

$$\lambda(x=0,y,t) = \frac{1 - \phi}{2} + \frac{1 + \phi}{2} \text{erf}\left(\frac{y-0.5}{\sigma}\right)$$

$$\gamma(x=0,y,t) = 1$$

(5.3a,b)

S-Z gradient

$$\nabla \lambda(0,y,t) = (0, \frac{\partial \lambda}{\partial y}(0,y,t))$$

$$\nabla \gamma(0,y,t) = (0,0)$$

(5.4a,b)

with

$$\frac{\partial \lambda}{\partial y}(x=0,y,t) = \frac{1 + \phi}{\sqrt{\pi} \sigma} \exp\left(-\frac{(y-0.5)^2}{\sigma^2}\right)$$

(5.5)

Product

$$Y_p(x=0,y,t) = Y_{p_{\text{max}}} \exp\left(-\frac{(y-0.5)^2}{\sigma^2}\right)$$

(5.6)

In the above profiles, as well as in the numerical simulations, the channel height is used as the space non-dimensionalizing scale. $\sigma$ is the standard deviation of the Gaussian profiles defining the inlet vorticity, gradient of the $\lambda$ variable and the product mass-fraction. Its relation to the scaling length ($H$) is given in a similar fashion to that described in Chapter Four: two wavelengths of the most unstable mode of the uniform density shear layer are required to fit within the channel height so that the channel can have the capability of
accommodating a paired eddy. Finally, it is noted that in the numerical simulations the velocity field is scaled with the top stream velocity \(U_1\) whereas the density and temperature fields by the common to both streams (see next paragraph) values of these properties \((\rho_o, T_o)\).

The profile for the \(\lambda\) Shvab-Zeldovich variable is obtained by assuming that each of the two fluid streams consists of a single reactant (i.e. \(\lambda_1=1, \lambda_2=-\phi\)) which at the inlet experiences an errorfunction type profile. (It should be noted that simulations for dilute reactants can straightforwardly be achieved by modifying this profile and accounting for the dilutant in the equation of the conservation of the mass-fractions (eq.(2.6))). Profiles of this type are not unlike the experimentally observed profiles for the two reacting species. For the \(\gamma\) Shvab-Zeldovich variable, the assumption is made that the temperature and product mass-fraction profiles are directly related, yielding a constant value profile. Under the behavior imposed by the governing equations such an assumption is valid for flows which prior to combustion were of uniform temperature and in which no product was present; a very physical and common condition.

In order to avoid having to deal with ignition phenomena at the inlet for the finite reaction speed case (note the temperature dependent nature of the reaction rate (eq.2.7))), a finite amount of product is introduced there. This is described by the Gaussian profile given above (eq.(5.6)) where \(Y_{P_{\text{max}}}\) is chosen as 0.4. The direct relation of the product mass-fraction and the temperature implies that the temperature at the inlet is raised and hence combustion becomes possible. In the infinite reaction speed case where reactants react on impact, ignition problems do not exist and the inlet product mass-fraction profile is uniquely defined by the Shvab-Zeldovich variables as explained in Chapter Two (eq.(2.9)). Hence, the scalar field inlet profiles specified above which are used in the numerical simulation of the flow, specify the inlet species profiles shown in figure 5.1. The related temperature and density profiles can straightforwardly be deduced from the product mass-fraction profile as earlier explained.
Initialization of the simulation is also carried out in accordance to the description given in Chapter Three. The vorticity layer between the two fluids, assumed to be initially flat, is discretized by distributing vortex-transport-product elements over nine material layers (lines) lying within the support of vorticity. The elements are of square area of side h=0.0195. Via the assumption that the inlet conditions persist throughout the domain the element discrete vorticity and λ gradient values are readily obtained from equations (5.2) and (5.5) respectively. The value of the core radius (δ) is found by the procedure described in Chapter Three and is δ=0.0234 (i.e.δ>h).

Finally, and as already pointed out, in some of the numerical simulations external forcing is implemented at the inlet. In the absence of forcing the evolution of the layer reflects the amplification of numerically-excited instability waves, resulting in the "natural"-unforced layer behavior. The forcing signal implemented in the forced layer case is very similar to the one used in Chapter Four to force the non-reacting variable density layer (see figure 4.1). It still consists of in-phase components of the most unstable mode of the uniform density layer and its subharmonic, but in this case a higher amplitude is assumed for both frequencies, i.e. A_f=A_s=0.025. The interaction of the two forcing frequencies gives rise to two types of eddies. The eddy which forms during the part of the cycle which the two components are in phase - the "fundamental" eddy - is larger than the one which forms in the second part of the subcycle - the "subharmonic" eddy - during which the two components are out of phase. As before, forcing is implemented by displacing elements at the inlet according to the forcing signal.

5.3. Numerical Results

Numerical simulations were carried out for both forced and unforced reacting shear layers with the aim of studying the dynamical effects of the combustion heat release. The bulk of the calculations were executed for forced layers and they included both finite and infinite reaction speed calculations. For unforced layers only infinite reaction speed
calculations were performed. The reason for this approach is that the forced flow, at least at its early stages, is highly repetitive and it thus allows better comparison between the various cases simulated. Analysis of the forced layer simulations (see Section 5.3.2) also shows that for the parameters used here, the effect of the reacting field on the flowfield is qualitatively similar for the finite and infinite reaction cases. This, together with the substantially smaller computational cost of the infinite reaction speed version of the numerical scheme (TREM reduces to TEM, see Chapter Three) motivated the latter's exclusive use for the unforced flow simulations. The time step for all calculations was $\Delta t=0.1$ while the length of the domain was varied between the values of $X_{\text{max}}=8$ and 5 for the unforced and forced cases, respectively. The shorter domains used for the forced cases are a manifestation of the fact that in these cases the destabilization of the flow takes place closer to the inlet due to the external forcing.

The fluid dynamical governing parameters were kept constant for all runs. The inlet velocity ratio is $r=\frac{U_2}{U_1}=0.5$ and the Reynolds number (and Peclet number since $Pe=Re$) based on the velocity difference across the layer ($\Delta U=U_1-U_2$) and on the vorticity layer's original thickness ($d=2\sigma$) is $Re=\frac{\Delta U d}{\nu}=500$. It should be noted that the Reynolds number could have also been defined with respect to the channel height $H$, since, as was earlier explained, $H$ is characteristic of the largest cross-stream scale of the layer. The resulting Reynolds number is $Re=\frac{\Delta U H}{\nu}=6400$. The chemical parameters (see Chapter two for definitions) were also kept constant with the exception of the enthalpy of reaction. The activation temperature is $T_a=\frac{E_a}{RT_o}=10$ the frequency factor $A_f=\frac{A_r H}{\Delta U}=100$ ($A_f=\frac{A_r H}{\Delta U}=1280$) and the mass stoichiometry ratio $\phi=1$. The non-dimensional enthalpy of reaction $Q_o=\frac{Ah_r}{cp T_o}$ (referred to in this text as "heat release") was varied between the values of 4 and 6. For the finite reaction speed calculations the corresponding Damköhler number ($Da=\frac{\tau_{\text{diff}}}{\tau_{\text{che}}}$ where $\tau_{\text{diff}}=\frac{d^2}{\alpha}$ is the diffusion time scale and $\tau_{\text{che}}=\frac{T_f}{A_f \exp(T_a/T_f)}$ the chemical reaction time scale) and the Karlovitz number ($Ka=\frac{\tau_{\text{che}}}{\tau_{\text{flw}}}$ where $\tau_{\text{flw}}=\frac{d}{\Delta U}$ is the flow time
are $Da = 595, 1026$ and $Ka = 0.84, 0.49$, respectively [$Da_H = 97414, 168110, Ka_H = 0.066, 0.038$]. While the values of these non-dimensional numbers are not far from physically realistic values the same is not necessarily true of the parameters used to create them. Specifically, the values of the activation temperature and the frequency factor, while higher than those used in previous work [25] are still quite low. The limitations on the values of these parameters are imposed by the numerical solution of the flow. Increases in the frequency factor yield higher reaction speeds thus requiring higher temporal resolution of the flow. Increases in the activation temperature, on the other hand, diminish the reaction zone size, which implies a higher spacial resolution. Both of these effects increase the computational cost of an accurate numerical solution overwhelmingly.

To assess the dynamical effect of the combustion heat release, the reacting calculations were repeated but this time the effects of the variable density field on the fluid dynamical field were ignored. That is, while the density was allowed to vary due to combustion, the density used in the evolution of the flowfield was kept constant and equal to its inlet value. Since, under the assumptions of our model, the variation in the density field is the only means by which the reacting field can influence the flowfield, then by keeping the flow density invariant the flowfield remains ignorant of the presence of the reacting field. While this approach might not be the most physically intuitive one, it is the one which isolates the dynamical effects of the heat release on both the flowfield and the reacting field to the greatest degree and allows their most detailed study.

The difficulty of choosing the relevant comparison case to study the dynamical heat release effects has been recognized before [66]. The usual approach is to compare cases with and without heat release. This is fine in the case where the reaction rate is chosen to be temperature independent [17]. In such a case, setting the heat release equal to zero will have no direct effect on the speed of the reaction. The reacting field is hence changed only via the altered flowfield. When a more physical, temperature dependent reaction rate is employed (e.g. an Arrhenius type rate), changing the heat release will not only alter the
flowfield, it will also have a direct chemical effect on the reaction rate (it basically alters the chemical reaction). This is manifested through the altered temperature field \( v \). A h is strongly linked to the heat released. Thus, a dual effect on the reactive field is experienced. Furthermore, setting the heat release to zero in such a case will not only decouple the flowfield from the reactive field, it will also terminate the reaction. A way around this latter problem was employed in ref [66] where the initial-global temperature was raised so that the sensitivity of the reaction rate to the temperature field was diminished (by lowering the activation temperature). In this case the reaction is not terminated, but the reaction speed is nevertheless altered. Hence, the dynamical and chemical effects of changing the heat release on the reacting field become indistinguishable, making cause-and-effect conclusions exceedingly difficult. To avoid this problem, in this work the chemical parameters were kept constant for the comparison cases and the decoupling of the flowfield from the reacting field was simply achieved by eliminating the effect of the variable density field on the flowfield. Note that the density was not assumed to be constant for both fields (i.e. in effect using a different equation of state where temperature and density are decoupled) because the density field itself contributes to the reaction and arbitrarily changing it would result in altered combustion characteristics. Thus any changes in the reacting field can be attributed to the modified flowfield. Once the dynamical effects of heat release have been established, then the more complex problem presented by the different heat release cases can be tackled.

In what follows the cases where the flow and combusting fields are decoupled in the manner described above, will be termed as the "uniform flow-density" cases. Evidently, as far as the flow is concerned these cases are indistinguishable from uniform density non-reacting calculations. Hence, in the analysis of the flowfield they will occasionally be treated as such. For the scalar field on the other hand these cases differ from uniform density calculations and hence they will be properly distinguished.
5.3.1. The Unforced Layer

Simulations of unforced, spatially developing, reacting shear layers at infinite reaction speed with and without incorporation of the effects of the combustion related density field on the flowfield were carried out at a single value of the heat release, $Q_o=4$.

Figure 5.2 displays a flowfield comparison of the two cases. The shear layer is depicted using the vortex elements and their local velocity vectors. The velocity is plotted with respect to the inlet mean velocity to highlight the relative motion within the layer. It is seen that in agreement with experimental observation, the flow, in both cases, is dominated by large scale coherent vortical structures. Their formation is a result of the destabilization of the initially flat vorticity region-layer existing between the two fluid streams, via the amplification of the Kelvin-Helmholtz instability and the subsequent non-linear rollup of the layer around itself. The figure also makes clear that density variation resulting from the combustion heat release significantly modifies the flowfield and causes a decrease in the layer growth. This appears to be a consequence of two effects: (i) A substantial delay in the onset of the flow instability, and (ii) an alteration of the evolution and interactions of the eddies.

For the uniform density case, the layer prior to rollup appears thinner than its variable density counterpart. Upon rollup its eddies also appear more rolled and coherent. Their interactions, further downstream, are by pairings i.e. the amalgamation of two eddies into a larger coherent structure initiated by the clockwise spiraling of these eddies around each other. For the variable density case, on the other hand, these pairings appear suppressed. Rather, the growth of the vortical structures is manifested by increases in size-volume of single eddies.

The effects of these instantaneous flow dynamics on the mean (time-averaged) behavior of the flow are shown in figures 5.3 and 5.4 where the vorticity thickness ($\delta_\omega$) and product thickness ($\delta_{pp}$) are shown, respectively. The vorticity thickness is defined with respect to the local free streams as
\[ \delta_{\omega} = \frac{U_1(x) - U_2(x)}{\left( \frac{\partial \bar{u}}{\partial y} \right)_{x, \text{max}}} \]  

(5.7)

where the overbar indicates a time-averaged property. Hence, this quantity is representative of the spatial cross-stream thickness of the layer. Figure 5.3 is in close agreement with the above described characteristics of the instantaneous behavior of the flow. Close to the inlet and before rollup the variable density case exhibits a slightly larger thickness to that of the uniform density case. This trend in the vorticity thickness profile is quickly reversed as the delay in the flow instability and the modification of the eddy evolution result in a smaller thickness for the variable density case. Close to the exit the vorticity thicknesses of the two cases tend to converge. This effect, though, is suspected to be a manifestation of the presence of the channel walls. This is because by this point in the evolution of the flow (i.e. the layer thickness is comparable to the channel height) the walls are expected to have a much more significant effect on the uniform density layer where growth is by eddy pairings than on the variable density layer where growth is by increase of eddy volume. As will be explained later (see Section 5.3.2) this eddy volume increase is not primarily due to entrainment of fluid from the free streams, but due to the expansion related with the combustion heat release. This latter effect is expected to be much less sensitive to the presence of walls as compared to the flow kinematics involved in an eddy pairing (i.e. clockwise spiraling of eddies around each other is physically obstructed by the walls).

The definition of the product thickness shown in figure 5.4 conforms to a more general definition of a scalar thickness which will be used throughout this discussion and is:
where in this particular case \( \Phi \) is the product density \( \rho_p = \rho Y_p \). Hence the product thickness is representative of the mass of product at a given channel cross-section. In figure 5.4 the product thickness of the variable density case is contrasted to two versions of the thickness of the comparison, uniform flow-density, case. It should be remembered that the comparison case is created by simply decoupling the density of the flowfield from the density of the reacting field which is allowed to vary. It should be recognized though, that while using a variable density in the determination of the reacting field is beneficial for the reasons given earlier, its use in the calculation of the mass of product, practically eliminates the effect of the change of volume from this latter quantity. Thus the comparison between the variable density and the uniform flow-density cases does not necessarily provide a measure of the relative difference in mass of product but rather it is more indicative of the relative size of the areas where product exists. For this reason the calculation of the product thickness for the uniform flow-density case is repeated using the uniform inlet density for the reacting field as well. This thickness is also shown in figure 5.4.

The figure is in general agreement with the behavior described in both, the instantaneous flowfield comparisons and the vorticity thickness. The delay in the flow instability as well as the modification of the eddy evolution in the presence of a variable density field result in a reduced mass of product downstream, hence diminishing the efficiency of burning. The effects of the walls close to the exit are also noted.

Hence, in this section it was shown that the numerical results are in agreement with experimental evidence and indicate diminished layer growth and amount of product formed in the case where heat release is allowed to modify the flowfield. Explanations for this behavior are difficult to clearly ascertain in the unforced case where the flow behavior is not
repeatable and does not allow direct comparisons between the flow features at the various stages of the flow. This, on the other hand, can be achieved when external forcing is implemented. Hence, in what follows, the study of the forced, exothermically reacting layer is used to determine the mechanisms by which density variation resulting from the combustion heat release modifies the flowfield. Understanding of these mechanisms is then used to provide explanations for the unforced layer behavior as well.

It should finally be noted that the study of the forced layer is also strongly motivated by the above seen significant effect of the combustion heat release on the initial instability of the flow. In a forced flow this effect is bypassed. Hence a study of the forced reacting shear layer can yield crucial information on the effect of the instability suppression and on whether the decrease in both the shear region size and amount of product formed can be reversed via external forcing.

5.3.2. The Forced Layer

Forced layer simulations were carried out for both finite and infinite reaction speed for the two values of the combustion heat release, $Q_0= 4$ and 6. The results are used both in a study of the dynamical effects of the combustion heat release on the flow and reacting fields, and in a comparison of the finite and infinite reaction speed models. In what follows, the finite reaction speed results are analyzed first. Subsequently the infinite reaction speed results are presented.

5.3.2.1. Finite Reaction Speed

5.3.2.1.1. Effect of the Heat Release on the Flowfield

5.3.2.1.1. Flowfield Description

Figure 5.5 displays a flowfield comparison between the uniform density layer and the variable density layer for which the heat release is $Q_0= 4$. The shear layer is depicted
using the vortex elements and their local velocity vectors, in a similar fashion to figure 5.2. To describe the evolution of the flowfield in time, three sequential time frames are shown.

It is seen that in both cases the flow is dominated by large scale coherent vortical structures. This was an anticipated finding, given the earlier noted presence of these structures in the unforced flow. While, as expected from previous experience [62.63], the external forcing results in a highly repetitive flowfield in each case, comparison between the two cases yields major differences. The figure clearly shows that density variation resulting from the combustion heat release, significantly modifies the flowfield by altering the shape, evolution and interactions of the vortical structures. As a result, dampening of the shear layer growth, earlier seen in the unforced flow, is experienced for the forced flow as well. During the initial rollup, the fundamental eddies appear less rolled and larger in overall size (area) than their uniform density counterparts. This increase in size though, appears to be mainly in the streamwise direction resulting in more elongated, more elliptical structures. Similar features are experienced by the subharmonic eddies which, additionally, appear much less coherent. Further downstream, where the eddies start to interact, major differences are experienced. In the uniform density flow, each subharmonic eddy interacts with its downstream fundamental eddy. The two, pair (by spiraling towards each other in a clockwise direction) to form a larger, coherent and highly elliptical structure which continues to rotate, exposing its major axis to the streamwise flow. This results in significant growth of the shear layer. When the density variation is accounted for, this process is fundamentally altered. Eddy pairing is resisted and the subharmonic eddy appears to be torn between its two neighboring fundamental eddies in a much more continuous process than pairing. (It should be noted that this type of behavior is in agreement with that of the unforced flow where a suppression of the pairing process was experienced.) The downstream fundamental eddy is still the one which absorbs most of the torn subharmonic eddy. This results in downstream structures with more dominant upper sides (close to fast stream). In addition, these structures appear less elliptic and coherent
than before and they tend to keep their major axis more aligned with the streamwise direction. This impairs the layer cross-stream growth significantly. As a final point, it is noted that in the regions between the eddies, even after complete tearing of the subharmonic eddy, the braids are thicker for the variable density case.

Figure 5.6, which displays a single time frame comparison between the uniform density case and the two different heat release cases ($Q_o=4$ and $6$), reveals further information about the flowfield. It is noted that the features of the $Q_o=4$ case described above, are experienced by the $Q_o=6$ case as well, but to a greater extent. Tearing of the subharmonic eddies occurs earlier and the fundamental eddies are larger, less coherent and more streamwisely elongated. Further downstream, the larger structures keep their major axis more aligned with the streamwise direction and their cross-stream asymmetry is more pronounced. The thickness of the braids is notably increased. But the figure reveals another point which on more careful inspection can also be seen in figure 5.5. The vortical structures appear to accelerate in the streamwise direction as more heat is released. This is seen in both their altered locations as well as their enhanced local velocity vectors: Compare, for example, the eddies indicated by arrows which were formed during the same subcycle of the forcing function.

Figures 5.7 and 5.8 offer further evidence of some of the major comments made above. In figure 5.7 the mean velocity profiles (at a fixed downstream location ($x=3$)) for the three cases of figure 5.6 are plotted against the cross-stream coordinate. The characteristics of the profiles shown, are qualitatively typical of most downstream locations within the computational domain. The steepening of the profiles with increasing heat release, which suggests smaller shear layer growth, is obvious. The shifting of the profiles to higher speeds, which was earlier suggested by the faster moving structures, is also noted. This shifting does not appear to be uniform across the channel (different effect on fast and slow streams), the non-uniformity being a function of the heat release. Thus, the velocity ratio across the layer is not constant but is weakly varying with distance and heat
release. It is interesting to note that with the presence of heat release -variable density- the mean velocity profile loses its monotonic nature, typical of uniform density shear layers. Instead, close to the fast free stream an overshoot, and close to the slow free stream an undershoot of the respective neighboring free stream values are experienced. This type of features of the mean velocity profile were also documented in ref.[17] for a reacting temporal shear layer and were attributed to the presence of the baroclinic generation of vorticity. Evidence supporting this argument was also provided in the earlier simulations of non-reacting variable density shear layers (see Chapter Three), where similar types of overshoots and undershoots were experienced.

In figure 5.8 the vorticity thickness (eq.(5.7)) is plotted versus the streamwise coordinate. (It should be pointed out that the definition of the vorticity thickness used here is not necessarily impaired by the non-monotonical nature of the velocity profile since the overshoots-undershoots are small (<2%ΔU). An alternative definition of δω from the points of the mean velocity profiles where the velocity varies by 5% of the free-stream value -i.e. the typical experimental approach- would give rise to similar results since the overshoots-undershoots would not be detected.) As expected, a drop in the vorticity thickness growth with increasing heat released is experienced for most of the domain. But, additionally, it is seen that close to the inlet quite the opposite is true. And for about half the computational domain the Qo=6 case exhibits more growth than the Qo=4 case. This type of behavior which is not unlike the one seen in the unforced flow, was also encountered in ref.[17] and was attributed to the expansion accompanying the changes in density. It is also seen that the largest drop in the growth of the vorticity thickness between the uniform density and the variable density cases occurs in the part of the domain where interactions of vortical structures take place. Thus, the modification of these interactions represents the most important mechanism by which heat release decreases the forced shear layer growth.
5.3.2.1.1.2. Density Field Description

Since the effect of combustion on the flowfield is felt solely via the resulting variable density field, one should be able to provide explanations for the various phenomena described above, through knowledge of the density field and the mechanisms by which this field influences the flowfield. Thus, while a detailed analysis of the reacting-scalar field is presented in Section 5.3.2.1.2, at this point some general information about the density field is presented.

Figure 5.9 presents the typical downstream (x=4) mean density profiles for the two different heat release cases considered. The profiles, which are Gaussian-like in shape, clearly indicate that the density decreases within the mixing region. The drop increases with increasing heat release - and hence, increasing temperature - but the spacial thickness of the profile can experience the opposite trend (a result of the decreased mixing seen in the decreased vorticity thickness).

To establish the overall effect on the density field, the "mean" density across the channel as a function of the streamwise direction is shown in figure 5.10. The definition of the "mean" density used here, conforms to the definition of a scalar thickness given earlier (eq.(5.8)) with \( \Phi=\rho \). The continuous decrease of the density thickness for both cases of figure 5.10 represents indirect evidence of the ongoing combustion and of the associated heat released. The figure also clearly shows that throughout the computational domain the higher heat release results in a lower density thickness.

Figure 5.11, which presents instantaneous two-dimensional plots of the temperature field for the case of \( Q_0=4 \) and for the corresponding uniform flow-density case, offers more detailed information on the nature of the variable density field (\( \rho=1/T \)). It is clearly seen that the region of variable density is strongly related to the region where vortical structures exist. As will be seen later, this is due to the fact that these structures represent the primary region of mixing of the two reactants and are, hence, the place where combustion can and does takes place. But the plot also provides the indication that
significant phenomena take place at scales smaller than those of the large scale vortical structures. It appears that the density variation is more closely related to the rollup of a material layer initially positioned between the two reactants, which, under the assumptions of our model, coincides with the vorticity layer mentioned earlier. The density experiences a minimum at the viscosity of this layer suggesting that the latter represents the region where most burning has taken place. Thus as a preliminary conclusion one can claim that the rollup of this layer represents the prime mechanism by which the reactants mix and burn. As will be seen in subsequent sections, analysis of both the reacting and flow fields can best be accomplished by considering the evolution of this layer.

5.3.2.1.1.3. Instantaneous Flow—Vorticity Dynamics

The equations of fluid motion suggest that the above described variable density field can influence the flowfield in a number of ways. Mass conservation (continuity) implies that the decrease of the density due to combustion causes volumetric expansion (flow divergence). Since the flow is confined, this increase in fluid volume causes a streamwise increase in the velocity field. This was seen in the shift of the mean velocity profiles of figure 5.7 which was also related to the increasing speeds of the vortical structures. (It should be noted here, that as will later be seen, the acceleration of the vortical structures downstream is not only due to volumetric expansion.) The increase of the shift with heat release should be expected since the drop in density is correspondingly larger. In figure 5.12, two-dimensional maps of the volumetric expansion for both \( Q_0 = 4 \) and 6 are shown. (The figure only displays positive values of divergence. Slightly negative values, which are the result of diffusion -cooling-, were artificially eliminated.) It can clearly be seen that, in general, both the intensity and locus of volumetric expansion differ between the two cases. As should be expected, the intensity is higher for the \( Q_0 = 6 \) case since the density variation is greater in this case. The regions where expansion is significant appear to shift, at least in the later parts of the domain from around the cores of the vortical structures (\( Q_0 = 4 \)), towards the braids (\( Q_0 = 6 \)). This provides an explanation for the substantially
thicker braids of the $Q_0=6$ case. As will be explained later (in the analysis of the reacting-scalar field) this shift is related to the change in the speed of the chemical reaction between the two cases which is introduced via the change of the heat release. It is also important to note that expansion in the cores of the vortical structures is minimal. This is an important feature because it provides some evidence why the structures are able to survive the combustion process. The two heat release cases appear much more similar in the very early parts of the domain where the expansion field is continuous and tends to follow the evolution of the material-vorticity layer. The inlet scalar profiles are such that they enable a zone of premixed, partially burned, reactants between the two streams. Enhanced combustion due to the presence of this region is the predominant reason for the increased divergence there. This significant volumetric expansion and the absence of significant rollup close to the inlet are the reasons why the vorticity thickness (fig. 5.8) tends to increase with heat release in this part of the domain. Further downstream, while expansion continues to be present, the evident dampening effects of the variable density field on the instability of the layer are much more significant, resulting in a decrease in the overall growth. In order to analyze these effects the rest of the equations of motion need to be considered.

The momentum conservation equations imply that the variable density field alters the material acceleration and the related pressure field in a non-trivial way. A better understanding of these effects can alternatively be achieved by considering the equation governing fluid rotation, the vorticity equation. Major motivation for this approach is offered by the highly rotational nature of the flowfield. This is exemplified by the already noted essential role played by the vorticity-material layer, its destabilization and rollup into large scale vortical structures. Understanding of its evolution, which is essentially governed by vorticity dynamics, appears to be an intuitive approach to analyze the flowfield.
The vorticity equation for this flow which was given earlier (eq.(2.14) or (3.1)) and is repeated here, i.e.

$$\frac{d\omega_k}{dt} + (\nabla \cdot \mathbf{u}) \omega_k = \frac{\nabla \rho \times \nabla p}{\rho^2} + \frac{1}{Re} \nabla^2 \omega_k$$  \hspace{1cm} (5.9)$$

implies that in a 2-D variable density field, the vorticity of a Lagrangian fluid element is modified by three different mechanisms. Volumetric expansion \((\nabla \cdot \mathbf{u}) \omega\), baroclinic generation \(\frac{\nabla \rho \times \nabla p}{\rho^2}\) and viscous diffusion \(\frac{1}{Re} \nabla^2 \omega\). In an exothermically reacting field like the one considered here, \(\nabla \cdot \mathbf{u}\) is generally positive. This implies that volumetric expansion is expected to decrease the element's vorticity. More information about this term can be obtained from its earlier noted absence from the circulation equation (see Chapter Three, eq.(3.14)). This is a result of the term's conservative nature and indicates that a Lagrangian fluid element under volumetric expansion (area expansion in 2-D), will experience a decay in vorticity which is equal and opposite to its increase in area, so that its circulation (or equivalently its angular momentum) remains constant. Pursuing this argument further, it is realized that the inability of volumetric expansion to alter the flow angular momentum, combined with the absence of the action of external body forces (and hence, torques) implies that the overall flow angular momentum should remain invariant. In other words, in this flow, combustion cannot alter the overall circulation. Finally it is noted that the expansion term in itself cannot change the sign of vorticity (direction of rotation) of the fluid element. It only decreases its absolute value (slows rotation down).

Baroclinic vorticity generation, on the other hand, which, as the corresponding term suggests, arises from misaligned pressure and density gradients, is capable of producing vorticity of either sign. A more fundamental explanation of the origin of the baroclinic term can be obtained by recognizing that the pressure gradient is mainly a manifestation of the fluid acceleration (see eq.(3.14)). Thus, the baroclinic term implies that rotationality (vorticity) results as neighboring regions of the fluid element experience differential
accelerations as a result of their different density. Because of its directional nature, baroclinic vorticity generation is strongly linked to the geometrical features of the flowfield. Hence, in order to understand its effect on the flowfield, the shape-geometry of the vorticity layer becomes crucial. This was clearly indicated in the study of baroclinic vorticity generation in the non-reacting variable density shear layer (Chapter Four) where kinematical arguments of the layer's evolution were used to determine the effect of baroclinicity on the flow.

The viscous diffusion term, as is commonly understood, acts to smooth the variation of vorticity in the flowfield. If the vorticity field is only of one sign, this term, like the expansion term, cannot on its own alter this sign. It should be noted though, that in a flow such as the one simulated here, where the viscosity is low, viscous diffusion is expected to have a marginal effect. Rather, the primary mechanisms by which the vorticity of a fluid element is expected to change are those of volumetric expansion and baroclinic vorticity.

Figure 5.13 presents the vorticity contours for the case where $Q_b=4$. Dotted lines indicate positive vorticity. As expected, the correlation with the vortical structures is evident. The field is seen to consist mainly of negative vorticity with islands of positive vorticity surrounding the vortical structures. The origin of the overwhelmingly negative vorticity field should come as no surprise since the inlet vorticity is negative (top stream is fastest, resulting in clockwise rotation). On the other hand, the fact that only baroclinic generation is capable of producing vorticity of both signs, suggests that the islands of positive vorticity must be a manifestation of the existence of this mechanism.

In an attempt to better understand the mechanism of baroclinic vorticity generation and motivated by the earlier conclusion that the vorticity layer's geometry plays an instrumental role in such a process, we consider the latter's kinematical evolution. The success of this approach in the study of the non-reacting variable density layer (Chapter Three) strongly motivates its implementation here as well. This is done in figure 5.15
where schematics of the geometrical evolution of the layer are presented and the baroclinic term is investigated by considering the cross product of the density gradient with the fluid acceleration (the pressure gradient is substituted with the acceleration by using the momentum equation and ignoring diffusion effects). It should be clear that the aim of this approach is to provide enhanced qualitative understanding of baroclinicity. The simultaneous modification of the vorticity field due to volumetric expansion, not accounted for in this analysis, limits the quantitative significance of any conclusions made.

During the initial rollup, the layer moves from a flat, to an "S" type configuration (fig.5.15a,b). Throughout this process fluid along the braids is accelerated along the layer towards the center of rotation of the evolving structure. (It should be noted that this implies that if more than one structures exist, then, in a frame of reference moving with the mean speed of these structures, a stagnation point exists along the braid connecting them. On either side of this point the fluid is accelerated in opposite directions away from the stagnation point and towards the corresponding structures.) The density field across the layer is such (minimum at center of layer, increasing on both sides and with small variation along it - see earlier analysis) that the density gradient is approximately normal to it and it changes sign across it. Furthermore, the thinning of the braids due to the local stretch ensures that the gradient size there, is large. Thus, in the braids, the enhanced density gradient and fluid acceleration are normal to each other and the contribution of the baroclinic term is significant. The arrangement of the vectors involved, results in the creation of positive vorticity on the upper side of the left braid and the lower side of right braid. Similarly, negative vorticity is created on the lower side of the left braid and the upper side of the right braid (fig.5.15a). As the fluid from the braids approaches the geometrical center of the structure it starts to decelerate. The size of the density gradients across the layer is decreased in this region due to the fact that, as a result of the accumulation of the incoming fluid from the braids, the layer becomes thicker. Additionally, layer curvature due to the rollup further modifies the gradient field by
changing both its size and direction. All these reasons result in diminished production of the baroclinic term as compared to the production in the braids. The produced vorticity is expected to have the opposite sign from that of the neighboring braids due to the change in sign of the acceleration vector (fig.5.15b). (It should be noted that this analysis implies that baroclinic vorticity generation tends to be symmetric about the eddy horizontal centerline. Thus, similar amounts of positive and negative vorticity are created and the effect on the overall vorticity should be small. This is a manifestation of the earlier noted fact that the overall circulation of the flow should remain invariant.) Further rollup, merges the regions of negative vorticity production around a core of weak positive vorticity and inside a region of the strong positive vorticity created in the braids. This is shown in figure 5.15c. It should be evident that adding an overall negative vorticity to this picture, as the initially negative vorticity field implies, would result to the type of vorticity field shown in figure 5.13. That is, a field of negative vorticity surrounded by positive vorticity. The analysis provided above for the nature of the baroclinic vorticity generation is checked in figure 5.14 where contours of the baroclinic vorticity production term are provided. As before, dotted lines indicate positive vorticity. The overwhelming agreement with what was described above, at least in the earlier part of the domain where the structures are similar to those of figure 5.15, validates this type of approach of analyzing this phenomenon. Further downstream, as the rollup continues, the cores of the structures, and hence the baroclinic vorticity generation there, become more complicated. But as already explained, the significant generation occurs in the braids and this will have a similar effect in the larger downstream structures as it did in the smaller structures upstream: The negative vorticity of the braids is entrained into the eddy while the positive is distributed around it.

This sign arrangement of the vorticity field should have significant implications on the nature of the flowfield. One could note, for example, that the positive vorticity around the eddies should decrease the entrainment of irrotational fluid into these structures. The
argument supporting this conclusion is as follows: The clockwise rotation of the eddies (overall negative vorticity field) implies that irrotational fluid from the free streams would start moving in a clockwise direction in order to be entrained. The positive (counterclockwise) vorticity around the eddies would counteract this effect. The extra negative vorticity entrained into the eddies would help it. But since the induced velocity from a vorticity field decays with distance ($\frac{1}{r}$, $r=\|x\|$), the effect of the positive vorticity, which is closer to the free streams, will be more significant than that of the negative vorticity. It should also be noted though, that since baroclinicity does not significantly alter the overall size of vorticity, then the layer should still be rolling with similar intensity. The combined influence of these two effects would be to give rise to smaller but still significantly rolled eddies. Admittedly, it is difficult to clearly distinguish such features in the flowfield. But as will be shown, this is only a result of the coexistence of expansion and the complications arising from the interactions of the two vorticity modification mechanisms. It should further be noted that the presence of the positive vorticity is also suspect for influencing the eddy interactions.

The sign arrangement of the vorticity field for the variable density case also provides an explanation for the shape of the corresponding mean velocity profile seen in figure 5.7. Figure 5.13 suggests that the time-averaged vorticity field would consist of a region (wedge) of negative vorticity in between two smaller regions of positive vorticity. This positive, counterclockwise vorticity gives rise to the overshoots and undershoots of the mean velocity profile. Thus, these features are a result of baroclinic vorticity generation.

The effect of the expansion term on the vorticity field of figure 5.13 is not as easy to detect. Rather, the plots of the diverging field of figure 5.12, can be better used to provide an indication of the regions in the flowfield where the instantaneous effect of expansion on the vorticity field is significant. It is important to note though, that even though the instantaneous contribution of the term takes place around the vortical structures
and in the braids, the overall effect of the term is to decrease the flow vorticity throughout the flowfield. This becomes evident when one considers that fluid from the braids is progressively entrained into the cores of the structures and thus the vorticity there, is effectively reduced. The decrease of the vorticity in the flowfield should result in diminished intensity of rollup, entrainment and downstream growth. It should also be born in mind that the streamwise acceleration of the flow due to expansion is also expected to cause a decrease in growth as similar events occur further downstream. Closer to the inlet, on the other hand, and before any major rollup, the thickening of the shear region due to expansion is expected to have a beneficial effect on the layer growth. Thus expansion should initially increase and then decrease shear layer growth as compared to the uniform density flow.

The limitations of the above approach of analyzing the vorticity field, namely investigating the different mechanisms of vorticity modification individually but in parallel, must have, by now, become apparent. Clear conclusions can usually only be made in certain regions of the flowfield (e.g. close to the inlet) where the flow features are simple and/or by identifying certain flow features which could only be attributed to one mechanism. As the flowfield becomes exceedingly complex with increasing streamwise coordinate, it becomes very difficult to recognize each mechanism's effect on the flowfield and on each other. It is not obvious, for example, how the two mechanisms interact to alter the layer growth. Most importantly, it is not clear whether the shift of the eddy interaction mechanism from pairing to tearing is a result of expansion, baroclinicity, or both. Arguments can be put forward which support all the above possibilities. To investigate these problems, the calculation for the case of $Q_o=4$ was repeated twice, but in each time one of the two mechanisms of vorticity modification was eliminated. There should be no doubt for the limitations of such an approach. The governing equation clearly indicates that the different mechanisms are non-linearly coupled. Decoupling them would result in flowfield solutions which may not necessarily be related to the actual flowfield.
Furthermore, since the flow and reacting fields are coupled, this approach will also alter the reaction which in turn will cause further modification of the flowfield. Despite these problems, this decomposition is attempted here, in the hope that more phenomena which can be attributed to mainly one mechanism can be identified.

Figure 5.16 displays the results of these calculations (c and d) together with the case where both mechanisms are active (b) and with the uniform density case (a). The fact that the new solutions belong to the same family as the ones obtained before, provides support to the hope that they can be used to deduce useful qualitative conclusions. The figure clearly shows that the altered interaction mode of the vortical structures experienced in the variable density case is a result of baroclinicity. In the expansion case the pairing mechanism appears to be the same as that of the uniform density flow. The vorticity layer thickens with increasing streamwise coordinate (volumetric expansion) and the rollup is increasingly slowed down (decreased vorticity). These type of features are in agreement with the earlier discussed effect of expansion on the flowfield. They also indicate to the fact that the large elliptical structures of the variable density case maintain their axes more aligned with the streamwise direction because of the decrease in the overall vorticity field due to expansion. As noted, this leads to significant decrease of the layer growth. In the baroclinic case, on the other hand, where expansion is eliminated, the interaction mechanism between the vortical structures is altered to that experienced by the variable density flow. The subharmonic eddies are torn between their neighboring fundamental eddies in a relatively continuous process. Large structures are formed as the fundamental eddies grow as they move downstream. The reason why baroclinicity has such an effect on the flow is not totally obvious. It appears that the positive, counterclockwise, vorticity surrounding the vortical structures inhibits the initialization of the rotation of each pair of fundamental and subharmonic eddies around each other (inhibits the initialization of pairing). This allows enough time for the stronger fundamental eddies to gain rotational fluid at the expense of the subharmonic eddies. The resulting decrease in size (thinning) of
the subharmonic eddies only acts to accelerate this process. The fact that the downstream fundamental eddy is more successful at acquiring fluid from the torn eddy must be a residual effect of the natural tendency of the layer (due to the inlet vorticity - effect of free stream velocities) to favor the interaction of these two eddies, as manifested in the uniform density case.

It is interesting to note that baroclinicity also appears to be responsible for the streamwise elongation of the eddies close to the inlet. This may appear rather surprising since one might have suspected the streamwise acceleration of the flow due to expansion to be the reason for this effect. But the expansion case clearly shows that this is not so, since the eddies, while larger, still retain the overall shape of those of the uniform density flow. The answer to this problem lies in the effect of baroclinicity on entrainment. First, one needs to recognize that the eddies become more elliptical not due to an increase of their major axis but due to a lack of increase of their minor axis. This implies that in the baroclinic case the eddies fail to entrain as much fluid as the ones in the uniform density flow, thus confirming earlier analysis. A comparison of the two first fundamental eddies of the baroclinic case clearly indicates that very little growth has taken place and that the elliptical shape of the eddies is a feature of their initial creation. It is also seen that these eddies are significantly rolled as was earlier speculated. Decrease in rollup is experienced mainly by the expansion case, an expected result. It is not evident what effect this has on entrainment since the size of the eddies is also changing. The effect on the vorticity thickness, on the other hand, is much easier to assess. Baroclinicity tends to decrease it by lateral thinning of the eddies and expansion to increase it by enlarging the eddies.

But figure 5.16 reveals another important point. It can be seen that the acceleration of the vortical structures in the streamwise direction is not only a result of volumetric expansion but also a result of baroclinicity. This conclusion is mainly arrived at, by noting that in the baroclinic case the structures move faster than those of the uniform density case. Pointing to the same conclusion is the fact that in the volumetric expansion case, the eddies
are slower than in the case where both mechanisms are active. (This second clue though, is not as irrefutable. One could claim that the slower eddies may be a consequence of decreased burning -and hence expansion-, resulting from altered mixing due to the absence of baroclinicity.) It is not totally clear how baroclinic vorticity generation induces this streamwise component of velocity to the vortical structures. In the study of the non-reacting variable density flow (Chapter Four) it was shown that vorticity generation of opposite signs across an eddy (in cross stream direction) can have such an effect. But in this case, baroclinic generation, at least in terms of sign, is symmetrical across the eddy. The only differences experienced between the two sides are due to the differences in shape. The most significant of these, is the one resulting from the unequal tearing of the subharmonic eddy between the two fundamental eddies. The fact that the largest part of this eddy tends towards the downstream eddy, results in larger upper braids than lower braids. This should result in more positive vorticity on the upper side than the lower side. (An indication of this can clearly be seen in the later stages the vorticity field of figure 5.14.) This arrangement of vorticity acts to accelerate the eddy in the streamwise direction.

It is interesting to note that baroclinicity, on its own, increases the strain in the field (which is proportional to the length of the material layers which in turn are proportional to the number of elements) while volumetric expansion decreases it. These two opposite trends result in approximately equal number of elements for the case where both mechanisms are active and the uniform density case. On the other hand, by observing figure 5.6 it can be seen that the same is not true for the case where $Q_0=6$. For this latter case the number of elements decreases which suggests that volumetric expansion is more significant than baroclinicity. This in turn, implies that the relative size of the effects of the two mechanisms is a function of heat release. This should not be surprising since the dependence of each mechanism on the variable density field, by definition, is not the same. Furthermore, their interactions act to amplify this phenomenon. For example, increasing the heat release, results at enhanced expansion close to the inlet which dampens the
instability of the layer. The decrease in the layer rollup, diminishes the baroclinic
generation and thus allows the effects of expansion to dominate.

5.3.2.1.1.4. Statistically Averaged Flow Dynamics

The approach used so far in analyzing the effects of the combustion heat release and
of the resulting variable density field, on the forced flowfield, consisted mainly of studying
the latter's unaveraged Lagrangian evolution. An alternative approach is offered by
considering statistically averaged quantities. In a variable density field this is usually done
using Favre (density weighted) averaging. The advantage of this type of averaging over
the more traditional Reynolds averaging is that it results in simpler averaged equations by
avoiding terms involving density fluctuations. Its major disadvantage lies in the fact that
the resulting extra terms in the governing equations, while fewer in number, are less
physically intuitive. Furthermore, they do not incorporate all the features of the fluctuating
(in the Reynolds sense) field, since fluctuating quantities are part of the Favre averaged
quantities, while at the same time they involve the effect of the mean density.

A Favre averaged quantity, $\bar{\beta}$, is defined as:

$$\tilde{\beta} = \frac{\rho \beta}{\bar{\beta}}$$  \hspace{1cm} (5.10)

where the tilde indicates Favre averaging and the overbar, Reynolds averaging. The
fluctuating quantities are, hence, defined as:

$$\beta'' = \beta - \bar{\beta}$$  \hspace{1cm} (5.11)

where the " superscript indicates the Favre fluctuation. It is a simple matter to show that
similar to Reynolds averaging the Favre average of this fluctuation is zero. i.e.

$$\tilde{\beta} = 0$$  \hspace{1cm} (5.12)

It should also be clear that in a uniform density flow, Favre averaging reduces to the
traditional Reynolds averaging.
In direct analogy to Reynolds averaging, the implementation of Favre averaging of the equations of motion results in extra terms formed by the products of the fluctuating quantities. In the two dimensional case considered in this work these quantities are:

$$\overline{\rho u v} (=\overline{\rho u^2}) , \quad \overline{\rho u^2} , \quad \overline{\rho v^2} \quad (5.13)$$

As pointed out in ref.[67] the first term, the turbulent stress term, represents the rate of transfer of momentum flux. The second and third terms are indicative of the flow's turbulent kinetic energy per unit volume in the streamwise and cross stream directions respectively and are representative of the turbulence intensity. The total flow turbulent kinetic energy can be defined as:

$$KE = \frac{\overline{\rho u^2} + \overline{\rho v^2}}{2} \quad (5.14)$$

It is important to note at this point that in order for the statistical analysis to be valid, a large enough sample of events over which the averaging takes place needs to be obtained. The more "ordered" the field, the fewer the events necessary. In this work, the flow was forced at the inlet with the earlier noted consequence that the resulting flowfield was highly repetitive. This allows a relatively small sample of events to result in representative statistical quantities. In the following analysis 100 events -timesteps- were used. During the time described by this sample, 16 eddies (8 pairs of fundamental and subharmonic) were formed by the forcing function. Increasing the sampling set by another 50 events for one of the cases studied ($Q_v=4$), did not have any significant effect on the obtained quantities. It should be clear though, that while forcing has the advantage of reducing the necessary size of the sampling set, it also has the drawback that it can destroy possible similarity of the profiles of the properties calculated. This is because the resulting repetitiveness of the flowfield requires similar events to take place at similar locations. A prime example of this, is seen in the case of the non-reacting shear layer. In the unforced flow, growth in the first part of the domain is by rollup of the shear layer via the Kelvin-Helmholtz instability. Further downstream, on the other hand, pairing takes place and is
the prime mechanism of growth. In the forced case the rollup is repeated identically with
the outcome that the resulting eddies mature and initiate pairing interactions at the same part
of the domain every time. This is expected to bias the fluctuating quantities and to destroy
the well known similarity of both the shear stress and the turbulence intensities profiles of
the unforced shear layer. Inspection of the profiles obtained in this work revealed that the
destruction of the similarity is mainly restricted in the streamwise intensity profiles. This
should have been expected, since this quantity is the one which mostly characterizes the
large scale structures of the flowfield [20]. Obviously, this will also have an effect on the
total turbulent kinetic energy. But it is found that the significant effect of the cross-stream
intensity on the kinetic energy is such that it manages to preserve a similar profile, at least
in the large scale features. For the heat release cases the problems mentioned here appear
diminished. This is because the mechanism of layer growth is much more gradual and
continuous throughout the flowfield for this case.

As noted earlier, due to the presence of heat release, the density decreases
significantly and this will result in decreased Favre turbulent quantities (eqs.(5.13) and
(5.14)). It should be clear though that this does not necessarily imply that the oscillating
nature of the flow is diminished. It only indicates to the fact that the mean density is
reduced. To clarify this point, the uniform flow-density case with the variable density of
its reacting field used in the calculation of the turbulent quantities, will be provided for
comparison. Since this latter case experiences the exact same flowfield as the non-reacting
case then the corresponding Reynold's turbulent quantities are identical. Hence, any
difference in the Favre turbulent quantities between the two cases can only be a
consequence of the variable density and will thus provide an indication of the effect of the
decreasing mean density.

Figure 5.17a presents a comparison of turbulent stress profiles between the case
with $Q_o=4$, the corresponding uniform flow-density case (as explained above) and the non-
reacting flow. Profiles are displayed at a fixed downstream location ($x=2.5$) and as
explained earlier are typical of the profiles experienced in the whole field. It is clearly seen that the region of significant fluctuations is related to the shear layer region. This implies that the shear layer represents the prime mechanism of turbulent mixing of the two streams. The bell-Gaussian shape of the profiles, in analogy to those of the Reynolds shear stress in a uniform density flow [20], clearly indicates that turbulent momentum transfer from the free streams to the shear region represents the latter's prime mechanism of growth. But the figure also clearly shows that this transfer is significantly diminished in the presence of heat release. Furthermore, it is seen, that the effect of the decreased mean density, while significant, cannot account for the whole drop in the turbulent stress. This suggests that heat release acts to dampen the oscillating nature of the flowfield.

A similar picture is seen in the turbulent kinetic energy profiles (figure 5.17b). They are plotted at the same downstream location as those of the turbulent stress. Again, it is seen that the presence of heat release, decreases the kinetic energy of the flow and that only part of this decrease can be attributed to the decrease in the mean density; the fluctuating field is dampened as well. As in the case of the shear stress, it is seen that the region of significant fluctuation corresponds to the shear region. It is interesting to note that a change in the shape of the profile takes place when heat is released. The single peak profile experienced by the non-reacting flow is transformed into a three peak profile in the heat release case. The fact that the uniform flow-density case profile experiences a single peak profile, suggests that the transformation is not due to the mean density or its fluctuation. Rather it is a result of the altered velocity field and it implies, as is the case, significant differences in the field's structure. The shift from a single to a three peak profile invites the speculation that this might be related to the alteration of the vorticity field in the cross-stream direction from an all negative (for uniform density) to a positive-negative-positive (for variable density) field noted earlier. As was seen this modifies the monotonic nature of the uniform density cross-stream mean velocity profile in such a way that its gradient experiences three peaks instead of one. Thus, it appears that the turbulent kinetic
energy could be related to the cross stream gradient of the mean velocity profile. It is important to note though that the similar behavior is exhibited by the shear stress.

5.3.2.1.5. Brief Conclusions

The effects of finite reaction speed combustion on the forced shear layer have been analyzed in detail. The analysis indicates that heat release decreases the growth of the shear region and the intensity of turbulence for most of the flow domain. Volumetric expansion increases the shear region close to the inlet, but decreases it further downstream by decaying the vorticity field and thus decreasing the intensity of rollup. It is also found to be responsible for the evident streamwise acceleration of the flow. Baroclinic generation which redistributes vorticity in such a way that positive vorticity appears surrounding the eddies, decreases the shear region both by decreasing entrainment and by altering eddy pairing interactions into tearings of subharmonic eddies by their closest neighbors. Furthermore, it is identified as the source of the overshoots and undershoots of the mean velocity profile and partly responsible for the eddy streamwise acceleration.

5.3.2.1.2. Effect of the Heat Release on the Reacting–Scalar Field

5.3.2.1.2.1. Product Formation

Figure 5.18 displays the effect of heat release on the product thickness ($\delta_{p_r}$) for the cases studied. The approach in plotting this thickness in both parts (a) and (b) of the figure, where the $Q_0=4$ and 6 are investigated respectively, is similar to that followed in plotting the product thickness for the unforced layer (fig.5.4). The product thickness of the actual heat release case is compared with that of the uniform flow-density case and with that constructed from this latter case by assuming a uniform density in the calculation of the product thickness. Both (a) and (b) clearly indicate that when combustion is allowed to modify the flowfield, the mass of products formed is reduced. On the other hand, the effect on the region where product exists (indicated by a comparison of the heat release case
with the uniform flow-density case) is not uniform throughout the field. In the early stages of the domain this region is enhanced. Further downstream, on the other hand, the opposite trend is experienced. By comparing both plots, it is seen that the modification of product formation in both sections of the field noted above, appears to increase with increasing heat release (i.e. more enhanced at the beginning and more decreased in the end). This is more clearly seen in figure 5.19 where the cases with heat release $Q_o=4$ and 6 are compared. This plot indicates that the above noted effects of the heat release on the product formation region are bound to lead to a similar behavior for the mass of product formed, if the difference in the overall density of the field between the cases compared, is not substantially different. It is also seen that at least to a large scale the spacial effects of the change of the reaction speed (due to the changing heat release) on the product thickness are not significant. Rather, it seems that the predominant effect is that of the increased heat released and the related modification of the flowfield.

In the uniform flow-density cases, the product thickness profile is characterized by two distinct regions of growth. The first region, close to the inlet ($x<2$), displays an ever increasing product thickness growth rate. It coincides with the region of the initial layer rollup up to the point where eddies mature and pairing is initiated (see fig.5.5). The second region, occurring further downstream where the paired structure evolves, displays an almost constant growth rate. When the variable density effects on the flowfield are taken into account this behavior is altered. The two regions are no longer distinguishable. This correlates well with the earlier flowfield analysis which showed that modification of the flow and in particular, of the interactions of the eddies, result in a more streamwise continuous evolution of the flowfield. Thus, it is seen that product formation is strongly related to the flowfield characteristics. This is not an unexpected result since flow induced scalar mixing brings reactants together and enables combustion to take place. Earlier information (fig.5.11) pointed to this fact and it showed that the vortical structures play an instrumental role in the mixing process. (It should be clarified at this point that the shear
and scalar mixing regions are not identical. It is usually found [65] that the mixing region -region of variable reactants- is larger than the shear region. But the differences are commonly small and the overall behavior of the two regions, as already noted, is strongly related. It should also be noted that the product thickness analyzed here, which is representative of the product mass at a cross section, is not the same as the product region thickness, that is, the spacial thickness of the region of varying product. This latter region is the one which should be closer to the scalar and shear regions. Nevertheless the two thicknesses should exhibit qualitatively similar features.)

A higher inlet product thickness growth rate (increasing with heat released) is experienced as the heat release is gradually increased (e.g. see fig.5.19 or compare with the uniform flow-density cases of fig.5.18). This implies higher burning there. Earlier results help provide an explanation for this point. In particular, it was seen that the shear region (vorticity thickness) was increased close to the inlet. This was shown to be the result of enhanced volumetric expansion there, which was linked to the combustion of the region of hot premixed reactants, specified by the inlet profiles. The enhanced shear region increases mixing which further increases the local burning.

Further downstream, but still in the first region, where the growth rate of the product thickness for the uniform flow-density cases increases significantly, the variable density case experiences a smaller growth rate. The result is that by the end of this region the product thickness is larger for the uniform flow-density case. The part of the flowfield where this takes place is the one which experiences initial eddy maturity. Thus, it is seen that alteration of this process is responsible for most of the decreased product thickness of the variable density case. This is so because once the larger structures have formed -second region- the growth rates for the uniform and variable density are not substantially different. (In fact the growth rate for the variable density case appears slightly higher towards the end of the domain.) This was a rather surprising result, considering the much more significant effect on the vorticity thickness in the same region. It should be born in
mind though that the tendency of the eddies of the variable density case to keep their major axes more aligned with the streamwise coordinate should result in a much more pronounced effect on the vorticity thickness (strictly related to the eddy cross-stream layer size) than the product thickness (loosely related to the eddy volume - burning area). To better understand this point one needs to consider the effect of the alteration of the eddy interaction mechanism. In the presence of a variable density field the resulting large eddy cross-stream dimension is reduced, thus decreasing the extend by which product protrudes into the free streams. At the same time, the large eddy streamwise direction is increased, thus the size of the regions between the eddies where very little product exists is decreased. In a time-averaged sense the combination of these two effects would result in a thinner product region but one in which the product concentration is higher. (This can clearly be seen in figure 5.20 where the time averaged product density profiles for the case of Q₀=4, with and without density variation on the flowfield are compared at a given downstream location.) Thus, the mass of product at a cross section is not as significantly decreased as the size of the product region. This is a very important point which exemplifies the importance of understanding the instantaneous flow dynamics in order to be able to deduce the mean flow behavior.

5.3.2.1.2.2. Instantaneous Reacting Field Description and Dynamics

More information about the nature of the combusting field can, hence, be obtained from instantaneous two-dimensional maps of the various properties. As already seen, in figure 5.11 such a map, comparing the temperature field for the Q₀=4 case with that of the corresponding uniform flow-density case, is shown. Under the assumptions of our model the figure can equivalently be considered as displaying product mass fraction fields. Figure 5.21 displays similar maps for the Q₀=6 case. The astonishing similarity of the product fields for the two uniform flow-density cases clearly points to the dominant effect of mixing and clarifies the reason why the product thickness profiles for these cases are so similar. It is seen that mixing and burning are strongly related to the evolution of the
material-vorticity layer and its rollup into elliptical vortical structures. As this layer becomes unstable and gets distorted, it experiences significant tensile strains. This is verified in figure 5.22 which displays the Lagrangian strain rate field for the cases of $Q_0=4$ and 6. The stretch of the layer increases its length and decreases its width. Both of these effects enhance mixing and burning. The increase of the layer length increases the surface of contact of the reactants. The decrease in width enhances the fluxes of reactants normal to it. Thus, the instability of the layer enhances burning. (This argument assumes that quenching, the collapse of the reaction zone due to excessive strains and the associated drop in temperature, does not take place. Figures 5.11, 5.21 and 5.22 clearly show that this assumption is valid in the cases analyzed here, since regions of high positive strain, are not associated with regions of low product-temperature. Thus, it can be concluded, that the flow and chemical parameters -or equivalently the Karlovitz number- are such, that quenching does not occur.) The argument becomes more complex as the layer winds around itself and forms the vortical structures - eddies. In such a case, only part of its length (the braids connecting the eddies) is clearly exposed to the free streams and will, hence, conform to the above argument. Inside the eddies this is not true any more and as the layer increases its length there, the efficiency of burning will depend on the local availability of reactants. Thus the mechanisms by which the layer is able to entrain reactants become important. Two such mechanisms are identified. Entrainment of unmixed reactants from the free streams by engulfment of irrotational fluid by the layer as it winds around itself, and entrainment along the layer of reactants premixed at the braids. As far as eddy core burning is concerned, the first type of entrainment is the most important. This is because reactants mixed at the braids get significantly burned by the time they reach the eddy core. But the quantity of reactants inside the eddies is not the only effect to be considered here. The related presence of products there, also complicates the problem. While the eddies are able to continuously entrain reactants they have no mechanism of getting rid of the products formed. Even worse, they, in addition, continuously entrain
products from the braids into the core. Thus they become regions of accumulation of products. This can reduce the efficiency of burning significantly by causing extinction, that is, the termination of reaction due to unavailability of reactants which results from an overaccumulation of products. Thus, it becomes evident that it is not only the presence of reactants in the eddy core which is important but their locus as well. This, in turn will depend on the eddy core structure and its ability to mix them.

Figures 5.11 and 5.21 clearly indicate the presence of entrainment of reactants from the free streams into the eddy cores. This is seen in the regions of low product mass fraction there, which persist throughout the computational domain for all cases, but which appear to increase with increasing heat release. For the uniform flow-density cases the major source of these regions appears to be the rollup of the fundamental eddy. As the layer winds around itself to form this eddy it engulfs two large islands of reactants, one from each stream. Further intense rollup of the layer inside the eddy (at x=2) mixes and consumes most of these reactants in what is clearly, very efficient burning. This is the reason why at this region the product thickness growth rate experiences a local peak. By the time pairing is initiated, the reactants in the eddy core are substantially depleted and the efficiency of burning decreases. The situation is quite different for the variable density cases. The rolling of the layer and, in particular, the formation of the fundamental eddy, is exceedingly inhibited with increasing heat release. The eddy is smaller and less rolled. The origins of these effects were earlier explained and attributed to the presence of expansion and baroclinicity. The entrainment into the eddy, as well as the length of the layer inside it, are decreased, thus decreasing the efficiency of mixing. But the delayed rollup of the layer means that the time allowed for entrainment before the eddy rolls completely around itself is increased. Thus, for the variable density cases the formation of the two islands of reactants inside the core takes longer with increasing heat release. The decreased rollup there, also decreases the speed by which they are consumed. These are the reasons why the islands of reactants inside the larger downstream eddies appear to
increase with heat release. Obviously, the diminished rollup inside the eddies, which decreases the mixing, will tend to decrease the burning there, despite the increasing presence of reactants. This, together with the decrease of the cross-stream dimension of the eddies with heat release are the major reasons why the product thickness is decreased with increasing heat release in the later part of the domain.

As expected, the effect of the eddy interactions on the combusting field differs significantly between the uniform flow-density and variable density cases. This is because as was earlier seen, the mode of interaction of the two cases, changes from pairing to tearing respectively. Tearing is a more or less continuous process for most of the field. It results in larger upper braids for the vortical structures and this can clearly be seen in both figures 5.11 and 5.21. As the eddy core keeps rotating it winds these braids around it. This results in more entrainment and further increases burning. Surprisingly enough, pairing does not appear, at least initially, to introduce large new reactant quantities into the eddy core. Rather, the reactant regions there, are the remainders of the ones introduced by the fundamental eddy and continue to be depleted but at slower rates due to significant accumulation of products. But, on closer scrutiny it can be seen that this assessment of the effect of pairing is actually incorrect. The paired eddies experience large scale rotation which should lead to significant entrainment downstream, as these structures wind around themselves in a similar fashion to the winding of the fundamental eddies. Furthermore, a second level of pairing interactions is anticipated when this happens, further increasing the mixing and burning. Unfortunately the computational domain is not long enough to witness this effect. In contrast, no such effects appear to be imminent for the larger structures resulting from tearing. Thus, it is here seen, that the earlier conclusion that the larger downstream structures of the uniform and variable density cases result in similar growth rates of the product thickness, is actually a misleading one and underestimates the efficiency of burning of the uniform flow-density case.
Verification of some of the above comments, as well as a deeper understanding of the combustion process can be obtained by studying the reacting field itself. Figure 5.23, presents two dimensional maps of the reaction rate for the \( Q_0 = 4 \) and 6 cases. It is important to realize that the property plotted here signifies reaction potential, that is, the ability to burn, rather than the amount of burning. In other words, for enhanced burning, a high reaction rate needs to be maintained for a certain amount of time. The higher the rate, the smaller the time required. The regions where the greatest amount of burning takes place, can better be identified through the changes of density which are expected to be higher there. The field of density change can equivalently be represented by the field of flow divergence. Thus, a better understanding of the reacting field can be obtained by analyzing both the reaction rate and the flow divergence. Maps of flow divergence for the two cases considered here, were provided in figure 5.12.

The substantial burning at the inlet, which is a consequence of the inlet profiles, is clearly witnessed. The high reaction rate there, as well as the slightly delayed (for the reasons explained above) divergence, bear witness to this fact. The ability of the layer to increase mixing and reaction by stretching is seen in both cases, both in the region before eddy formation, as well as in the braids. The absence of quenching is evident through the substantial reaction rates at the braids where strain is highest. (See fig.5.21 for strain field for the two cases.) In contrast, the flow divergence exhibits significant differences between the two cases when it comes to the braids. The \( Q_0 = 6 \) case shows significant divergence there, while the \( Q_0 = 4 \) case, very little. Rather, most of the divergence for this case takes place around the eddies. On closer inspection though, some differences in the reaction rate field of the braids can be noted as well. In contrast to the \( Q_0 = 4 \) case, the \( Q_0 = 6 \) case experiences diminished reaction in the centerline of the braids. The high concentration of products there (fig.5.20), implies that the phenomenon experienced, is extinction. This implies that, for this case, the rate of product formation due to reaction, is higher than the rate of product removal due to the flow-induced strain. Two mechanisms are at work here.
First, and most important, the rate of product formation is increased over that of the \( Q_o = 4 \) case, because the speed of the reaction is higher. This is a result of the higher temperatures of the field which are, in turn, related to the higher heat release. Second, the rate of product removal is reduced due to the decreased strain (as seen in fig.5.21) which again is a consequence of the increased heat release. Thus, reactants which get mixed at the braids burn to a much greater degree there, for the \( Q_o = 6 \) case. This agrees with the conclusion made from the flow divergence maps. Further indication of this effect is provided by the fact that by the time fluid from the braids reaches the outskirts of the eddies the reaction rate decays significantly. This implies that braid mixed reactants have almost completely burned by this point. For the \( Q_o = 4 \) case, on the other hand, while burning starts at the braids, the decreased reaction speed, as well as the diminished residence time of the mixed reactants there, decreases the amount of burning. Rather, the mixed reactants are transported to the eddies before they have a chance to burn significantly. As they reach the outskirts of the eddies they decelerate (see earlier flow analysis). The increased reactant residence time in this region leads to more substantial burning there. This is verified from both the flow divergence plots which show this region to be the region of greatest expansion, as well as the reaction rate plots which show significant values in this region and they indicate the first signs of layer centerline extinction.

Burning inside the vortical structures conforms to earlier analysis. The two islands of reactants inside the fundamental eddies can be identified as the two regions of insignificant reaction rate. Between them the region where they mix and burn is clearly seen. The intensity of burning is increasing with heat release as expected. The perseverance of the regions of reactants, as well as of the mixing-burning region between them, further downstream, is also noted. The absence of significant flow divergence in the same region is rather surprising and implies fast transport of the reacting mixture to the outskirts of the eddy. While it is not totally clear how this takes place, it is nevertheless verified by the substantially diminished presence of products in the eddy cores.
5.3.2.1.2.3. Brief Conclusions

In the above analysis it has been seen that the modification of the forced flowfield due the combustion heat release can have significant effects on the reacting field itself. Close to the inlet and before the flow gets destabilized, heat release increases burning over that of the uniform flow-density case by volumetric expansion induced mixing. As the flow gets destabilized and the vorticity layer starts to roll, burning for the variable density flow is decreased. This is due to both, decreased rollup and entrainment of the initial eddies and the modification of the eddy interaction mechanism from pairing to tearing. For the uniform flow-density case, both the initial and paired eddies grow in a similar fashion. They experience large scale rotation which engulfs two large islands of reactants, one from each free stream. Further, intensive mixing inside their cores quickly consumes these reactants. For the variable density case the initial eddies are less rolled and they experience reduced rates of entrainment from the free streams. The decreased rollup allows longer time for entrainment which is finally able (at a further downstream location) to entrain significant amounts of reactants. Burning of these reactants is not as efficient due to decreased mixing at the eddy core. In contrast to the uniform flow-density case, the larger downstream structures resulting from tearing experience a different growth mechanism from the upstream eddies. Entrainment is mainly achieved by winding of the upper larger braids around the eddy core. This results in diminished entrainment and thus diminished burning.

It was shown, that positive strain rates can be related to enhanced combustion (no quenching experienced for cases studied) only outside the eddies where the layer is exposed to the free streams. As the speed of the reaction increases the amount of burning at the braids increases. For slow reactions, reactants mixed at the braids are transported to the eddies before they have the chance to substantially burn at the braids.
5.3.2.2. Infinite Reaction Speed

Significant similarities exist between the results of the finite and infinite reaction speed calculations. Hence, in order to avoid repetition, in the following analysis such similarities are simply pointed out and the phenomena involved, are not discussed in detail. Since the numerical schemes used in the two cases are different in a number of aspects, the above mentioned similarities will, when appropriate, be used to provide qualitative verification of the numerical consistency of the schemes used. Despite the similarities, significant differences also exist. These are analyzed in more detail and explanations for their existence are proposed.

5.3.2.2.1. Effect of the Heat Release on the Flowfield

5.3.2.2.1.1. Flowfield Description

Figures 5.24 and 5.25 are analogous to figures 5.5 and 5.6 of the finite reaction speed calculations. That is, figure 5.24 presents a comparison of the uniform flow-density flowfield with that of the variable density field for which $Q_0=4$, at three sequential times. Figure 5.25, on the other hand, displays a comparison of the uniform density flowfield and the two heat release cases, $Q_0=4$ and 6. The similarities with figures 5.5 and 5.6 are significant. For the variable density cases the decrease in rolling and coherence of the initial eddies (as compared with those of the uniform density case), as well as the apparent streamwise elongation of the fundamental eddies is clearly seen. The alteration of the eddy interaction mechanism from pairing to tearing is evident. The acceleration of the vortical structures in the streamwise direction with increasing heat release is also seen. But subtle differences are experienced as well. The variable density initial eddies are more coherent and rolled than their finite reaction speed counterparts. The subharmonic eddies appear to be more resistant to tearing and can commonly still be detected quite downstream. This results in an inability of the layer to create the larger downstream structures of the finite reaction speed cases and, hence, in a further decrease in layer growth. The enhancement of
these effects with increasing the heat release appears to be diminished. The intensity of the
strain field (noted through the number of elements) is significantly higher than that of the
finite speed calculations.

In order to obtain a deeper understanding of these differences, more information
about the flowfield needs to be provided. In figures 5.26 and 5.27 the mean velocity
profiles (at a downstream location (x=3)) and the vorticity thickness respectively, are
plotted for the cases of figure 5.25. The profiles of figure 5.26 are very similar to those of
figure 5.7. That is, with increasing heat release, they are steepened and experience
overshoots and undershoots close to the fast and slow free streams respectively. The
similarity suggests that the processes at work are the same. It is noted that the overshoots
and undershoots appear more pronounced for the infinite speed cases. Since these
characteristics of the profiles were attributed to the presence of baroclinicity then one is led
to the conclusion that this process is more pronounced for these cases.

The vorticity thickness behavior of figure 5.27, in similarity to figure 5.8, clearly
indicates the downstream decrease with increasing heat release. It is further noted that this
decrease is more significant for the infinite speed case. (This is not an unexpected result
since, as was seen in figures 5.24 and 5.25, the creation of the larger downstream
structures for this case is inhibited through the persistence of the subharmonic eddy.) But
close to the inlet the behavior is different from that of figure 5.8. The heat release cases do
not experience higher thicknesses than the uniform density case and the $Q_o=6$ case only
slightly, and very close to the inlet, is able to exceed the $Q_o=4$ case. The increased vorticity
thickness of the finite reaction speed heat release cases, was attributed to the expansion
associated with the introduction of a reactant premixed region, by the inlet profiles. The
decrease of the inlet expansion effects for the infinite speed calculations verifies this
conclusion. This is because the inlet profiles for this latter case do not allow for premixed
reactants at the inlet (see fig. 5.1). The smaller difference between the two heat release
cases must, additionally, be related to the fact that, in contrast to the finite reaction speed cases, the speed of reaction is the same (infinite).

5.3.2.2.1.2. Density Field Description

Combustion alters the flowfield via the modification of the density field. Thus, some information is provided here about the density field to aid the analysis of the flowfield. Figure 5.28 presents two dimensional mass fraction plots for the $Q_o=4$ case (b), together with the same case without the effect of variable density on the flowfield (a), and the $Q_o=6$ case (c). As earlier explained, under the assumptions of our model the mass fraction is directly related to the temperature and through the equation of state to the density. This figure clearly indicates that like the finite reaction speed cases the density field is directly related to the evolution of the material-vorticity layer existing between the two fluid streams at the inlet. The implications of figure 5.28, particularly when considered in conjunction with the noted flowfield similarities between the finite and infinite reaction speed cases, are that the density field must, in general terms, be similar for the two cases. The overall higher intensities of the product mass fraction of figure 5.28 as compared to figures 5.11 and 5.21 indicate that the density field must experience lower densities in the infinite reaction speed cases. The reason for this lies, in the fact that under the assumptions of this case a line where only products exist (i.e. $Y_p=1$) always exists between the two streams. This line represents the reaction zone which is infinitely thin, and the temperature there is the adiabatic flame temperature. For the finite reaction calculation this is not true. The coexistence of reactants and products in the finite size reaction zone lowers the temperature there. The higher temperatures of the infinite reaction speed case imply lower densities. This is also verified in figure 5.29 where the averaged density profiles for the case with $Q_o=4$ for both the finite and infinite reaction speed are compared at a downstream location ($x=3$). (This comparison is typical for most downstream stations). It is clearly seen that the density experiences a lower minimum for the infinite reaction speed case. This latter case also displays a smaller cross-stream
thickness which should be an expected consequence of the decreased vorticity thickness. Both of these effects should contribute to larger density gradients. It should be clarified though, that the lower densities of the infinite reaction case do not directly imply more enhanced combustion because the inlet profiles are different for this case as well, and they specify lower densities than those of the finite reaction speed (see fig.5.1).

5.3.2.2.1.3. Instantaneous Flow–Vorticity Dynamics

In similarity to the finite reaction speed analysis, the flowfield characteristics are discussed in terms of vorticity dynamics. Figure 5.30 displays the vorticity field for the $Q_\alpha=4$ case. The similarity with figure 5.13, which presents the corresponding finite reaction speed case, is obvious. Eddies of negative vorticity are surrounded by islands of positive vorticity. As explained earlier, the positive vorticity is a result of baroclinicity. The vorticity generated by baroclinicity is shown in figure 5.31 and exhibits the same type of features as those of figure 5.14. This is particularly true in the first half of the domain where the similarities of the flowfield are substantial. (Further downstream differences in both the flowfield and the density field make comparison more difficult.) Thus, it is here seen, that to a significant qualitative detail, the effect of baroclinicity is very similar for the two cases. It should be noted that this similarity also provides an internal consistency check of the numerics. The most fundamental difference between the finite and infinite reaction speed numerical schemes lies in the calculation of the product field. Because of this difference, the way by which the density gradient is obtained is different between the two cases (see Chapter Three). The fact that the two schemes, while different, result to the same type of solution, confirms the correctness of the numerical approach used.

But while figures 5.31 and 5.14 are qualitatively similar, they also imply that, quantitatively, baroclinicity is more dominant for the infinite reaction speed case (i.e increased number of contours). The increased importance of baroclinicity for the infinite reaction speed case was already noted in the discussion of the mean velocity profiles and can also be detected in the larger islands of positive vorticity of figure 5.30 (as compared to
those of figure 5.13). This effect is primarily related to the larger density gradients involved in the infinite reaction speed case.

Differences in the effects of volumetric expansion between the vorticity fields of figures 5.30 and 5.13 are not easy to detect. The simultaneous action of baroclinicity is the source of the difficulty. Some information for the effect of the expansion is provided via figure 5.32 which displays the flow divergence field for the cases of $Q_o=4$ and $6$. The figure clearly indicates that for both cases expansion takes place primarily at the braids (note in particular the braids very early and very late in the computational domain which are more easily distinguishable). This behavior is more similar to the $Q_o=6$ case of the finite reaction speed calculations (see fig 5.12b). The origin of this similarity lies primarily in the reaction speed and will be discussed in more detail in the next section. Expansion at the braids, as explained in the analysis of the finite reaction speed $Q_o=6$ case, is the reason why they appear thick downstream. Comparison of figures 5.31 and 5.12 also shows that while the intensity of the expansion term tends to be higher for the infinite reaction term cases, the area of the field which it takes place, is substantially decreased. Competition of these two effects suggests that the overall divergence in the field is not necessarily increased for these cases.

To establish a clearer understanding of the effect of baroclinicity and expansion on the flowfield, and in analogy to the approach followed the finite reaction speed analysis, calculations for the case of $Q_o=4$ with the mechanisms of baroclinicity and volumetric expansion in turn eliminated, are carried out. Results from these calculations are shown in figure 5.33, together with the case where both mechanisms are active, and the one where both are disabled. The similarity of this figure with figure 5.16 is overwhelming. The fact that tearing is a result of baroclinicity is clear. The expansion, case experiences the same pairing interaction as the uniform density flow but in a delayed fashion (decreased rollup) due to the streamwise thickening of the layer and the associated drop in vorticity. The streamwise acceleration of the vortical structures is seen, again, to be a consequence of
both expansion and baroclinicity. The baroclinic case clearly documents the decreased entrainment and the resulting elongation of the fundamental eddies. The larger upper braids are also seen but the subharmonic eddies appear to be able to maintain some form of structure further downstream than those of the finite reaction speed case. Obviously, this must be related to the differences in the density field between the two cases but this effect is so small that its origin at this point is inconclusive. Nevertheless, it is noted here, that the earlier conclusion that the subharmonic eddies of the infinite reaction speed calculations are more resistant to tearing, is a result of a modification of the baroclinic vorticity generation. A crude visual comparison of the expansion cases of figures 5.33 and 5.16 (i.e. checking the effect on layer thickness, eddy pairing, eddy streamwise acceleration and flow strain - number of elements) reveals that, quantitatively, the overall field expansion of the two cases must not be greatly dissimilar. In contrast, the enhanced baroclinicity of the infinite reaction case is evident (particularly through the substantially enhanced strain and size of larger downstream structures). The fact that baroclinicity plays a more important role in the infinite reaction case was established earlier from a number of different sources and explained in terms of the density field. Here this effect is also related to the more intense strain, noted earlier in the analysis of the flowfield.

5.3.2.2.1.4. Statistically Averaged Flow Dynamics

A statistical approach in analyzing the flowfield only acts to reinforce some of the above conclusions. In figure 5.34 the Favre averaged turbulent shear stress (a), and the turbulent kinetic energy (b), for the case of \( Q_o = 4 \) are shown at the same downstream location as that of figure 5.17 (i.e. \( x = 2.5 \)). The similarities of the finite and infinite reaction results are substantial. The shapes of the profiles are basically the same, implying the similarities of the phenomena involved. The size of the turbulent quantities is decreased for the infinite reaction case implying the decay of the turbulent field for this case. This is in agreement with the above documented inability of the layer to further grow by interaction of the eddies.
5.3.2.2.1.5. Brief Conclusions

The analysis of the effect of the combustion heat release on the flowfield for the forced infinite reaction cases has shown that the more basic features of the flow as well as the phenomena involved, are similar to those of the finite reaction cases. Some minor differences were pointed out. Volumetric expansion effects close to the inlet are substantially reduced due to the absence of the introduction of premixed reactants by the inlet profiles. Tearing of the subharmonic eddy is delayed and hence the formation of the larger downstream structures is inhibited. This further decreases the growth of the shear region. The delay of the subharmonic eddy tearing is a result of the nature of the density field and the associated baroclinic vorticity generation. The effect of this mechanism of vorticity modification is more significant for the infinite reaction speed cases because of the more intense density gradient field.

But as noted above, these differences are small and hence it can be concluded that the infinite reaction speed model offers a computationally efficient way of investigating the dynamical effects of the combustion heat release on the flowfield.

5.3.2.2.2. Effect of the Heat Release on the Reacting–Scalar Field

5.3.2.2.2.1. Product Formation

The product thicknesses for the two cases studied, are shown in figure 5.35. The figure is arranged in direct analogy to figure 5.18 of the finite reaction speed results. Parts (a) and (b) display values for the cases of $Q_\alpha=4$ and 6 respectively and they contrast the actual heat release case with the uniform flow-density case and with a recalculation of the thickness of this latter case using a uniform density. The figure makes clear that the modification of the flowfield by combustion, influences the reacting field in such a way that
the amount of product formed is decreased. Figure 5.36 presents a comparison of the $Q_0=4$ and 6 cases.

While the similarities with figure 5.18 are significant, differences also exist. Most notable amongst these is the decrease (or even total elimination) of the region close to the inlet where expansion increases burning. Furthermore, the product thickness profiles for the variable density cases have similar shapes to those of the uniform flow-density case. They are characterized by the two regions of growth noted in the uniform flow-density profiles of the finite reaction speed cases. This implies changes in the profiles throughout the field and not just in the first section of the first region ($x<1$) where the inlet expansion effects are experienced. The second section of the first region ($1<x<2$) which is characterized by fundamental eddy growth and maturity, still displays one of the highest growth rates of the whole domain. Further downstream, while the growth rate is decreased for both uniform and variable density, it appears to be more so for the latter cases. While this is different from the behavior exhibited by the finite reaction speed results, it should be pointed out that the differences are seen to be small. Furthermore they should be expected. As was seen, the finite reaction speed cases have, by this point, totally torn the subharmonic eddy and created the larger coherent structures. The infinite reaction speed cases, on the other hand, are not usually able to complete this process within the computational domain. The inability of the infinite reaction speed cases to form the larger downstream structures will decrease the burning there.

5.3.2.2.2. Instantaneous Reacting Field Description and Dynamics

A more detailed understanding of the nature of the reacting field, can be achieved through use of the product mass fraction maps of figure 5.28 in conjunction with maps of the $\lambda$ Shvab-Zeldovich variable. These are shown in figure 5.37 and correspond to the cases of figure 5.28. As earlier explained, under the infinite reaction speed assumption, reactants burn on contact and thus their coexistence is prohibited. This implies that the reaction zone shrinks to a line - the reaction interface. Along this line only products are
present (i.e. \( Y_p=1 \), \( Y_1=Y_2=0 \) and thus it can be defined as the line where \( \lambda=0 \). Burning is achieved via the diffusion of reactants towards the reaction interface. The fundamental role played by the reaction interface on the combusting field can easily be assessed through a comparison of figures 5.28 and 5.37. The figures clearly indicate that reactant's mixing and product formation are closely related to the locus of this interface. The fact that flow mixing is the primary mechanism which governs the interface's evolution points to the former's important effect on the efficiency of mixing. In analogy to the finite reaction speed analysis, the straining of the interface can enhance burning in two ways: Elongation of the interface, which provides more length for burning, and thinning of the diffusion region surrounding the interface which enhances the local reactant diffusion fluxes. (It should be evident that the infinite reaction speed assumption removes the dependence of the reaction on the temperature so quenching is not possible. Extinction, on the other hand, can and does happen.) These processes are certainly valid at the initial stages of the rollup (before eddy formation) and at the braids. Since the reaction speed is infinite, burning at this regions is instantaneous. This can clearly be seen in figure 5.32 where the volumetric expansion (i.e. changes in density) is shown for the two heat release cases. The significant burning at the early parts of the domain and at the braids, is evident. (It should be noted that this behavior verifies the conclusion drawn in the finite reaction speed analysis that burning at the braids becomes more significant as the reaction speed increases.) As the layer rolls into eddies the ability of the flow to enhance burning is also dependent on the local availability of reactants and the relative accumulation of products. During the early stages of the rollup which are dominated by the growth of the fundamental eddy, the availability of reactants is practically unimpaired (through entrainment of reactants from the free streams), and the accumulation of products is small. Thus, in this region the increases in product formation can be related to the stretching of the reaction interface. It should be noted that the features of the combusting field in this region are very similar to those of the finite reaction speed cases. The decrease of the rollup and entrainment of the fundamental
eddy can be clearly seen in both figures 5.28 and 5.37. As explained above, this will result in decreased product formation in this region a fact already documented by the product thickness profiles. Further downstream, where the eddies interact, accumulation of products and the unavailability of reactants in the eddy cores are more prominent. Thus stretching of the reaction interface in this region does not necessarily result in proportional increases in the amount of burning. This is the reason why the growth rate of the product thickness profiles is decreased in this region for all cases. The fact that the growth rate of the product thickness is still higher for the uniform density cases becomes understandable when one compares the difference in the length of the reaction interface together with the acknowledgment that, in contrast to the finite reaction speed results, the entrainment of reactants into the eddies is not much more significant for the heat release cases. The difference in reactant entrainment into the eddy core between the finite and infinite reaction speed cases at the later part of the domain is attributed to the differences in the flowfield characteristics experienced there. Still, in contrast to the finite reaction speed results, the amount of burning at the core centers (as seen in figure 5.32) is more significant. This, again is a result of the different reaction speeds. Reactant mixing in the eddy cores was also seen in the finite reaction speed results, but the mixture was not allowed significant time there for burning and was shifted to the eddy outskirts. Obviously, such a phenomenon could not be experienced in the infinite reaction speed cases where reactants burn on contact.

5.3.2.2.3. Brief Conclusions

Thus, it has been established that the effect of heat release on the infinite reaction speed combusting field is to reduce product formation throughout the domain. This is slightly different from the behavior of the finite reaction speed cases. Two major reasons are seen to cause this difference. The absence of a reactant premixed region at the inlet (different inlet profiles) and the inability of the layer to form the larger downstream structures (i.e. to complete the eddy interactions within the computational domain)
documented in the finite reaction speed cases. This latter effect was earlier seen to be a result of baroclinicity. In similarity with previous results it is established that flow mixing plays an instrumental role in the burning process.

The numerical results indicate to the effectiveness of the infinite reaction speed model in capturing the effects of the combustion heat release on the scalar field.

5.4. Conclusions

The dynamical effects of the combustion heat release on a spatially developing reacting shear layer have been investigated under both forced and unforced conditions. Results of the unforced flow indicate the presence of large scale vortical structures which survive and combustion process. Mixing and combustion coincide with the regions where these structures exist. The heat release decreases the growth and efficiency of burning of the unforced layer via a significant delay of the onset of the flow instability and via a suppression of the eddy interactions-pairings downstream. These results are in qualitative agreement with experimental observations.

External, high amplitude forcing does not fundamentally alter the trends in layer growth and amount of product formed, experienced in the unforced flow. Even though the effect of the delay of the instability is bypassed in forced flows, heat release still substantially modifies the interactions of the eddies. Eddy pairing is resisted and instead, a tearing of subharmonic eddies by their fundamental neighbors is experienced. This causes a significant drop in the shear layer thickness and reduces the amount of product formed.

It is seen that the evolution of both the flow and reacting fields is closely related to the evolution of the vorticity-material layer separating the two fluids at the inlet. Thus, the flowfield modification in the presence of combustion heat release is related to the two major mechanisms by which the resulting variable density field can alter the evolution of this layer: Volumetric expansion and baroclinic vorticity. Volumetric expansion increases the shear region close to the inlet by thickening of the layer but decreases it further downstream
by decaying the vorticity field and, hence, impairing the intensity of the layer rollup. Baroclinic vorticity generation, on the other hand, rearranges the vorticity of the layer in such a way that positive vorticity appears on the outskirts of the eddies. This effect is responsible for the suppression of eddy pairing and for diminished entrainment into the eddies, both of which result in decreased growth of the shear region.

Finally, results indicate that the infinite reaction speed model represents a good, numerically cost efficient model under which the effects of the combustion heat release on the flowfield may be investigated.
Figure 5.1 The inlet mass-fraction profiles for the finite, (a), and infinite, (b), speed of reaction cases.
Figure 5.2 Single time frame flowfield comparison between the uniform (a) and variable (b) density cases for which the reaction speed is infinite, $Q_0=4$, and no forcing is implemented at the inlet. The length of the domain is $X_{max}=8$. 
Figure 5.3 Comparison of the streamwise evolution of the vorticity thickness between the uniform and variable density, Qo=4, infinite reaction speed, unforced cases.

Figure 5.4 Comparison of the streamwise evolution of the product thickness between the variable density and the uniform flow-density, Qo=4, infinite reaction speed, unforced cases. The thickness of the latter case using a uniform density for the scalar field is also shown.
Figure 5.5 Flowfield comparison between the uniform density (left) and the variable density (right) reacting, forced shear layers for which the reaction speed is finite and $Q_e=4$. The layer is depicted using the vortex elements and their local velocity vectors. Three sequential time frames (increasing from top to bottom) are shown.
Figure 5.6 Single time frame forced flowfield comparison between the non-reacting, uniform density case (a), and the two finite reaction, variable density cases, which are at different heat release, $Q_0=4$ (b) and $Q_0=6$ (c).
Figure 5.7 Comparison of the time-averaged velocity profiles between the uniform density and the $Q_0=4 \& 6$ variable density, finite reaction speed, forced cases. The streamwise location is $x=3$.

Figure 5.8 Comparison of the streamwise evolution of the vorticity thickness between the uniform density and the $Q_0=4 \& 6$ variable density finite reaction speed, forced cases.
Figure 5.9 Comparison of the time-averaged density profiles between the $Qo=4$ & 6, finite reaction speed, forced cases. The streamwise location is $x = 4$.

Figure 5.10 Comparison of the streamwise evolution of the density thickness between the $Qo=4$ & 6, finite reaction speed, forced cases.
Figure 5.11 The product mass-fraction field (or equivalently the temperature field) for the finite reaction speed, \( Q_0 = 4 \), forced cases. (a) is the uniform flow-density case and (b) the variable density case. The time is \( t = 10 \) for both. Ten shade intensities (white to black) equally subdivide the mass fraction scale \( 0 < Y_r < 1 \) (or the temperature scale: \( 1 < T < 3 \))
Figure 5.12 Comparison of the flow-divergence fields between the $Q_0=4$, (a), and $Q_0=6$, (b), forced cases for which the reaction speed is finite. The time $t=10$ for both cases. Ten shade intensities (white to black) equally subdivide the plotting scale which ranges from 0 to 0.2
Figure 5.13  Vorticity contours for the finite reaction, Q₀=4, case, at time t=10. Dotted/continuous lines indicate positive/negative vorticity. The contour increment is 0.4.

Figure 5.14  Contours of the baroclinic vorticity generation term for the finite reaction, Q₀=4, case, at time t=10. Dotted/continuous lines indicate positive/negative vorticity. The contour increment is 0.4.
\[ \dot{\omega}_b = a \times \frac{\nabla \rho}{\rho} \]

Figure 5.15 Schematic illustration of the effect of vorticity generation. \( \omega_0 \) is the initial vorticity of the layer and \( \omega_b \) the vorticity generated by the baroclinic torque. \( \nabla \rho \) is the density gradient and \( a \) the material acceleration.
Figure 5.16  Investigation of the effect of expansion and baroclinicity on the flowfield for the finite reaction speed, \( Q_o = 4 \), case. In (a) both mechanisms are eliminated. In (b) they are both active. In (c) only expansion is present and in (d) only baroclinicity.
Figure 5.17 Comparisons of the Favre-averaged turbulent shear stress (a) and kinetic energy (b) profiles, between the uniform density case and the Qo=4, variable density and uniform flow-density (but with the reacting field density in the calculation of the averaged quantities), finite reaction speed cases. The streamwise location is x=2.5.
Figure 5.18  Comparison of the streamwise evolution of the product thickness between the variable density and the uniform flow-density, finite reaction speed, forced, $Q_0=4$ (a) and $Q_0=6$ (b) cases. The thicknesses of the uniform flow-density cases using a uniform density for the scalar field are also shown.
Figure 5.19 Comparison of the streamwise evolution of the product thickness profiles between the Qo=4 & 6, finite reaction speed, forced cases.

Figure 5.20 Comparison of time averaged product density profiles of the finite reaction, Qo=4 case and the corresponding uniform flow-density case. The streamwise location is x=4.
Figure 5.21 The product mass-fraction field (or equivalently the temperature field) for the finite reaction speed, forced, $Q_o=6$ cases. (a) is the uniform flow-density case and (b) the variable density case. The time is $t=10$ for both. Ten shade intensities (white to black) equally subdivide the mass fraction scale $0 < Y_r < 1$ (or the temperature scale: $1 < T < 4$)
Figure 5.22  Lagrangian strain contours for the finite reaction Qo=4, (a), and Qo=6 (b) cases. The time is t=10. Dotted/continuous lines indicate positive/negative strain. The contour increment is 0.1.
Figure 5.23 The finite reaction-rate field for the Qc=4, (a), and Qc=6, (b) forced cases. The time \( t=10 \) for both cases.

Ten shade intensities (white to black) equally subdivide the plotting scale which ranges from 0 to 0.0001 A.
Figure 5.25 Single time frame forced flowfield comparison between the non-reacting, uniform density case (a), and the two infinite reaction, variable density cases, which are at different heat release, $Q_0=4$ (b) and $Q_0=6$ (c).
Figure 5.26 Comparison of the time-averaged velocity profiles between the uniform density and the $Q_0=4$ & $6$ variable density, infinite reaction speed, forced cases. The streamwise location is $x=3$.

Figure 5.27 Comparison of the streamwise evolution of the vorticity thickness between the uniform density and the $Q_0=4$ & $6$ variable density infinite reaction speed, forced cases.
Figure 5.28 Product mass-fraction fields for forced cases with infinite reaction speed. (a) and (b) are the uniform and variable density, $Q_0=4$, cases respectively and (c) is the variable density, $Q_0=6$, case. The time is $t=10$ for all cases. Ten shade intensities (white to black) equally subdivide the mass fraction scale $0<Y_r<1$. 
Figure 5.29 Time-averaged density profile comparison between the finite and infinite reaction speed, $Q_0=4$, forced cases. The streamwise location is $x=3$. 
Figure 5.30  Vorticity contours for the infinite reaction, \( Q_0 = 4 \), case, at time \( t = 10 \). Dotted/continuous lines indicate positive/negative vorticity. The contour increment is 0.4

Figure 5.31  Contours of the baroclinic vorticity generation term for the infinite reaction, \( Q_0 = 4 \), case, at time \( t = 10 \). Dotted/continuous lines indicate positive/negative vorticity. The contour increment is 0.4
Figure 5.32 Comparison of the flow-divergence fields between the $Q_0=4$, (a), and $Q_0=6$, (b), forced cases for which the recation speed is infinite. The time $t=10$ for both cases. Ten shade intensities (white to black) equally subdivide the plotting scale which ranges from 0 to 0.2
Figure 5.33 Investigation of the effect of expansion and baroclinicity on the flowfield for the infinite reaction speed, $Q_0=4$, case. In (a) both mechanisms are eliminated. In (b) they are both active. In (c) only expansion is present and in (d) only baroclinicity.
Figure 5.34 Comparisons of the Favre-averaged turbulent shear stress (a) and kinetic energy (b) profiles, between the uniform density case and the Qo=4 variable density and uniform flow-density (but with the reacting field density in the calculation of the averaged quantities), infinite reaction speed, forced cases. The streamwise location is x=2.5.
Figure 5.35 Comparison of the streamwise evolution of the product thickness between the variable density and the uniform flow-density, infinite reaction speed, forced, $Q_0=4$ (a) and $Q_0=6$ (b) cases. The thicknesses of the uniform flow-density cases using a uniform density for the scalar field are also shown.
Figure 5.36 Comparison of the streamwise evolution of the product thickness profiles between the $Q_0=4$ & 6, infinite reaction speed, forced cases.
Figure 5.37 $\lambda (=Y_1-\phi Y_2)$ fields for forced cases with infinite reaction speed. (a) and (b) are the uniform flow-density and variable density, $Q_0=4$, cases respectively and (c) is the variable density, $Q_0=6$, case. The time is $t=10$ for all cases. Ten shade intensities (white to black) equally subdivide the plotting scale, $-1<\lambda<1$. The white contour indicates the locus of $\lambda=0$ and denotes the reaction interface.
6. AN UNSTEADY STRAINED FLAMELET MODEL FOR
   FAST COMBUSTION IN A SHEAR LAYER—EFFECT OF
   STEADY AND PERIODIC STAIN ON DIFFUSION FLAMES

6.1. Introduction

In previous chapters a numerical methodology was presented and implemented in
the determination of a shear layer flow experiencing moderately fast, or infinitely fast
combustion. The numerical problems associated with extending this methodology to very
high but still finite speed combustion were discussed in Chapter Six. Therein it was
pointed out that in such a case both higher temporal and spacial numerical resolutions
become necessary. The need for a higher temporal resolution is a direct consequence of the
smaller reaction time scale. The higher spacial resolution is a manifestation of the fact that
under fast combustion conditions the reaction zone becomes exceedingly thin. These
increased resolution requirements substantially amplify the cost of accurate numerical
solutions.

In this chapter an alternative approach in dealing with the fast but finite reaction
speed regime is introduced. A new numerical scheme yielding the reacting-scalar field by
segmenting the flame (reaction region) along its length into a series of Lagrangian strained
diffusion flamelets, is considered. Herein the part of the scheme describing the individual
characteristics of a flamelet is presented and it is used in a study of flat, strained diffusion
flames. The remaining features of the scheme, namely the determination of the global
reacting-scalar field from the flamelet solutions and the evaluation of the flowfield (which is
to be provided by the Vortex Element Method) are to be presented in future work.

The basis of the strained diffusion flamelet model lies on the earlier noted fact that
as the reaction speed increases the reaction zone thickness decreases. This results in a thin
flame whose surface area is a strong function of the turbulent flow and is governed by the
competition between flame area generation due to stretch and consumption due to burning.
To a smaller scale, and in a frame of reference local to itself, this flame may appear laminar and can be approximated as a flat and one dimensional structure which is stretched by the local flowfield (see figure 6.1). Hence, the concept of a flamelet arises: a small, flat, one-dimensional piece of a laminar flame which senses the surrounding flow via the local Lagrangian strain.

Diffusion flamelets have been used before in the study of flow-combustion interactions in the presence of fast reaction [68]. (For other regimes, see ref. [69]). Most studies have only considered the effect of steady strains on the burning rate or quenching of the strained flamelet [70]. Exceptions include ref.[71] where the effect of small amplitude oscillation was considered using asymptotic analysis, ref.[72] where the effect of unsteady strain on a fuel strip was evaluated and ref.[73] where ignition computations were presented. Turbulence exerts an unsteady strain on the reaction zone, which can be modeled as a superposition of a mean and an oscillating strain with a characteristic time scale and amplitude. The amplitude and frequency of the oscillating strain component can impact unsteady chemical processes, such as ignition and quenching, whose initiation depends on local instantaneous values of strain, temperature and species concentrations. In this work, unsteady processes resulting from the application of a steady strain, and the effects of oscillating strains are analyzed.

Steady strain models ignore several fundamental features of turbulence-combustion interactions. In particular, the unsteady response of combustion and transport processes to the variations in the turbulent field is removed. In a turbulent flow, the strain field varies with a time scale determined by the flow time scale and a flamelet is not subjected to a constant strain for a time longer than such a scale. Whether this transient is long enough to cause quenching, if the strain exceeds the quenching strain, is not clear; and if it leads to local quenching, how long does the flamelet take to re-ignite? The re-ignition time depends on the local conditions, i.e. the prevailing strain rate, reactants premixing, and the temperature or ignition source. It is important to understand and quantify the impact of
these unsteady mechanisms on flamelet properties such as ignition and quenching times and how they relate to the characteristics of the ignition source.

Another question which arises in the application of flamelet models is the effect of periodic strain, being a more realistic model of a turbulent flow, on the burning rate. Since chemical kinetics are nonlinear functions of temperature, the steady burning rate computed using a mean steady strain need not be the same as the burning rate evaluated by averaging the instantaneous response of the burning rate to a periodic strain. This nonlinearity is compounded by the continuous adjustment of the reaction zone structure, which depends on the local flow conditions and species distribution, according to the imposed unsteady strain.

In this work, we use a one-dimensional, one-step Arrhenius-kinetics flamelet model to quantify the effects of steady and periodic strains on diffusion flamelets. These effects are shown to play a dominant role in the development of unsteady chemical processes, namely ignition, quenching and extinction. The importance of properly accounting for these mechanisms in flamelet models is one of the conclusions of this study.

6.2. Formulation

The assumptions defining the flamelet model require a formulation of the governing equations which differs from the one presented in Chapter Two. The same is also true for the associated nomenclature. Hence, in this chapter a new formulation is introduced and in an attempt to avoid confusion with previous chapters the related nomenclature is explicitly given in Section 6.5.

In a coordinate system moving with the flame front, with axes (x,y) that are locally tangential and normal to its surface, respectively, the continuity, species and energy equations are:
Table 6.1

Continuity
\[ \frac{\partial \rho}{\partial t} + \rho \mathbf{v} + \frac{\partial (\rho \mathbf{v})}{\partial y} = 0 \quad (6.1) \]

Chemical Reaction
\[ \phi_f \chi_f + \chi_o \rightarrow (\phi_f+1) \chi_p \quad (6.2) \]

Equation of State
\[ \rho T = \text{constant} = \rho_{in} T_{in} \quad (6.3) \]

Temperature
\[ \frac{\partial T}{\partial t} + \mathbf{v} \cdot \frac{\partial T}{\partial y} = \frac{1}{\rho c_p} \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \frac{h_f \dot{w}_f}{\rho c_p} \quad (6.4) \]

Species
\[ \frac{\partial Y_j}{\partial t} + \mathbf{v} \cdot \frac{\partial Y_j}{\partial y} = \frac{1}{\rho} \frac{\partial}{\partial y} \left( \rho D_j \frac{\partial Y_j}{\partial y} \right) + \frac{\dot{w}_j}{\rho} \quad j = f, o \quad (6.5) \]

\[ Y_p = 1 - (Y_f + Y_o) \quad (6.6) \]

Reaction rate
\[ \dot{w}_f = - (\phi_f B / W_f) \rho^2 Y_f Y_o \exp (-T_o/T) \quad (6.7a) \]

\[ \dot{w}_o = \frac{\dot{w}_f}{\phi_f} \quad (6.7b) \]

where the symbols are defined in Section 6.5. Solutions are sought along the stagnation line \( x = 0 \).

In the case of equal mass diffusivities, \( \rho^2 D = \text{constant} \), and a unity Lewis number, the equations governing the Shvab-Zeldovich variables \( \lambda = Y_f - \phi_f Y_o \) and \( \gamma = \frac{T}{T_{in}} - \frac{h_f}{c_p T_{in}} Y_f \), are devoid of source terms. A series of coordinate transformations is applied to transform the governing equations into a diffusion equation for \( \lambda \) and \( \gamma \) and a reaction-diffusion equation for \( Y_f \).

(1) The density is eliminated using the Howarth-Dorodnitzyn transformation,

\[ (y,t) \leftrightarrow (\zeta,t) : \]

\[ \zeta = \int_0^y \tilde{\rho} \, dy \quad \text{where} \quad \tilde{\rho} = \frac{\rho}{\rho_{in}} \quad (6.8) \]
(2) A transformation \((\zeta, t) \leftrightarrow (\tilde{\zeta}, \tau)\) is implemented to absorb the stretch,

\[
\tilde{\zeta} = \zeta \exp\left(\int_0^t \epsilon(\hat{t}) \, d\hat{t}\right) \quad \text{and} \quad \tau = \int_0^t \exp\left(2\int_0^\hat{t} \epsilon(\hat{t}) \, d\hat{t}\right) \, d\tilde{\tau} \quad (6.9)
\]

(3) A translation \((\tilde{\zeta}, \tau) \leftrightarrow (\xi, \tau)\) is used to move the coordinates with the original material interface:

\[
\xi = \tilde{\zeta} - \int_0^t V(t') \, dt' \quad \text{where} \quad V(t) = (\rho V)_{y=0} \exp\left(\int_0^t \epsilon(t') \, dt'\right) \quad (6.10)
\]

The solution of the diffusion equations for \(\lambda\) and \(\gamma\) is written in terms of the similarity variable \(\eta = \frac{\xi}{\sqrt{4D_{\text{lin}} \tau}}\), and the boundary conditions, \(y \to \infty\), \(Y_f \to 1\), \(Y_0 \to 0\), and \(T \to T_{\text{in}}\) while \(y \to -\infty\), \(Y_f \to 0\), \(Y_0 \to 1\), and \(T \to T_{\text{in}}\), are incorporated to find:

\[
\lambda = \frac{(1+\phi_f)}{2} \text{erf} \eta + \frac{(1-\phi_f)}{2}, \quad (6.11)
\]

\[
\gamma = 1 - \frac{hr}{2cpT_{\text{in}}} \left(1 + \text{erf}\eta\right), \quad (6.12)
\]

while, equation (6.5) becomes:

\[
\frac{\partial Y_f}{\partial \tau} = D_{\text{lin}} \frac{\partial^2 Y_f}{\partial \xi^2} + \frac{dt}{\partial \tau} \frac{\dot{Y}_f}{\rho} \quad (6.13)
\]

Equation (6.13) is numerically integrated using a Crank-Nicolson scheme, and its solution is combined with the solutions of the Shvab-Zeldovich variables (eqs.(6.11) & (6.12)) to yield \(Y_0\) and \(T\). The change of \(Y_f\) is determined by a competition between diffusion and reaction rates. Their ratio defines a Damkohler number, \(Da = \tau_{\text{flow}}/\tau_{\text{chem}}\). (The difference between this definition of the Damkohler number and the one used in previous chapters should not go unnoticed. The Damkohler number used here is in fact an inverse Karlovitz number.) The fast chemistry solution, obtained in ref.[70,74], applies exactly when
Da \to \infty, or approximately when Da >> 1. For low Damkohler numbers, equation (6.13) is integrated.

6.3. Results

Computations were performed to illustrate the effect of the competition between a steady and a periodic strain and finite-rate kinetics on the burning rate, quenching and extinction, and to investigate the role of the ignition, or flame stabilization source in these processes. We used the following parameters in all the computations, \( T_{in} = 300^\circ K, T_a = 10, T_f = 6, D_m = 10^{-4} \text{ m}^2/\text{s}, \phi_f = 1, B = 3.18 \times 10^7 \text{ s}^{-1}, \) leading to a chemical time scale \( \tau_{chem} = 10^{-6} \text{ s}. \) The flow-time scale was taken as \( 1/\epsilon_s. \) The initial conditions were determined by allowing the two reactants to diffuse for several time steps producing a thin, mixed zone. The mixture was then ignited by raising its temperature so that it reaches the adiabatic flame limit, \( T_f, \) in the middle of the mixing zone and falls off to the ambient temperature, \( T_{in}, \) at the boundaries of the mixing zone according to a Gaussian curve. It was found that the thickness of the initial diffusion zone has no effect on the long-term behavior of the problem. The effect of the ignition mechanism on the flame history was investigated by changing the duration of the ignition source.

6.3.1. Simple Spark Ignition–Steady Strain

In this model, the strain rate is held constant and the spark is allowed to last for a single time step, \( \Delta t = 10^{-7} \text{ s}. \) Figure 6.2 shows the burning rate, \( m'', \) from the moment of sparking until a steady state is reached. For zero strain, the reaction rate reaches a maximum and then decays to zero due to the depletion of reactants within a mixing zone of increasing thickness. For low strains, \( m'' \) rises to a maximum and falls off to reach a plateau which increases with strain. The high value of \( m'' \) during the transient is due to high initial concentration of reactants within the mixing zone. It takes longer for the flame to reach steady state under conditions of strong strain, i.e. a strained flame resists ignition.
The ignition time increases substantially close to quenching. At \( \varepsilon_s = \varepsilon_{\text{spark}} = 5.5 \times 10^4 \text{ s}^{-1} \), which corresponds to \( \text{Da}_{\text{spark}} = 18.2 \), the flame simply cannot ignite using a short-duration spark. This transition is abrupt and, as shown below, the critical value, \( \varepsilon_q \), depends on the ignition mode.

Figure 6.3 shows the change of the steady-state burning rate, \( m_s^* \), and the corresponding maximum temperature, \( T_{\text{max}} \), with the steady strain. \( m_s^* \) increases continuously with \( \varepsilon_s \) as more reactants are convected/diffused towards the flame. The reaction rate reaches a maximum at the point of quenching when the heat released by the chemical reaction can no longer sustain the reaction. This occurs as \( T_{\text{max}} \) decreases slowly, then at a faster rate as the strain rate increases. Sudden quenching is due to the nonlinear dependence of \( m^* \) on the temperature. The lower part of this curve corresponds to very low reaction rates sustained at low temperatures. The behavior of strained flames is qualitatively similar to combustion in a well-stirred reactor in which \( m^* \) reaches a maximum which depends on the chemical time scales and then falls off sharply to very small values as the flow rate is increased.

6.3.2. Pilot Flame Ignition

6.3.2.1. Steady Strain

The critical dependence of the flame response on temperature suggests that the burning history strongly depends on the duration of the ignition source and its temperature. In the pilot-flame ignition, the temperature within the reaction zone is maintained until the maximum \( m^* \), estimated by gradually raising the strain of a sustained flame until it quenches, was achieved and then the ignition source is removed. From extensive experimentation, we found that this ignition mode is sufficient for the establishment of a self-sustained strained flame, if at all possible.

Figure 6.4 shows the burning history of a strained flame ignited by a pilot-flame. The flame can sustain higher strain before it quenches at \( \varepsilon_{\text{q, pilot}} = 12 \times 10^4 \text{ s}^{-1} \),
corresponding to $Da_{\text{PILOT}} = 8.3$. This value of $\varepsilon_q$ is the maximum possible steady strain that the flame can sustain without quenching, hence it is a characteristic value of the problem, $\varepsilon_{qc}$. $T_{\text{max}}$ and $m^s_*$ are shown in figure 6.3. For small strains, $m^s_*$ is identical to that of the spark-ignited case. Thus, as previously stated, $m^s_*$ of the sustained flame is independent of the ignition mode. However, the quenching strain for the pilot-ignited-flame is almost twice as large as that of the spark-ignited flame.

As the strain approaches $\varepsilon_{qc}$, $m^s_*$ approaches a constant value. This is due to two competing effects, both induced by the strain field. As $\varepsilon_s$ increases, the reactants concentrations within the reaction zone increase but $T_{\text{max}}$ decreases. Thus, some reactants leave the reaction zone unburnt. This process is qualitatively similar to the well-stirred reactor response to increasing the reactants flow rate.

Application of a strong strain changes the steady-state thickness of the combustion zone in the manner illustrated in figure 6.5. Both the reaction zone thickness, $\delta_w$, defined as the region where $\dot{\omega}_f > 1\%\dot{\omega}_{f_{\text{max}}}$, and the product thickness, $\delta_p$, defined as the region where $0.01 \leq Y_p \leq 0.99$, are shown. $\delta_p$ defines a diffusion zone, while $\delta_w$ determines a chemical activities zone. Strain reduces both values with the reduction being more pronounced for $\delta_p$. The reduction is accompanied by a rise in the concentration of $Y_f$ and $Y_o$ within the reaction zone resulting in a net increase in $m^*$, i.e. the rise of $Y_fY_o$ compensates for the drop in $T_{\text{max}}$ and reaction zone thickness. Near quenching, the thickness of the reaction zone approaches that of the products and reaches a characteristic value, $\delta_{w qc}$ which could be used as a length scale of a diffusion flame [68]. Figure 6.5 also shows the ignition time, $\tau_{ig}$, defined as the time it takes $m^*$ to reach its maximum value, for spark and pilot ignition modes.

6.3.2.2. Periodic Strain

Here, we assume that the diffusion flame is subjected to the passage of a train of vortices which exert a periodic strain rate on top of the mean strain induced by the mean flowfield and use the following relationship for the strain rate:
\[ \varepsilon(t) = \varepsilon_s + \varepsilon' \sin(2\pi ft) \]  \hspace{1cm} (6.8)

The flow time scale is defined as \(1/\varepsilon_s\). Results indicate that as long as \(\varepsilon_{\text{max}} = \varepsilon_s + \varepsilon' < \varepsilon_{\text{qc}}\) and \(\varepsilon_{\text{min}} = \varepsilon_s - \varepsilon' > 0\), where \(\varepsilon_{\text{qc}}\) is the steady-state quenching strain rate computed above, the burning rate averaged over many strain cycles, \(m_{\text{av}}\), is well approximated by the rate of burning under constant strain, \(\varepsilon_s\), despite the fact that the instantaneous behavior may vary drastically. Otherwise, we observe two different phenomena: quenching which occurs due to flame cooling when \(\varepsilon_{\text{max}} > \varepsilon_{\text{qc}}\), and extinction which occurs when \(\varepsilon_{\text{min}} < 0\) and the supply of reactants diminishes. The results of unsteady strain are summarized in figure 6.6 where \(m_{\text{av}}\) is plotted against \(\varepsilon'\). To explain these results, we distinguish between the following two cases:

(i) \(\varepsilon_s > \varepsilon_{\text{qc}}/2\) and \(\varepsilon_s + \varepsilon' > \varepsilon_{\text{qc}}\). Typical results of this case are shown on the right-hand side of figure 6.6 where curves are plotted for different strain oscillation frequencies, \(f\). In all cases, \(\tau_{\text{chem}} = 10^{-6} \text{ s}\). We use \(\varepsilon_s = 1/\tau_{\text{flow}} = 8.0 \times 10^4 \text{ s}^{-1}\), and \(f = \frac{1}{n \tau_{\text{flow}}}\) with \(n = 4, 8, 16\) and 24. Figure 6.6 shows that, for high-frequency fluctuation \((f = \frac{1}{4 \tau_{\text{flow}}})\), \(m_{\text{av}}\) is almost independent of \(\varepsilon'\). For lower \(f\), \(m_{\text{av}}\) decreases with \(\varepsilon'\) and suffers a sharp drop as the total strain exceeds the quenching strain. As shown below, the drop in \(m_{\text{av}}\) is due to partial quenching of the unsteady flame, which results in a substantial decrease in the instantaneous \(m''\). This process is followed by re-ignition of the flame during low strain part of the cycle. For very high amplitudes, quenching is permanent, i.e. the flame does not have time to re-ignite in the low strain part of the cycle. The effect of oscillating strain is stronger when \(f\) is low, i.e. high frequency fluctuating strain, even when its amplitude is high, weakly affects the flame. On the other hand, the lower \(f\) is, the more pronounced the oscillating strain effect becomes and permanent quenching occurs even at lower oscillation amplitudes.

Detailed results of two cases, which are typical of burning and quenching flames due to the change in \(\varepsilon'\) at a fixed \(f\) and labeled as cases 1 and 2 in figure 6.6, are shown in figures 6.7 and 6.8. For cases 1 and 2, \(f = \frac{1}{16 \tau_{\text{flow}}}\), and \(\varepsilon' = 2 \times 10^4 \text{ s}^{-1}\) and \(7 \times 10^4 \text{ s}^{-1}\),
respectively. While, as indicated in figure 6.6, case 2 suffers permanent quenching following the initial ignition phase due to high $\varepsilon'$, case 1 exhibits periodic out-of-phase undulation of $m''$ and $T_{\text{max}}$. The effect of $f$ on the reduction of $m''$ is shown in figure 6.9, which details case 3 of figure 6.6. Case 3 has the same value of $\varepsilon'$ as case 2, but higher frequency, $f = \frac{1}{8 \tau_{\text{flow}}}$. In this case, the high frequency strain oscillation guards against permanent quenching, and periodic variation of $m''$ and $T_{\text{max}}$ are established. However, $m_{\text{av}}''$ is smaller than that of a flame subjected to the steady mean strain. The response of $m''$ to high amplitude oscillation is characterized by sharp peaks and valleys, and significantly departs from the shape of the sinusoidal strain component. The non-linear dependence of $m''$ on the temperature and the disparity between chemical, flow and diffusion time scales all contribute to this effect. The results also show how the mean and instantaneous behavior may vary substantially between cases which have the same mean and oscillating strain but differ in the frequency.

(ii) $\varepsilon_s < \varepsilon_{qc}/2$ and $\varepsilon_s - \varepsilon' < 0$. Typical results for this case are shown on the left-hand side of figure 6.6, where curves are plotted for different strain oscillation frequencies. In this case, we use $\varepsilon_s = 1/\tau_{\text{flow}} = 2.0 \times 10^4 \text{ s}^{-1}$, and $f = \frac{1}{n \tau_{\text{flow}}}$ with $n = 1, 2, 4$ and 16. The figure shows that increasing the amplitude of the fluctuating strain, while fixing the mean value, decreases $m''_{\text{av}}$ at a slow rate until $\varepsilon_s - \varepsilon' < 0$, i.e. when compressive strains are established. In this regime, $m''$ drops due to extinction of the flame. Extinction occurs due the depletion of reactants as compressive strains reduce the transport fluxes of reactants into the "reaction zone" although the temperature there remains high. Extinction is not permanent and the reaction resumes as soon as positive strains are recovered since the temperature in the reaction zone is high.

Detailed results of a representative case, which is typical of partial extinction and labeled case 4 in figure 6.6, are shown in figure 6.10. For case 4, we set $\varepsilon' = 8.0 \times 10^4 \text{ s}^{-1}$ and $f = \frac{1}{4 \tau_{\text{flow}}}$. In this case, the total strain never exceeds the quenching strain, $\varepsilon_{qc}$, but a compressive strain subcycle is imposed so that extinction may occur. Here too, out-of-
phase variation of $m''$ and $T_{\text{max}}$ are observed. As the strain decreases below its mean value, the temperature reaches a maximum when all the reactants are burnt. At this point, extinction occurs. Intermittent extinction reduces $m''$ below the value obtained for the mean strain applied continuously, as shown in figure 6.6. At lower frequency, the extinction part of the cycle lasts longer.

6.4. Conclusions

(1) The ignition delay time required to reach steady burning increases exponentially with strain when the mixture is ignited by a short-duration source. This delay is substantially reduced when the ignition source is sustained. The latter also increases the value of the quenching strain.

(2) The burning rate depends on the fluctuating strain amplitude and frequency. Weakest dependency occurs when positive strains, bounded by the steady quenching strain, prevail. In this case, the averaged burning rate is close to the steady burning rate obtained using the mean strain.

(3) For high amplitude strain fluctuation, the flamelet is quenched as the total strain exceeds the quenching strain. For low frequency oscillations, permanent quenching is more likely to occur as high strain is maintained for a long duration. Partial quenching is encountered when the frequency is increased. The averaged burning rate approaches the burning rate corresponding to the mean strain as the frequency increases.

(4) Compressive strains inhibit reactants' diffusion into the reaction zone, and lead to partial extinction of the flamelet. Extinction is not permanent since the flamelet reignites as soon as positive strains resume. Intermittent extinction results in an average burning rate smaller than the steady burning rate obtained using the mean strain.
The results show that the modeling of unsteady processes is of major importance especially in turbulent combusting flows, in which rapidly varying modes of instability may develop simultaneously. Hence, a successful numerical determination of turbulent combustion at high Damköhler numbers can be achieved via the implementation of a time dependent flamelet model, like the one presented above, in conjunction with a flow simulation which accommodates rapid strain variations, like the Vortex Element Method.

6.5. Nomenclature

B
pre-exponential factor

c_p
specific heat at constant-pressure

D_a
Damköhler number ($\tau_{\text{flow}}/\tau_{\text{chem}}$)

D
mass diffusivity

f
frequency

h_r
enthalpy of reaction per unit mass of fuel

k
thermal diffusivity

m''
burning rate per unit flamelet area

(x,y)
local normalized coordinates

(u,v)
velocity

T
temperature

T_a
activation energy divided by the gas constant

T_{fl}
adibatic flame temperature

t
time

W
molecular weight

\dot{w}
mass burning rate

Y
mass fraction

Greek Symbols
\( \Delta t \) time step

\( \delta_p \) and \( \delta_w \) product and reaction thickness

\( \varepsilon \) strain rate in the direction of the flame front \( x \)

\( \varepsilon' \) oscillating strain component

\( \phi_f^* \) and \( \phi_f \) molar and mass stoichiometry

\( \lambda, \gamma \) Shvab-Zeldovich variables

\( \eta \) similarity variable

\( \rho \) density

\( \tau \) transformed time

\( \tau_{\text{flow}} \) flow time scale \( (\equiv 1/e_{\delta}) \)

\( \tau_{\text{chem}} \) chemistry time scale \( (\tau_{\text{chem}} = \left[ \frac{\phi_f B \rho_{\text{in}} \exp(-T_{a}/T_{\text{fl}})}{W_f} \right]^{-1}) \)

\( \zeta, \tilde{\zeta}, \xi \) transformed y coordinate

**Subscripts**

\( q, q_c \) quenching, characteristic quenching

\( o, f \) and \( p \) oxidizer, fuel and product

\( \text{max, min} \) maximum, minimum

\( \text{av} \) average

\( s \) steady

\( \text{fl} \) flame

\( \text{ig} \) ignition

\( \text{in} \) initial
Figure 6.1 Schematic illustration of the approximate representation of the thin diffusion flame by a number of one-dimensional strained flamelets.
Figure 6.2  Evolution of the burning rate for a spark-ignited diffusion flame subjected to steady strain. The value of the strain rate is indicated.
Figure 6.3  Effect of steady strain on the steady burning rate and maximum flame temperature in both, the spark-ignited and pilot flame ignited cases.
Figure 6.4 Evolution of the burning rate for a pilot-ignited diffusion flame subjected to steady strain. The value of the strain rate is indicated.
Figure 6.5 Effect of steady strain rate on the steady product and reaction zone thicknesses for pilot-ignited flames. The ignition time for both spark-ignited and pilot-ignited flames are also plotted.
Figure 6.6 Effect of periodic strain amplitude on the mean burning rate in a pilot-ignited diffusion flame. The amplitude of the mean strain component and the frequency of the oscillating component are indicated.
Figure 6.7 Evolution of (a) strain rate, (b) maximum temperature, and (c) burning rate, for a diffusion flame subjected to a periodic strain with $\varepsilon_s = 8 \times 10^4$ s$^{-1}$, $\varepsilon' = 2 \times 10^4$ s$^{-1}$, and $f = \frac{1}{16} \frac{1}{\tau_{flow}}$. 
Figure 6.8  Evolution of (a) strain rate, (b) maximum temperature, and (c) burning rate, for a diffusion flame subjected to a periodic strain with $\varepsilon_s = 8 \times 10^4$ s$^{-1}$, $\varepsilon' = 7 \times 10^4$ s$^{-1}$, and $f = \frac{1}{16 \tau_{flow}}$. 
Figure 6.9  Evolution of (a) strain rate, (b) maximum temperature, and (c) burning rate, for a diffusion flame subjected to a periodic strain with $\varepsilon_s = 8 \times 10^4$ s$^{-1}$, $\varepsilon' = 7 \times 10^4$ s$^{-1}$, and $f = \frac{1}{8 \tau_{flow}}$. 

(a) STRAIN: $\varepsilon_s = 8 \times 10^4$ [1/s], $\varepsilon' = 7 \times 10^4$ [1/s], $f = 0.125/\tau_f$
Figure 6.10 Evolution of (a) strain rate, (b) maximum temperature, and (c) burning rate, for a diffusion flame subjected to a periodic strain with $\varepsilon_s = 2\times 10^4$ s$^{-1}$, $\varepsilon' = 8\times 10^4$ s$^{-1}$, and $f = \frac{1}{4 \tau_{flow}}$. 
CONCLUSIONS

The Transport–Reaction Element Method (TREM), a numerical scheme which resolves an exothermically reacting scalar field, was developed as an extension of the earlier proposed [38] non-reacting Transport Element Method (TEM). The new scheme is used in conjunction with the Vortex Element Method (VEM) which is capable of resolving a post-transitional flowfield. The two schemes solve the unaveraged, time dependent and coupled scalar transport-reaction and Navier-Stokes equations respectively, in their scalar-gradient and vorticity forms. They are both Lagrangian grid-free and adaptive, i.e. a set of computational elements evolves with the flowfield to capture the time dependent scalar-gradient and vorticity distributions. The trem exploits the Shvab-Zeldovich formulation to concentrate computational effort on the solution of only one transport-reaction scalar equation. It also readily provides solutions for both moderately fast and infinitely fast reaction speeds. For finite reaction speeds Arrhenius kinetics were assumed.

The developed methodology was implemented in simulations of both non-reacting and reacting turbulent shear layers. Simulation results for the non-reacting variable density shear layer, i.e. the flow evolving between two fluids of different velocities and densities, followed experimentally established trends. The rate of growth of the layer was found to increase as the slow stream became denser. The same was true of the ratio of volume of fluid entrained from the fast and slow streams. In contrast, the speed of the vortical structures (eddies) characterizing this flow, was decreased as the density of the slow stream was increased. The eddy speed was also found to coincide with the phase speed of the instability waves predicted by the linear stability analysis. Explanations for most of these effects where traced to the mechanism of baroclinic vorticity generation, the only added mechanism of vorticity modification in the presence of a variable density field. It was found that baroclinicity redistributes the vorticity in such a way that positive (counterclockwise) vorticity appears on the denser stream side.
External forcing of the flow instability at both the fundamental and subharmonic frequencies was found to alter the growth characteristics of the layer. It was established that the forced growth behavior correlates with, and is a consequence of, the momentum ratio between the two fluid streams. The lack of an apparent relation of the growth of the unforced layer with the momentum ratio was attributed to the nature of the initial conditions and the instability characteristics of the flow.

Reacting shear layers were simulated for different values of the enthalpy of reaction for both finite and infinite reaction speeds, and the effects of the combustion heat release on the flow were investigated. It was established that the growth of the layer was decreased in the presence of heat release. This was a consequence of both a substantial delay in the destabilization of the flow as well as a suppression of the interactions of the vortical structures. The reduced layer growth, coupled with the decreased density within the shear-mixing region, resulted in diminished product formation and hence efficiency of burning. When the flow was externally forced in such a way as to promote pairing interactions of the vortical structures, the reduction in shear layer growth and amount of product formed persisted. The growth reduction was, in this case, mainly a consequence of a modification of the eddy interaction mechanism from pairing, which continued to be resisted, to tearing of smaller eddies by larger neighbors.

Explanations for these effects were sought by investigating the effects of volumetric expansion and baroclinic vorticity generation, the two main mechanisms by which the combustion-related density field modifies the flowfield, on the downstream evolution of the vorticity-material layer separating the two fluids at the inlet. Both the flow and reacting fields were found to be strongly related to the locus of this layer. It was determined that volumetric expansion reduces the shear region growth, by decaying the vorticity field and hence decreasing the layer rollup. Baroclinic vorticity generation, on the other hand, was found to be responsible for the suppression/modification of the eddy interactions by
rearranging the vorticity of the layer in such a way that positive vorticity appears surrounding the eddies.

Comparison of results for finite and infinite reaction speeds have indicated that the infinite reaction speed model offers a simple, computationally cost effective approach in ascertaining the effects of the combusting field on the flowfield.

Finally, a strained flamelet model was developed as a basis of a future methodology which will deal with very fast but finite reaction speeds. The model was used in an investigation of the effects of steady and periodic strains on diffusion flames. Flame ignition time was found to increase exponentially with increasing strain, the ignition delay decreasing as the duration of the ignition source was increased. The mean burning rate of the flame was substantially modified by unsteady strains only in the cases where abrupt transient phenomena like quenching extinction and re-ignition were experienced to some degree.
APPENDIX A

Derivation of the Discrete, Desingularized Integrals for Vortical and Expansion Velocity

These integrals are manifestations of the integration of Poisson equations, i.e.

\[ \nabla^2 \psi = - \omega \quad \Rightarrow \quad \text{Vortical velocity} \quad (u_\omega = \nabla_x(\psi \hat{k})) \]

\[ \nabla^2 \phi_e = - \frac{1}{\rho} \frac{d\rho}{dt} \quad \Rightarrow \quad \text{Expansion velocity} \quad (u_e = \nabla \phi_e) \]

where all symbols as earlier defined.

In 2-D cylindrical (polar) coordinates these equations can be written in the generic form

\[ \frac{1}{r \frac{d}{dr}} \left( r \frac{\partial \Phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \Phi}{\partial \theta^2} = W \]

where for \( \Phi = \psi \), \( W = - \omega \) and for \( \Phi = \phi_e \), \( W = - \frac{1}{\rho} \frac{d\rho}{dt} \).

The velocity field set up by one element is first considered. The total field is subsequently obtained by summing all the individual element fields.

For simplicity the element is positioned at the origin. The vorticity and substantial density derivative fields in the neighborhood of the element are given by the radially symmetric core function \( f_\delta \) i.e.

\[ P = P_i A_i f_\delta \]

where

\[ f_\delta = \frac{1}{\pi \delta^2} \exp \left(-\frac{r^2}{\delta^2}\right) \]

\( P \) is \( \omega \) or \( - \frac{1}{\rho} \frac{d\rho}{dt} \) and \( P_i \) and \( A_i \) are the strength and area of the element respectively. Thus, \( W \) (which is directly related to \( P \)) is radially symmetric and the solution for \( \Phi \) in an infinite domain will also be radially symmetric (i.e. \( \frac{\partial}{\partial \theta} = 0 \)). Thus, the Poisson equation reduces to:

\[ \frac{1}{r \frac{d}{dr}} \left( r \frac{\partial \Phi}{\partial r} \right) = W \]

which after rearranging and integrating is transformed to:
\[
\frac{\partial \Phi}{\partial r} = \frac{1}{r} \int_{r}^{r'} W \ r' \ dr'
\]

Substituting for \( W \) and performing the integration:

\[
\frac{\partial \Phi}{\partial r} = \frac{W_i A_i}{2 \pi r} \left( 1 - \exp \left( -\frac{r^2}{\delta^2} \right) \right)
\]

(A)

**Vortical Velocity**

For this case \( \Phi = \psi \) and \( W_i = - \omega_i \) and the relationship between the vortical velocity and the streamfunction dictates that

\[
\frac{\partial \psi}{\partial r} = - v_\theta
\]

where \( v_\theta \) is the component of velocity in the \( \theta \) direction. Thus, equation (A) is rewritten as

\[
v_\theta = \frac{\Gamma_i}{2 \pi r} \left( 1 - \exp \left( -\frac{r^2}{\delta^2} \right) \right)
\]

where \( \Gamma_i = \omega_i \ A_i \). The components of this velocity in cartesian coordinates are given by

\[
u = v_\theta \cos(\theta) = v_\theta \ \frac{x}{r}
\]

\[
v = v_\theta \sin(\theta) = v_\theta \ \frac{y}{r}
\]

where \( r = \sqrt{x^2 + y^2} \). Thus, the vortical velocity due to the element, in cartesian coordinates is given by

\[
u = (u, v) = \frac{\Gamma_i}{2 \pi} \left( \frac{y, x}{r^2} \right) \left( 1 - \exp \left( -\frac{r^2}{\delta^2} \right) \right)
\]

The corresponding expression for an element not at the origin is straightforwardly arrived at, by shifting the origin to the element location, i.e.

\[
u = \frac{\Gamma_i}{2 \pi} \left( \frac{-(y-y_i), (x-x_i)}{(r-r_i)^2} \right) \left( 1 - \exp \left( -\frac{(r-r_i)^2}{\delta^2} \right) \right)
\]

The total vortical velocity field is obtained through a summation of the contributions of all the elements. This can be written as:
\[ u_\omega = \sum_{i=1}^{N} \Gamma_i K_\delta(x-x_i) \]

where \( N \) is the total number of elements and

\[ K_\delta(x) = \bar{K}(x) \frac{F(r)}{\delta} \]

with

\[ \bar{K}(x) = -\frac{(y_r-x_r)}{2\pi r^2} \quad \text{and} \quad F(r) = 1 - \exp(-r^2) \]

which is the discrete desingularized form given in the main text.

**Expansion Velocity**

For this case \( \Phi = \phi_e \), \( W_i = \left( -\frac{1}{\rho} \frac{dp}{dt} i \right) \) and the relationship between the expansion velocity and the expansion potential dictates that

\[ \frac{\partial \phi_e}{\partial r} = v_r \]

where \( v_r \) is the velocity in the radial (r) direction. Hence, equation (A) is rewritten as:

\[ v_r = \frac{-\frac{1}{\rho} \frac{dp}{dt} A_i}{2\pi r} \left( 1 - \exp\left( -\frac{r^2}{\delta^2} \right) \right) \]

Noting that the components of the radial velocity in cartesian coordinates are given by

\[ u = v_r \cos(\theta) = v_r \frac{x}{r} \]

\[ v = v_r \sin(\theta) = v_r \frac{y}{r} \]

then the element-induced expansion velocity vector is given by

\[ u = (u, v) = \left( -\frac{1}{\rho} \frac{dp}{dt} \frac{A_i}{2\pi} \frac{(x, y)}{r^2} \left( 1 - \exp\left( -\frac{r^2}{\delta^2} \right) \right) \right) \]

For an element not at the origin the corresponding expression is obtained as was shown for the vortical velocity case, by shifting the origin to the element location. The total expansion velocity is obtained by summing the contributions of all the elements and is thus given by:
\[ u_e = - \sum_{i=1}^{N} \left( - \frac{1}{\rho} \frac{d\rho}{dt} \right)_i A_i \nabla G_{\delta}(x-x_i) \]

where

\[ \nabla G_\delta(x) = \nabla \overline{G(x)} \frac{F(\xi)}{\delta} \]

with

\[ \nabla \overline{G(x)} = - \frac{(x,y)}{2\pi r^2} \quad \text{and} \quad F(r) = 1 - \exp(-r^2) \]

which is the form of the discrete-disingularized integral given in the text.
REFERENCES


