NUMERICAL SIMULATION OF TURBULENT FLAMES USING VORTEX METHODS

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SUMMARY

During the year of 1986-1987, we have developed the vortex element method and the transport element method, for the numerical simulation of the Navier-Stokes equations and the energy and species conservation equations, respectively. These methods are based on a Lagrangian, grid-free, time-accurate simulation of the governing equations at high Reynolds and Peclet numbers, without resorting to turbulence modelling. Finite-rate chemical reactions, finite compressibility and finite heat release rates are also considered in the formulations of the numerical schemes. To validate these methods, we are obtaining solutions for reacting shear layers, both homogeneous and heterogeneous, under various idealizations, and comparing the numerical results with experimental data. The solutions are also analyzed to investigate the mechanisms of turbulence-combustion interactions.
During the year of 1986-1987, we have developed the vortex element method and the transport element method for the numerical simulation of the Navier-Stokes equations and the energy and species conservation equations, respectively. These methods are based on a Lagrangian, grid-free, time-accurate simulation of the governing equations at high Reynolds and Peclet numbers, without resorting to turbulence modelling. Finite-rate chemical reactions, finite compressibility and finite heat release rates are also considered in the formulations of the numerical schemes. To validate these methods, we are obtaining solutions for reacting shear layers, both homogeneous and heterogeneous, under various idealizations, and comparing the numerical results with experimental data. The solutions are also analyzed to investigate the mechanisms of turbulence-combustion interactions.
OBJECTIVES

The goal of this research program is to develop, test and apply methods of numerical simulation, based on vortex dynamics, to reacting flows with finite chemical reaction and heat release rates. In particular:

I. The development of accurate and efficient numerical methods which can be utilized in the simulation of the time-dependent, multi-dimensional Navier-Stokes equations at high Reynolds number, and can be extended to solve the energy and species conservation equations in cases where the chemical reaction rates are finite and fast and when the associated heat release is large and hence dynamically important.

II. The application of these numerical algorithms to turbulent reacting shear layers, for both homogeneous and heterogeneous reactants, to validate the numerical methods against experimental results, and to study the underlying mechanisms of entrainment and mixing and how they affect the rates of product formation.

III. The investigation of the mechanisms of turbulence-combustion interactions based on rigorous fundamental models, and how these interactions can be manipulated to provide more efficient burning. In particular, the effect of turbulent fluctuations and flow stretch on the rate of chemical reaction, flame stability and extinction.
PERSONNEL

Three graduate students have completed their master's theses under the sponsorship of this program. Their names and thesis titles are listed at the end of the report. Currently, five graduate students are continuing their doctorate work under the partial or full support of this project. Their names, listed according to seniority, are

(1) Ghassem Heidarinejad
(2) Omar Knio
(3) Habib Najm
(4) Anantha Krishnan
(5) Luis-Fillipe Martins

EQUIPMENT

To meet the computational needs of this work, we have built the following system around a VAX 11/750:

(1) An array processor MAP-6420.
(2) Two MicroVAX II workstations, and a MicroVAX cpu.
(3) A local area network with communication interface to a supercomputer.
(4) Graphics terminals, a laser printer, and a color film recorder.

The system has been hard-wired into the Campus-wide network to allow easier access to other computational facilities available within and outside M.I.T., especially the John von Neumann supercomputer center at Princeton.
WORK STATUS

In the following, the vortex and transport element methods are briefly described and the results of their preliminary applications are discussed.

THE VORTEX ELEMENT METHOD

In this method, Lagrangian particles are treated as finite vortex elements that accurately discretize the vorticity field. We have shown that the accuracy of the method is governed by: the shape function of individual elements, the core radius and the distance between neighboring elements. To preserve the accuracy as the flow develops strong strain fields, particle distribution must change to accommodate distortions of the vorticity by the strain field, leading to a natural growth in the number of vortex elements with time as the flow develops stronger gradients, or fine scales, via stretch. We are implementing a new algorithm to limit the number of interactions between N vortex elements to \( O(N) \), instead of \( O(N^2) \) in direct interactions, using multipole expansion of the contribution of groups of elements.

In Appendix I, the scheme is described in detail, and results for the evolution of a temporal shear layer are analyzed. A temporal shear layer model allows one to limit the computations to a fixed number of large eddies as they evolve from a perturbation to a coherent vortex structure. The accuracy of the computations reveals the detail of the inner structure of the large eddies and the development of secondary instabilities which force the core into several rotations, as well as the severe strain which material line are exposed to within the eddy core. The application of the scheme to a spatially developing shear layer is presented in Appendix II. The improvement of the accuracy over schemes which utilize a fixed number of elements can be realized by comparing these results with results shown in
Appendix III. In the vortex element method, the number of elements grows as the strain field develops, letting one capture the areas where the strain field, and thus the large scalar gradients develop.

Extension of the vortex element method to three dimensional flow simulation has been accomplished by utilizing spherical vortex elements that discretize a three dimensional vorticity field and undergo stretching along the direction of the vorticity vector, as described in Appendix IV. The application of the scheme to study the evolution of azimuthal instabilities on vortex rings has shown that these structures are unstable to a particular wave number, causing the ring to develop into a star-like structure with lobes of vorticity extending in the radial direction of the ring. Results also show that these azimuthal instabilities can excite higher frequency modes by vortex stretching, generating a turbulent cascade of the energy into higher wave numbers. Results of the simulation compared favorably with experimental data. The computations are currently being extended to simulate the evolution of streamwise vorticity in a planar shear layer and a turbulent jet.

THE TRANSPORT ELEMENT METHOD

To achieve an efficient, self-adaptive Lagrangian algorithm for the solution of the energy and species conservation equations, scalar gradients are discretized using core functions similar to those used in the vortex element method. However, contrary to the scalar concentration, gradients are not conserved along a particle path since stretching and tilting material layers enhance the gradients and change their direction. This effect is implemented by changing the strength of the transport elements according the variations of a small material line that coincides with the center of the transport element. Adding a chemical source term requires
changing the local gradients with time. This amounts to transporting several scalar gradients with each element and integrating the source term within each element to compute its instantaneous strength according to a given chemical kinetics scheme. At low Mach number, volumetric expansion due to heat release produces an irrotational velocity field, and generates non-baroclinic vorticity due to the interaction between the density and pressure gradients.

In Appendices I and II, the mathematical formulations of the transport element method are described for a non-reacting flow and a reacting flow, respectively. In Appendix I, the method has been applied to compute the temperature profiles in an initially-thermally stratified temporal mixing layer, showing how entrainment leads to intermittency within the eddy core and to mixing enhancement by generating large gradients as the material layers stretch. Statistics of mixing of a passive scalar in a spatial shear layer have been compared with experimental results in Appendix III, where only a simplified version of the scheme, the scalar element method, was used. The comparison is favorable, considering the fact that no turbulence modeling was implemented to obtain these results. The accuracy of the computations falls off around the boundaries of the layer due to the small number of scalar elements which were used in this simulation. The transport element method avoids this problem by transporting the gradients, instead of the scalar, and is expected to yield better predictions for the mixing statistics. This is currently being tested.

Results for the development of an eddy in a reacting shear layer are presented in Appendix II. Initially, reactants and products are on the top and bottom sides, respectively. As the eddy grows by entraining more reactants, the flame is stretched and wrinkled, leading to a rise in the
rate of product formation over that of the corresponding laminar flame. The ratio of the total amount of products formed in the two cases scales with the square of the flame length in the turbulent case.

To validate these results, computations will be performed for a spatially developing, reacting mixing layer, and statistical information derived from the simulations will be compared with experimental measurements.

**TURBULENCE-COMBUSTION INTERACTIONS**

Slowing down the rate of chemical reaction in the reacting mixing layer leads to local and temporary extinction, as shown in Appendix II. As the Damkohler number of the reacting mixture is lowered, the rate of product formation is decreased. Moreover, the reaction is observed to cease completely for short periods of time. The lower the Damkohler number, the earlier the reaction is temporarily extinct. Local extinction is observed around areas of largest strain field. The extinction occurs temporarily since on the other side of the layer, products at high temperature heat up the reactants and resume the reaction after a short pause. To explain why extinction is correlated with the strain field, we inspected plots of the temperature, strain rate and expansion rate along one of the layers within the flame zone. It was found that a negative correlation existed between the strain rate and expansion rate, and between the temperature and strain rate. Thus, it was concluded that as the strain lowered the temperature by enhancing the diffusion flux via strong gradients, it led to flame extinction. The temperature drop was due to the fact that chemistry was slow so that it could not make up for the increase in the diffusion fluxes with stretch.
Other parameters, e.g., the Peclet number, Lewis number and the activation energy, can affect the interaction between turbulence and combustion. Work is underway to investigate their influence on the mechanism described above.
THESES PRODUCED DURING 1984-1987:


PAPERS PUBLISHED DURING 1984-1987:


Symposium (International) on Combustion, Munich, West Germany, August 1986. Proceedings to be published.


PRESENTATIONS DURING 1984-1987:


**INTERACTIONS DURING 1984–1987**


2. NASA Lewis Research Center, Combustion Fundamentals (Dr. C. John Marek) and Computational Fluid Mechanics (Dr. John Adamczyk), June 1984.

3. California Institute of Technology, Combustion Laboratory of Prof. E. Zukoski, to explore their experimental work on pressure oscillations in dump combustors and couple to our numerical studies, July 1985.

4. Army Research Office, Mathematical Sciences Division (Dr. J. Chandra) (to visit the Laboratory on October 4, 1985, and explore avenues for interactions).

5. Pennsylvania State University, Combustion Laboratory of Dr. Dominic Santavicca, to couple his experimental investigation on the effect of turbulence on flame propagation (supported by AFOSR) to our numerical simulation activities (to visit the Laboratory on November 6th).

6. Sandia National Laboratory, couple experimental work on flame structure (Dr. R. Green) and engine efficiency (Dr. F. Dyer) with our numerical simulation studies.

7. Columbia University, N.Y., Combustion Laboratory of Drs. R. Bill and R. Cheever, to couple their experimental work on stability of V-shaped
flames and axisymmetric shear layers to our numerical simulations (to visit during this academic year, 1985-1986).

8. AFWAL Aeropropulsion Laboratory, Wright-Patterson AFB, OH, Dr. W.M. Roquemore, structure of turbulent jet flames.
Appendix I

The paper on "Numerical simulation of a thermally stratified shear layer using the vortex element method" describes formulation the vortex element method and the transport element method for a non-reacting flow. Results for the application of the methods to a non-reacting, thermally stratified temporal shear layer are presented.
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NUMERICAL SIMULATION OF A THERMALLY STRATIFIED SHEAR LAYER
USING THE VORTEX ELEMENT METHOD

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ABSTRACT

In computing the development of an unstable inviscid shear layer, it is
found that using a fixed number of vortex elements can lead to large errors
due to the strong strain field which develops and acts to distort the
original vorticity contours. It is suggested that the vorticity should be
redistributed among elements which are arranged in the local principal
direction of strain in order to capture this distortion accurately. Mixing
within an initially stratified layer, which results from the combined action
of convection and diffusion, is computed using a similar scheme to integrate
the energy equation. Calculations illustrate the evolution of the
temperature profile during the growth of the instability.
I INTRODUCTION

I.1. BACKGROUND

Numerical simulation of inviscid two-dimensional incompressible flow using vortex discretization of the Euler equations has been discussed extensively in recent literature (Leonard [1], Beale and Majda [2], Hald [3] and Ghoniem and Ng [4]). The method is based on distributing the vorticity field among elements which carry radially-symmetric, compact supports of vorticity (Chorin [5]). By choosing the extent of the support, or the core radius of each element to be larger than the distance of separation between neighboring elements, the fields of individual elements overlap and high order discretization of the vorticity field can be achieved. Vortex elements move with the local flow velocity evaluated at their geometrical centers, which is computed as the summation over the contributions of all elements that exist in the field. The motion of a vortex element does not change its circulation and, in most applications, vortex elements possess invariable core shape and size.

The attraction of these Lagrangian, grid-free methods is that, by construction, computational vortex elements are expected to be, at all times, concentrated around zones of high velocity gradients. When properly exploited, this property endows the scheme with the resolution necessary to study interesting phenomena that arise when molecular diffusion is small relative to convective transport. For instance, at high Reynolds numbers, vorticity exists on small patches of the fluid and it suffices to distribute computational elements within these patches and hence avoid wasting labor on zones of very small vorticity. That the elements move to capture large velocity gradients is particularly important in unsteady and nonlinearly unstable flows where the evolution of the instability causes a substantial
distortion of the vorticity distribution. Moreover, using a Lagrangian formulation of the equations of motion avoids the convective non-linearity and enables the construction of computational schemes which are explicit in time. The employment of moving Lagrangian grids (Fritts and Boris [6]), or grid-free schemes such as contour dynamics (Zabuski et al. [7]), are other successful ways of accomplishing the same goal.

I.2. BRIEF REVIEW

Analysis of the convergence of inviscid vortex methods shows that three factors govern their accuracy: (1) the scheme of discretization of the initial vorticity; (2) the form of the core function; and (3) the ratio of the core radius to the separation between vortex elements (Chorin et al. [8], Del-Prete and Hald [9], Hald [3,10], and Beale and Majda [2,11,12].) Results of these analyses have been supported by numerical tests (Nakamura et al. [13], Roberts [14], and Perlman [15]). In the following, all three factors are briefly discussed.

To initialize the strength of vortex elements, Del-Prete and Hald [9] used the average vorticity within an area element around the center of the element, while Beale and Majda [2] suggested using the vorticity at the center of the element. Nakamura et al. [13] minimized the global error between the continuous and the discrete vorticity distribution to evaluate the latter. Anderson and Greengard [16] proposed the use of a non uniform mesh to discretize the vorticity field. Using the procedure in [2] or [9], one should expect almost a second-order accuracy for short time if the core function is chosen to be a second order Gaussian. A fourth order Gaussian was shown to improve the accuracy. In both cases, a critical parameter is the ratio of the core radius to the distance of separation between the
centers of the elements, which must be chosen larger than unity to preserve the accuracy for long time.

As the elements move, their separation exceeds their initial value if strong strain field arises. This, in effect, decreases the critical ratio of core/separation, leading to a deterioration of the accuracy. The fact that large strains cause deterioration in the accuracy of vortex methods has been observed explicitly in analysis, e.g., Leonard [1]. Thus, for most inviscid vortex methods, which are based on using a fixed number of vortex elements with invariant cores, the evolution of large local strains can lead to large errors. For example, a circular patch of vorticity may deform into an elliptical shape with its major axis aligned with the principal direction of strain. If a small fixed number of computational elements is used, they may not be able to accommodate these severe changes. Anderson [17] and Krasny [18], when discretizing non-smooth vorticity, employed a very large core radius so that as vortex elements moved away from each other due to stretch, reasonable overlap could still be maintained to satisfy the requirements for accuracy. One may also be forced to consider schemes of redistributing the vorticity among a different set of elements under conditions of large strain. Similar schemes have been used in methods of contour dynamics to preserve the accuracy of the integration around the vorticity contours (Zabuski and Overman [19].) Krasny [20], in an independent effort, used a similar procedure in simulating the evolution of a vortex sheet by a desingularized Biot-Savart integral.

Extension of Lagrangian element methods to integrate a scalar conservation equation has been applied to several problems in one dimension (Chorin [21], Ghoniem and Oppenheim [22,23] and Ghoniem and Sherman [24].) These schemes were based on using the scalar gradient, in analogy to
vorticity, in the transport process. Anderson [16,25] constructed a scheme to solve for a two dimensional thermal in the inviscid Boussinesq approximation by discretizing the density equation in its vortex form. This was done by casting the equation in gradient form and discretizing the density gradients among elements that could be transported. This scheme, while preserving the advantages of the vortex method, suffers from a major problem: A large strain field, while it may lead to the generation of large gradients, depletes the area of computational elements which are used to transport these gradients.

I.3. ORGANIZATION

In this paper, we apply the inviscid vortex methods to the problem of a temporal shear layer at high Reynolds number. This problem is characterized by a well-defined smooth vorticity field at time zero, and has well-documented stability properties. At later times, the shear layer develops into a complicated structure which resembles a turbulent eddy, and a very strong strain field is generated around this eddy. We use the analytical solution of a temporal shear layer to measure the accuracy of the results at the initial stages of development, and test the schemes for initializing the vortex elements. At longer times, we observe the effect of the strain field on the accuracy of the computations and suggest ways to cope with it. We then proceed to compute the temperature field as fluids with different temperatures are entrained, stretched and mixed.

In Section II, the formulation of the vortex method is described, and is extended to solve for a flow with a strong strain field. The scheme is applied to compute the evolution of a vorticity layer subject to periodic boundary conditions. The growth of the instability and its effects on the flow field are investigated. In Section III, the concepts of the vortex
method are generalized to solve the energy equation and to obtain the temperature profile across the shear layer during its development. The paper ends with conclusions in Section IV.
II INVISCID INCOMPRESSIBLE FLOW

II.1. THE VORTEX METHOD

For an inviscid incompressible flow, the vortex transport equation is:

$$\frac{\partial \omega}{\partial t} + \mathbf{u} \cdot \nabla \omega = 0$$  (1)

$$\Delta \psi = -\omega$$  (2)

where \( \mathbf{u} = (u,v) \) is the velocity, \( \omega = \nabla \times \mathbf{u} \) is the vorticity, \( x = (x,y) \) are the streamwise and cross stream directions, respectively, \( t \) is time, \( \nabla = (\partial/\partial x, \partial/\partial y) \) and \( \Delta = \nabla \cdot \nabla \). Variables are normalized with respect to the appropriate combination of a characteristic velocity and length scale. \( \psi \) is the stream function defined so that \( u = \partial \psi / \partial y \) and \( v = -\partial \psi / \partial x \). The solution of Eq. (1) can be written as:

$$\omega(x(x,t),t) = \omega(x,0)$$  (3)

while \( x \) is governed by:

$$\frac{dx}{dt} = u(x(x,t),t)$$  (4)

where \( x(x,0) = x \). In the vortex method, the vorticity field \( \omega(x,0) \) is discretized between elements centered at \( x_i, i=1,..,N \), so that:

$$\omega(x,0) = \sum_{i=1}^{N} \Gamma_i f_\delta(x-x_i)$$  (5)

where \( \Gamma_i = \omega_i h^2 \) is the circulation of an element of strength \( \omega_i \) and \( f_\delta \) is the core function. \( f_\delta(x) = 1/\delta^2 f(r/\delta) \), where \( r^2 = x^2 + y^2 \), and \( \int f_\delta dx = 1 \). \( \delta \) is the core radius, and \( f_\delta \) is a fast decaying function so that most of the vorticity is concentrated within \( r < \delta \). To approximate the initial vorticity distribution accurately, \( \delta \) should be greater than \( h \), where \( h \) is...
the initial separation between vortex centers. The core function $f$ plays a similar role as interpolating polynomials in finite-difference schemes and base functions in finite-element formulations. By requiring $f$ to be radially symmetric, the approximation in Eq. (5) is at least second order.

Using Eq. (3) and the incompressibility condition, the vorticity distribution at any time is given by

$$\omega(x,t) = \sum_{i=1}^{N} \Gamma_i f_\delta(x-x_i)$$

(6)

where $dx_i/dt=u(x_i,t)$ and $x_i(x_i,0)=X_i$.

The stream function of a single vortex element is obtained by integrating Eq. (2). Using polar coordinates, for a vortex element placed at $x=0$, $\partial \psi_\delta/\partial r = -\kappa(r/\delta)/r$, where $\kappa(r) = \int_0^r r' f(r') \, dr'$. Moreover, $u_\theta = -\partial \psi_\delta/\partial r$. The velocity field induced by a distribution of vortex elements, of shape $f_\delta$ and strength $\Gamma_i$ located at $X_i(x_i, t)$ is:

$$u_\omega(x,t) = \sum_{i=1}^{N} \Gamma_i K_\delta(x-x_i)$$

(7)

where

$$K_\delta(x) = -\frac{(x_*-x)}{r^2} \kappa(r/\delta)$$

(8)

Vortex elements move without changing their circulation (strength) or core shape, at a velocity computed from Eq. (7).

In the calculations, we used mostly a second order Gaussian core:

$$f = \frac{1}{\pi} e^{-r^2}$$

$$\kappa = \frac{1}{2\pi} (1 - e^{-r^2})$$

(9)
When applying the vortex scheme to a flow field with boundary conditions other than \( u(\infty, t) = 0 \), a potential flow is added to satisfy these conditions. In this work, we perform computations for a periodic shear layer. The velocity field induced by vorticity outside the computational domain \( 0 \leq x \leq \lambda \), where \( \lambda \) is the longest wavelength of the perturbation, must be added to \( u \). The total velocity is:

\[
\mathbf{u} = \sum_{i=1}^{N} \frac{\Gamma_i}{2\pi} \left[ \sum_{j=0}^{\pm 1} \frac{1}{\delta^2} \left( \gamma_i - (x+j\lambda) \right) \exp \left( -\frac{(x+j\lambda)^2 + y^2}{\delta^2} \right) \right] + \sum_{i=1}^{N} \frac{\Gamma_i}{\delta \lambda} \left( -\sinh(2\pi y/\lambda), \sin(2\pi x/\lambda) \right)
\]

where \( N \) is the total number of vortex elements in the computational domain \( 0 \leq x \leq \lambda \). Note that since \( \delta \ll \lambda \), the effect of the core was included only for the nearest sister vortices.

The initial vorticity distribution across the shear layer can be well represented by a Gaussian curve (which should not be confused with the Gaussian core of individual vortex elements) with a spread \( 2\sigma \):

\[
\omega(x) = \frac{\Delta U}{\sqrt{\lambda \sigma}} \exp(-y^2/\sigma^2)
\]

where \( \Delta U \) is the velocity difference across the layer and \( \sigma \) is the standard deviation of the Gaussian. The corresponding velocity distribution is:

\[
U(x) = \frac{\Delta U}{2} \operatorname{erf}(y/\sigma)
\]

where \( \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-r^2) \, dr \) is the error function. We take \( \Delta U \) and \( \sigma \) as the characteristic velocity and length scales of the problem, respectively.
As it was pointed out in the Introduction, using either a pointwise discretization, $\omega_i = \Omega(X_i)$, or an area average value $\omega_i = \int_{h \times h} \Omega(X) \, dX$, where $X_i, i=1,2,..,N$ are the centers of a square mesh of side $h$, to discretize the vorticity of the shear layer among vortex elements produced a large error in the initial growth of the perturbation. Instead, the following scheme was used:

$$\Omega(X_i) = \sum_{j=1}^{N} \omega_i \, h^2 \, f_\delta(X_i-X_j)$$

for $i=1,2,...,N$. The error associated with this distribution was used as a measure of the accuracy of the initial discretization. In all cases, the error $|e_\omega| = \int |\Omega(X) - \omega(X,0)| \, dX < 10^{-5}$. The error $e_\omega$ increased rapidly as $\delta/h$ was decreased below one, which is consistent with the result of the convergence theory which shows that the overlap between neighboring elements is necessary for accurate discretization of vorticity. For $\delta/h > 1$, the error was less sensitive to its exact value, up till $\delta/h = 1.5$. In the following calculations, we used $\delta/h = 1.1 - 1.4$.

To measure the effect of the accuracy of the initial discretization of vorticity among vortex elements on the flow field for short times, we will use the rate of growth of the perturbation. The growth of the initial perturbation can be characterized by an integral parameter $I$ as:

$$I = \int_0^\lambda \int_{-\infty}^{\infty} |u(x,t) - U(x)| \, dx$$

which is used in the linear theory analysis of the perturbation.

At $t = 0$, the layer was perturbed by a sinewave with amplitude $\varepsilon$, taken as $0.001 \lambda$, $0.01 \lambda$, and $0.1 \lambda$. In Fig. 1, we compare the growth of the perturbation with the prediction of the linear theory of stability (Michalke
[26].) to assess the accuracy of the vortex method for short times. For most of the computations, $\lambda = \lambda^* = 13.2 \sigma$, which corresponds to the wave with the maximum growth rate. Eq. (4) is integrated using a second order Heun’s method with $\Delta t = 0.1$, and $h = \lambda / 44 = 0.3$, and $N(0) = 572$ vortex elements. The figure indicates that for $\varepsilon = 0.01$ and $0.001$, the layer behaves linearly and the computed growth rate $\dot{\gamma} = d\ln \gamma / dt = 0.215$ agrees well with the results of the linear theory, $\dot{\gamma} = 0.22$. The latter was computed as the eigenvalue of the linearized Euler equations (Betchov and Criminale [27]). Using $h = \lambda / 24$, i.e. $N(0) = 168$, and a second order time integration scheme, $\dot{\gamma} = 0.23$. For $N(0) = 572$ and a first order time integration, $\dot{\gamma} = 0.24$. Within this linear stage of development, the maximum distance between neighboring element in the direction of maximum strain $\Delta x < 1.5 h$, i.e. the flow is developing mild stretch. For $\varepsilon = 0.1$, the perturbation leads directly to the nonlinear range.

In Figs. 2, 3 and 4, the vortex elements and their velocity vectors are plotted for $\varepsilon = 0.001 \lambda$, $0.01 \lambda$, and $0.1 \lambda$, respectively. In the first two cases, the end of the linear range corresponds to the beginning of the rollup of the interface, defined here as the line which coincides with $y = 0$ at $t = 0$, and the formation of a spiral center at the midpoint of the wavelength. Concomitantly, the interface starts to stretch near the boundaries of the domain and two saddle points are established at the beginning and end of the wavelength, $x = 0$, and $\lambda$. Beyond the linear range, the perturbation continues to grow with more layers rolling around the spiral center and stretching near the saddles. Within this nonlinear range of development, special care must be exercised or the numerical accuracy deteriorates quickly, as exhibited by the evolution of irregular motion near the saddles and the loss of organization of the evolving structure.
II.2. EFFECT OF STRETCH

The loss of organization, which is associated with the development of strong stretch, illustrates one of the fundamental problems of the vortex method. Vortex elements, which start as cores with radial symmetry, may not properly represent the vorticity field after it has developed strong local strains. As the effective distance, $\Delta x$, between neighboring elements increases, the ratio $\delta/\Delta x$ (equivalent to $\delta/h$) reaches levels where the vorticity discretization becomes inaccurate. One obvious remedy is to restart the calculations with smaller values of $h$ to allow a larger number of weaker elements to represent the strong distortion. However, that only delays the onset of the crisis at the expense of using more elements at the initial stages when they are not needed. Several remedies may be suggested: (1) utilizing deformable cores; (2) employing large cores; or (3) using more elements as the distance between the original elements increases.

The first scheme, utilizing deformable cores, depends on assuming that the core structure will become elliptical as stretch develops, with the major axis of each element aligned with the local principal direction of strain. The vorticity distribution within the core must also adapt to the geometrical boundaries of the cores. If elements with constant vorticity within the cores and zero outside, i.e. Rankine vortex elements, are used then these elements will become Kirchhoff vortices which have analytical expressions for the induced velocity field. However, there is an obvious limitation on maintaining one ellipse as a single element if the ratio between its axes exceeds a reasonable value. Thus, this scheme is discarded.

The second scheme, in which one uses large cores, did not yield accurate predictions for the growth rate within the linear range, in
accordance with the results of the convergence theory. Moreover, it will fail at the point where $\delta/\Delta x < 1$ due to stretch. It does, however, delay the deterioration of accuracy since it maintains a reasonable overlap between neighboring elements for longer times.

The third option, redistributing the vorticity field among an increasing number of elements arranged along the direction of principal direction of strain, is employed here. One monitors the distance between neighboring elements in the direction of maximum positive stretch $\Delta x$. If $\Delta x > \beta h$, where $1 < \beta < 2$, an extra element is placed halfway between the original elements and the vorticity is redistributed to compute the share of the new element. Ideally, this redistribution should not perturb the existing vorticity field, that is

$$\omega(x,t) = \sum_{i=1}^{N} \Gamma_i \delta(x-x_i) = \sum_{i=1}^{N+n} \Gamma_i \delta(x-x_i)$$

where $n$ is the number of new particles, and $\sim$ indicates the new value of the strength and location of the vortex elements. Unfortunately, this is a large dense system of linear equations to be solved every time step. Therefore, its benefit does not warrant the added cost.

A more economical scheme is based on equally interpolating the strength of the two original elements among the three elements, i.e. assuming uniform stretch between the two original elements. This amounts to splitting the original vortex dumbbell formed of two vortex discs into three discs when the distance between the centers of the two discs exceeds a threshold, as shown in Fig. 5. To minimize the interpolation errors, the maximum interdistance between neighboring elements is taken as $1.5 h$. This will also keep the ratio $\delta/\Delta x$ within reasonable limits.
To illustrate the degree of stretch experienced by this flow, we plot the growth of the length of the interface, and the total number of vortex elements, $N(t)$, used to capture this stretch for three perturbations $\epsilon = 0.001\lambda$, 0.01$\lambda$, and 0.1 $\lambda$ in Figs. 6, 7, respectively. Within the linear range the layer is subjected to mild stretch and $N$ remains almost constant. Beyond that, the length of the line grows linearly and $N$ multiplies accordingly. From the plots of the location of vortex elements, we noticed that most of the stretch is concentrated around the spiral center and the saddles at the boundaries of the domain.

II.3. SHEAR LAYER DYNAMICS

Figures 1, 2, 3 and 4 reveal that the growth of the perturbation and the development of the eddy structure can be divided into four stages: (1) linear growth; (2) rise to a maximum amplitude; (3) decay to a constant amplitude; and, (4) very slow decrease of amplitude. The first stage has been discussed. The strongest stretch and fastest multiplication of the vortex elements occur during the second stage where an eddy is forming in the middle of the wavelength and two braids are evolving between each two neighboring eddies. During this stage, the core maintains almost a circular configuration and the stretch is concentrated within the braids.

In the third stage, the eddy deforms into an elliptical structure, while the size of the perturbation decreases from its maximum value. This is accompanied by more stretch along the braids and within the core, and a slowdown of the eddy rotation. By the end of this stage, the thickness of the braids at the saddle points has become extremely small. At the final stage, the envelope of the core reaches a dynamic equilibrium, i.e., it does not rotate any more, while its boundaries keep on stretching as the fluid within the eddy starts to move in the main directions of the streams.
Although there are signs of that, it is difficult to confirm that the flow has reached a steady state.

The kinetic energy of perturbation \( u' \cdot u'/2 \), where \( u' = u - U \), and the total kinetic energy in the flow within the computational domain, \( u \cdot u/2 \), are plotted in Figs. 8a and 8b. The first quantity rises with the growth of the perturbation and the formation of the eddy, then falls with the collapse of the eddy and the return of the fluid to the main streams (Corcos and Sherman [28]). The total kinetic energy is conserved since the flow is inviscid.

Using larger values for \( h \) while keeping \( \delta/h \) the same caused a slight fattening of the core at latter times, while the main features of the flow were reproduced almost exactly. A similar modification of the structure is observed when using a first order time integration scheme, or increasing the time step. It was concluded that the errors introduced by using a small number of elements or a low order time integration scheme were numerical-diffusion-like errors. We also found that the dependence on the value of \( h \), or the initial number of elements, becomes much less pronounced when the scheme of increasing the number of elements with stretch is employed.

Figure 9 shows a qualitative comparison between the experimental results of Roberts et al. [29] and the computational results. Here we use a Galilean transformation to compare the experimental results of the spatially-developing layer and the computational results of the temporal layer.

The physical parameters that govern the flow field are \( \lambda \) and \( \varepsilon \).

Results for the rollup of a layer with \( \lambda = 10.5 < \lambda^* \) are presented in Figs. 10 and 11, showing the growth of the perturbation and the vorticity field. \( \lambda^* \) is the wavelength of the most unstable perturbation. The computed growth rate \( \hat{\lambda} = 0.214 \) while the analytical value is 0.208. More vorticity remains
in the braids between the eddies which are not strong enough to accomplish the same stretch as in the case of $\lambda^*$.  

Figures 12 and 13 show results for $\lambda = 2 \lambda^*$ with $\epsilon = 0.01\lambda$ and $0.1\lambda$, respectively. In the first case, $\bar{i} = 0.18$ while the analytical result is 0.173. The core is smaller and weaker than for the case of $\lambda^*$ and hence the braids are thicker and maintain more of the original vorticity. At later times, a small scale rollup is observed near the boundary of the domain due to the instability of the vorticity layer that forms the braids. This rollup occurs only at the fourth stage of development when the midsection of the braids becomes almost stationary, i.e. when the motion produced by the braids is neutralized. Comparing Figs. 12 and 13, we see that contrary to the most unstable case, the effect of the initial perturbation is more pronounced here in terms of the size and shape of the eddy and the braids. Higher amplitudes of perturbation tend to form a larger core and thinner braids. The ratio between the major and minor axes of the elliptical core increases with $\epsilon$ and small amplitude waves start to appear on the braids.  

Figures 14 and 15 show results for $\lambda = 3 \lambda^*$ with amplitudes $\epsilon = 0.01\lambda$, and $0.1\lambda$, respectively. The effect of the amplitude is emphasized further since at larger $\epsilon$, the core splits into two eddies. This bifurcation phenomenon was observed before by Pozrikidis and Higdon [30]. The braid instability is manifested here by the long waves that appear at the later stages of development of the layer.  

With the presence of two perturbation wavelengths, a new process is observed. Figures 16 and 17 depict results for a layer subject to two perturbations superimposed at $t = 0$, at $\lambda^*$ and $2\lambda^*$ with $\epsilon = 0.1\lambda^*$ for both perturbations. The results show that when the amplitude of the two perturbations are equal, pairing starts at the end of the second stage and
before any substantial elongation of the eddies. The growth of the subharmonic perturbation closely resembles that of the fundamental, as shown in Fig. 17. The eddies continue to deform while they pair until the "vortex fluid" contained within each structure start to rotate around a common center and their original boundaries become indistinguishable. Similar qualitative observations were shown in the computations of Corcos and Sherman [28] and Riley and Metcalfe [31].
III THE TEMPERATURE DISTRIBUTION

III.1. THE TRANSPORT ELEMENT METHOD

In an inviscid incompressible flow, the temperature distribution evolves according to the following form of the conservation of energy:

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = 0$$  \hspace{1cm} (15)

where $T$ is temperature. This is equivalent to the statement that $T(X(X, t), t) = T(X, 0)$, where $X(X, 0) = X$ and $\frac{dX}{dt} = u(X, t)$. To solve this equation using a Lagrangian element scheme, we start by introducing the temperature gradient $\mathbf{q} = \nabla T$, where $\mathbf{q} = (p, q)$ is a vector proportional but opposite to the heat flux vector $-k \mathbf{q}$, $k$ being the thermal conductivity. The transport equation of $\mathbf{q}$ is obtained by taking the gradient of Eq. (15) and rearranging:

$$\frac{\partial \mathbf{q}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{q} = - \mathbf{q} \cdot \nabla \mathbf{u} - \mathbf{q} \times \mathbf{\omega}$$ \hspace{1cm} (16)

where $\mathbf{\omega} = \omega \mathbf{e}_z$ and $\mathbf{e}_z$ is the unit vector normal to the $(x, y)$ plane. Thus, along a particle path $X(X, t)$, the temperature gradient changes according to the local strain field and turns with the local rotation of the fluid element. Using the vortex method described in the previous section, the velocity gradient may be computed directly from the vorticity distribution as: $\mathbf{Vu} = \mathbf{V} \int \Gamma \mathbf{v}_p (X - X_i) + \mathbf{Vu}_p$, where $u_p$ is the irrotational component of the velocity.

The scheme proceeds in the same way as the vortex algorithm. The initial temperature gradient is discretized among a number of elements located at the centers of a square mesh of side $h$ so that:
\[ q(x,0) = \sum_{i=1}^{N} q_i \, h^2 \, f_\delta(x-X_i) \]  

(17)

where \( q(x,0) \) is the initial distribution of the temperature gradient, \( q = \nabla T(x,0) \). To initialize \( q_i \), a similar procedure to that used in computing the strength of the vortex elements is employed here, i.e. Eq. (12) with \( q_i \) instead of \( \omega \), is solved to find \( q_i(0) \). To update \( q_i(t) \), Eq. (16) is solved in two fractional steps: in the first step, the elements are transported without changing their strength or their core shape or size. In the second step, the strength of the elements is updated according to:

\[ \frac{dq_i}{dt} = -q_i \cdot \nabla u_i - q_i \times \omega_i \]  

(18)

Thus, a system of ordinary differential equations must be integrated to update the strength of the gradient elements as they move along particle paths. The local gradient at time \( t \) is computed from:

\[ q(x,t) = \sum_{i=1}^{N} q_i(t) \, h^2 \, f_\delta(x-X_i) \]  

(19)

The core function \( f_\delta \) may be different for the vortex elements and the gradient transport elements. In this work, we use the same form for both. The temperature can be calculated by direct integration of the gradient along a determined path. As pointed out by Anderson [17], a convenient expression can be obtained by expressing the temperature as a Poisson integral in the temperature gradient, \( T = \int \nabla G(x-x') \cdot \nabla T(x-x') \, dx' \). Using Eq. (19) for \( q_i \), we get:

\[ T(x,t) = \sum_{i=1}^{N} q_i(t) \cdot \nabla G_\delta(x-X_i) \]  

(20)
where

\[ \nabla G = \frac{(x, y)}{r^2} \kappa \left( \frac{r}{\beta} \right) \]

while the relationship between \( f \) and \( \kappa \) is as before. This expression is convenient when used in connection with the vortex method since all the functions involved in the summation must be computed for the transport of the vortex elements and with simple programming tricks, the increase in cost can be minimized.

Results obtained for the temperature distribution in the shear layer of Figs. 2, 3 and 4 are shown in Figs. 18, 19 and 20, respectively. At \( t = 0 \), the temperature distribution is described by an error function, with \( T(x, 0) = 0.5 \left( 1 + \text{erf}(y) \right) \). This choice is motivated by the fact that this is the fundamental solution of the diffusion equation. Therefore, an initial discontinuity in temperature would develop into an error function before the perturbation grows and convection effects become important. The layer is first perturbed by a sinewave by displacing the elements according to \( y = \tilde{y}(x) \), and then the temperature gradient \( \Omega(x) \) is computed. The discrete values \( \theta_i(0) \) are obtained as follows: Since the temperature is constant along the streamlines after the perturbation \( y = \tilde{y}(x) \), then \( T(x, 0) = \Theta(x) = 0.5(1 + \text{erf}(y - \tilde{y}(x))) \). From this equation we can recover the initial distribution of \( P(x, 0) \), and \( \Omega(x, 0) \) as follows:

\[
\begin{align*}
P(x) &= \frac{\partial \Theta}{\partial x} = -\text{Gau}(y - \tilde{y}(x)) \frac{d\tilde{y}}{dx} \\
Q(x) &= \frac{\partial \Theta}{\partial y} = \text{Gau}(y - \tilde{y}(x))
\end{align*}
\]
where Gau is a Gaussian similar to Eq. (11a). These expressions are then used in Eq. (17) to compute \( q_i \). The values of \( q_i(0) \) were initialized one column at a time, i.e. for fixed values of \( X \), to avoid solving \( N^2 \) simultaneous equations, and instead solve \( N_X \) of \( N_Y \) simultaneous equations. The error associated with this approximation was very small since the perturbation was kept at a low value.

In the computations, we used the same particles to transport vortex elements and elements of the temperature gradient. This represents a substantial saving since the kernel functions appearing in the expressions of the velocity, velocity gradients, and temperature can be computed all at once and the velocity is computed only for one set of elements.

**III.2. ENTRAINMENT IN A SHEAR LAYER**

To quantify the overall change in the temperature distribution, we define a quantity \( T \), similar to the growth \( I \), as:

\[
T = \int_0^\lambda \int_{-\infty}^\infty |T(x,t) - \Theta(x)|
\]

\( T \) can be regarded as an average thermal thickness of the shear layer. Within the linear range, the temperature distribution remains essentially the same, except for getting shifted up or down depending on the local sign of the perturbation. In Fig. 21, the natural logarithm of \( T(t) \) is shown for three values of the initial amplitude of the perturbation. The accuracy of the calculation of the temperature profiles depends on the initialization of the vorticity and temperature gradient, and on the value of \( \delta/h \).

During the second stage, and with the rollup of the interface and the establishment of a spiral center at the midpoint of the wavelength, a complex temperature gradient develops as a result of the motion of the cold fluid upwards and the hot fluid downwards around the spiral center. Within
this stage, if the number of transport elements remained the same, i.e. stretch was not accommodated by introducing elements where the local strain is large, the temperature distribution would collapse very quickly. In the problem of periodic shear layer, this collapse leads to values of $T(x, +, t) < 1$ and $T(x, -, t) > 0$. The reason of the loss of accuracy is clear from Eq. (16). When the elements move apart, the accuracy of computing the velocity gradient $\nabla u$ deteriorates, and hence the new values of $q_i$ accumulate large errors. Thus, while the calculation of the velocity field at the early stages of strong stretch using a fixed number of vortex elements may be acceptable for a short period of time, the calculations of the velocity gradient and the evolution of a passive scalar will show unacceptable errors.

To continue beyond the linear stage, the distance between neighboring elements in the principal direction of strain, $\Delta x$, must to be monitored. If $\Delta x > \beta h$, where $\beta > 1$, one extra element is added between the two original elements and the total value of $q_i$ is redistributed equally between the three elements. In the calculations, we used $\beta = 1.5$. Numerical convergence, in which one systematically refines the numerical parameters until no more changes are observed, was used to obtain these results.

The effect of the shear layer rollup on the temperature distribution is seen in Figs. 18 and 19. Immediately after the interface reaches a vertical position, an S-shape starts to form indicating that cold fluid has been transported from the lower stream into the upper stream and vice versa. This phenomenon, known physically as engulfment or entrainment, relies solely on convective transport and is observed when molecular diffusion, which acts to dissipate the sharp gradients, is small. Fast entrainment with small diffusion leads to "unmixedness" of hot and cold fluids within
the eddy core. With more fluid being transported to the opposite stream the
S-shape grows, reaching a maximum amplitude when the interface becomes
horizontal. At this moment, fluid with the maximum and the minimum
temperature has been entrained into the core, i.e. entrainment has reached
all the way to the free streams to bring fluid into the core of the eddy.
This is the stage of maximum entrainment when the core size reaches its
largest size and cannot accommodate any more fluid. In the case of $\epsilon = 0.1\lambda$, it corresponds to $t = 8.0$, which is at the end of the second stage of
development. To make the correspondence between the temperature profiles
and the evolution of the interface of the layer clear, we plot the latter in
Fig. 22, showing the actual vortex elements that were used in the
computations of the interface. At this time, the interface has rotated $180^\circ$
around the spiral center. This is the first step in the process of
homogenization of the core.

As the core rotates further into the third stage, the inner part of the
interface develops a secondary instability that rolls up in a very similar
manner to the primary instability. This secondary instability is in phase
with the primary instability and can be envisioned by zooming in on the
intersection between the interface and the horizontal centerline of the
layer. Due to the elongation of the outside envelope of the core, the
wavelength of the secondary instability grows with time, as seen from Fig.
22. However, the amount of fluid within the elliptical envelope remains
constant, or decreases slowly as seen from Fig. 21 for the temperature
thickness of the layer. The growth of the secondary instability provides a
mechanism of internal entrainment within the core. During the growth of the
secondary instability, an inverted S-shape, or a Z-shape, forms in the
middle of the temperature profile, Figs. 18-20. The entrainment associated
with this instability turns the fluid in a clockwise fashion, making the inside of the core more uniform. This is seen from the decay of the peaks in the temperature profile as this Z-shape grows.

With another 180° turn of the interface at the spiral center, a smaller S-shape forms in the middle of the profile due to the onset of an even shorter wavelength instability that is in-phase with the primary instability. While the existence of the secondary instability was not observed before in numerical simulations, its presence is clearly seen in the experimental results in Fig. 9.

The onset and subsequent growth of successively shorter wavelength instabilities continues, leading to a more uniform temperature distribution within the eddy core. An asymptotic limit to this process can be foreseen: it is the formation of a temperature profile with the following shape: \( T = T_\text{m} \) at \( y > \Delta/2 \); \( T = T_- \) at \( y < -\Delta/2 \), and \( T = (T_\text{m} + T_-)/2 \) in between, where \( \Delta \) is the minor axis of the elliptical envelope at \( x = \lambda/2 \). This shape has been measured experimentally by Konrad [32], (see also Broadwell and Breidenthal [33],) for mixing layer flows at high Reynolds numbers. This is, to our knowledge, the first time it has been computed numerically.

By the end of the third stage, the layer cannot absorb any more energy and a relaxation process occurs, during which the kinetic and thermal energy are fed back into the main flow streams. This reverse action is accompanied by the fluid leaving the core and moving back into the main streams at a very slow rate.

III.3. EFFECT OF MOLECULAR DIFFUSION

The generation of large temperature gradients within the core as successive instabilities evolve gives rise to large molecular diffusion fluxes which act to smooth out some of these gradients. While for most
cases of interest the diffusion transport is very small relative to the convective transport, i.e. the Reynolds number is high, diffusion plays an important role since mixing at the molecular scales can only be accomplished via molecular diffusion. Thus, the combined action of convective entrainment and molecular diffusion leads to the homogenization of the temperature within the eddy core. To simulate the effect of diffusion for small values of $\alpha$ in the current model of a shear layer, Eqs. (15) and (16) are modified by adding a diffusion term:

\[
\frac{\partial T}{\partial t} + u \cdot \nabla T = \alpha \nabla^2 T 
\]

and

\[
\frac{\partial q}{\partial t} + u \cdot \nabla q = -q \nabla u - q \times \omega + \alpha \nabla^2 q
\]

where $\alpha$ is the non dimensional molecular diffusivity, or the inverse of the Peclet number. At high speed flow, the Peclet number is typically $10^3$-$10^5$.

To solve Eq. (24) using the scheme that we have developed, a third fractional step must be added, in which the value of $q$ is updated according to:

\[
\frac{\partial q_i}{\partial t} = \alpha \nabla^2 q_i
\]

without changing the shape of the core function or the value of $q_i$. By taking $\delta = \delta(t)$, and substituting Eq. (19) into Eq. (25), we find that $d\delta^2/dt = 4\alpha$. Thus, the core radius must change according to:

\[
\delta^2 = \delta_0^2 + 4\alpha t
\]
where \( \delta_0 \) is the core radius at \( t = 0 \) (for more discussion, see Leonard [1], Ashurst [34]). The cores of the vortex elements and of the temperature gradient elements become different with time.

Results in Fig. 23 show the temperature profile at \( T = 20 \) for the case of \( \lambda^* \) and \( c = 0.1 \lambda^* \), evaluated for \( \alpha = 0.0, 0.00001, 0.0001, 0.001, 0.01 \) and 0.1. Note that the temperature profiles of the first two cases are almost identical, indicating that the effective diffusivity of the inviscid calculation is of the order of \( 10^{-5} \). In the last case, the temperature profile is similar to the case of pure diffusion, indicating that diffusion proceeds at a rate faster than the instability. It is also noticed that for moderate values of \( \alpha, 0.0001 < \alpha < 0.01 \), diffusion only affects the core of the eddies, making them achieve a homogeneous state faster.

Greengard [35], in his analysis of the core-spreading vortex method in which a fixed number of elements are used to perform the convective transport and their cores are expanded to account for the effect of diffusion, showed that the scheme does not converge to the correct equation of motion except when the flow field outside the region \( |\omega| > 0 \) is uniform. We have used a core spreading scheme to simulate the effect of diffusion in the energy equation with two modifications: (1) the number of transport elements which discretize the gradient field is increasing with time; and (2) \( \alpha \) is kept small. Utilizing an increasing number of elements to perform the convective transport is essential since it is important to determine the gradient field accurately, in terms of the location and strength of the elements, before the diffusion effect can be added. In essence, adding transport elements at areas of high strain allows the computational elements to capture all the vorticity, and temperature gradient carrying fluid at all times, even after the vorticity has been fragmented by the action of the
strain field. Without this step, strain will create areas which are void of elements, thus, diffusion cannot be represented.

In the particular application of a shear layer at high Reynolds number, the flow field is uniform outside the area where $|\omega| > 0$, and this area expands slowly by diffusion if $\alpha < 1$. Limiting the simulations to small values of $\alpha$: (1) reduces the errors associated with the fractional step scheme used to solve Eq. (24) (Beale and Majda [36]); and (2) reduces the errors concomitant with convecting an element with the velocity evaluated at its center while its core radius is growing. To accommodate this growth, which causes the spread of vorticity in the direction normal to the streamlines, one may be forced to add elements in the direction normal to the maximum principal strain direction, and then redistribute the vorticity. It is, therefore, clear that the scheme is only applicable when $\alpha < 1$ and for short time, i.e., at $< 1$. If these two conditions are not satisfied, one must divide each element whose core radius is larger than a critical value into a number of separate elements so that the convective transport can be performed accurately. Since most interest in shear layer flows is at high Reynolds number, or $\alpha < 1$, and within the short time of development of the convective instability, we feel that the current scheme is sufficient for this application.

To define a quantitative measure of mixing in a single phase fluid with thermal stratification, we observe first that mixing is only achieved by molecular diffusion. Large entrainment fluxes bring the unmixed fluid layers in contact along a larger interface; however, molecular diffusion across this interface is what accomplishes the actual mixing. A measure of mixing can be defined as:
\[ M(t, \alpha, \epsilon) = \int_{-\infty}^{\lambda} |T(x, t, \alpha, \epsilon) - T(x, t, 0, \epsilon)| \, dx \]

Note that \( M(t, 0, \epsilon) = 0 \), while \( M(t, \alpha, 0) \) is due to diffusion only. In Fig. 24 \( M(t, \alpha, 0.1) \) is plotted for various values of \( \alpha \) and for \( \lambda^* \). It represents mixing due to the combined action of entrainment and diffusion. At very small values of \( \alpha \), mixing is limited by the amount of diffusion across the fluid layers which have been entrained into the eddy core. Since for these values of \( \alpha \) the convective transport is faster than the diffusive transport, mixing increases approximately as \( \sqrt{\alpha} \). However, as \( \alpha \) increases, and at longer times, mixing proceeds at a slower rate since it becomes bounded by entrainment of unmixed fluid into the eddy core which almost ceases by the end of the second stage of rollup.
IV CONCLUSIONS

In this work, the vortex element method is used to compute both the early and late stages of development of an inviscid temporal mixing layer. In this method, the vorticity is initially discretized among overlapping element of radially symmetric cores. We find that using a scheme which depends on equating the vorticity at the centers of the elements with the accumulative value induced by all elements is necessary to obtain accurate results for initial vorticity discretization. We also find that to ensure the accuracy of the solution for short times, the ratio of the core/separation should be larger than one. Very large cores introduce a strong perturbation in the vorticity field, while smaller cores cause a fast deterioration of accuracy. Using fourth order Gaussian cores results in better accuracy over second order Gaussian cores. However, we feel that the improvement in accuracy does not warrant the added cost.

As time proceeds, the distance between neighboring elements exceeds its initial values due to the generation of strong stretch. This leads to the computation of inaccurate velocities and is manifested by the irregular motion of the vortex elements. To overcome this problem, the vorticity is constantly redistributed among elements inserted along the principal direction of strain to capture the local deformation of the vorticity field and to improve the resolution of the calculations. This is achieved by an insertion-and-interpolation process, which is applied where the distance between the neighboring centers along the principal direction of strain exceeds a threshold value. We show, using solutions for a shear layer perturbed at different wavelengths and amplitudes, that this process yields accurate solutions for the vorticity distribution at long times and after strong strain fields have caused a severe distortion of the streamlines.
This scheme enables one to accurately compute the local velocity gradient which, while it is not required in connection with vorticity convection, is necessary for the accurate evaluation of the convection of a passive scalar.

The temperature gradient, distributed over transport elements which resemble in their structures the vortex elements, are used to compute the temperature distribution as the rollup evolves. Contrary to vorticity, scalar gradients are not conserved along particale paths, thus, the strength of these transport elements is changed according to the straining and rotation of the material elements. The scheme is capable of capturing very sharp gradients that develop within the core since the elements migrate towards these zones by convection. The multiplication of these elements via stretch, which inadvertently mimics the physical process by which large scalar gradients are generated, provides a naturally adaptive grid to compute these gradients. By expanding the cores of the transport elements, the effect of small diffusivities can be simulated as a small perturbation to the convection field. Diffusion, even at high Peclet number, is responsible for generating areas of uniform temperature inside the eddy since it acts to smooth out the sharp gradient created by convection.

The application of vortex methods to problems in which the no-slip boundary condition along solid walls must be satisfied can be accomplished using the random vortex method (Chorin [37], and Sethian and Ghoniem [38].) In this method, extra vortex elements are generated along the solid walls to cancel the slip velocity, and the diffusion of vorticity is simulated by the random walk of the vortex elements. At high Reynolds number, a strong strain field is expected to cause similar problems as described in this work, i.e., areas of large stretch will be depleted from vortex elements and accurate resolution of the vorticity field may be lost around these areas. Extending
the insertion-and-interpolation scheme described in this work to the random vortex method requires: (1) adding a third fractional step, which must be performed after the convection and before the diffusion steps, for the redistribution of the vorticity field among elements arranged in the direction of principal strain; and (2) computing the strain field at the center of the vortex elements in a Lagrangian form since, due to random walk, neighboring vortex elements and neighboring material elements change as time evolves. The implementation of these two steps must be preceded by careful formulation, and will require lengthy computation.
REFERENCES


Figure 1. The growth of the perturbation amplitude I with time for the most unstable case, $\lambda^*$, for three values of the initial perturbation $\varepsilon/\lambda = 0.001$, 0.01 and 0.1, showing the linear range and the saturation of the perturbation. Each curve is normalized with respect to the corresponding value of I at $t = 0$.

Figure 2. The location and velocity of the vortex elements during the rollup of a temporal shear. $\lambda = \lambda^*$, with $\varepsilon/\lambda = 0.001$. $N(0) = 572$, $h = 0.3$, $\delta = 0.375$, and $\Delta t = 0.1$.

Figure 3. The location and velocity of the vortex elements. Wavelength is $\lambda^*$, and $\varepsilon/\lambda = 0.01$. At $t = 0$, $N = 440$, $h = 0.33$, $\delta = 0.4$ and $\Delta t = 0.1$.

Figure 4. The location and velocity of the vortex elements for $\lambda = \lambda^*$, and $\varepsilon/\lambda = 0.1$. All the numerical parameters are the same as in Fig. 3.

Figure 5. Schematic diagram showing how the vorticity is redistributed among three elements when the distance between two neighboring elements exceeds a pre-specified value. $(x_n', y_n')$ are the coordinates of the new elements.

Figure 6. The total length of the interface, originally at $y = 0$, with time for the cases presented in Figs. 2, 3, and 4, normalized with respect to its length at $t = 0$.

Figure 7. The number of vortex elements used to represent the vorticity field during rollup for three initial perturbations, normalized with respect to the corresponding value at $t = 0$.

Figure 8. (a) The total kinetic energy of the perturbation based on the perturbation velocity, $(U(x)-u(x,t))^2$, and (b) The total kinetic energy of the flow, $u^2$, for $\varepsilon/\lambda = 0.001$, 0.01, 0.1.
Figure 9. The evolution of the vorticity field with time, compared with the experimental results of Roberts et al. [29] for the spatial development of a small perturbation of a shear layer.

Figure 10. The growth of the perturbation amplitude for $\lambda = 10.5$, $\varepsilon/\lambda = 0.01$. $N(0) = 455$, $h = 0.3$, $\delta = 0.375$ and $\Delta t = 0.1$.

Figure 11. The location and velocity of the vortex elements used in the calculations of the case shown Fig. 10.

Figure 12. The vorticity field for $\lambda = 2\lambda^*$, $\varepsilon/\lambda = 0.01$. $N(0) = 540$, $h = 0.44$, $\delta = 0.5$, $\Delta t = 0.1$.

Figure 13. The vorticity field for $\lambda = 2\lambda^*$, $\varepsilon/\lambda = 0.1$, using the same numerical parameters as in Fig. 12.

Figure 14. The vorticity field for $\lambda = 3\lambda^*$, $\varepsilon/\lambda = 0.01$. $N(0) = 818$ and the values of $h$, $\delta$, and $\Delta t$ are the same as in Fig. 12.

Figure 15. The vorticity field for $\lambda = 3\lambda^*$, $\varepsilon/\lambda = 0.1$, using the same numerical parameters as in Fig 14.

Figure 16. The location and velocity of the vortex elements for two perturbations, $\lambda_1 = \lambda^*$ and $\lambda_2 = 2\lambda^*$, with $\varepsilon = 0.1\lambda^*$ for both perturbations. $N(0) = 336$, $h = 0.55$, $\delta = 0.6$ and $\Delta t = 0.5$. A fourth order time integration scheme is used to transport the elements.

Figure 17. The total amplitude of the perturbation of the case in Fig. 16.

Figure 18. The temperature distribution across the layer at the center of the core, for $\lambda^*$ and $\varepsilon/\lambda = 0.001$. The numerical parameters are the same as in Fig. 2.
Figure 19. The temperature distribution across the layer at the center of the domain for $\lambda^*$ and $\epsilon/\lambda = 0.01$. The numerical parameters are the same as in Fig. 3.

Figure 20. The temperature distribution across the layer at the center of the core for $\lambda^*$ and $\epsilon/\lambda = 0.1$. The numerical parameters are the same as in Fig. 4.

Figure 21. The variation of the logarithm of the temperature thickness $T$ with time for the cases in Figs. 2, 3, and 4.

Figure 22. The rollup of the interface, defined by the layer which coincides with $y = 0$ at $t = 0$ for the case shown in Fig. 4.

Figure 23. The effect of thermal diffusion on the temperature distribution across the layer. Temperature is shown at $t = 20$ for the case shown in Fig. 4.

Figure 24. Total mixing, $M(t, \alpha, 0.1)$ due to the combined action of entrainment and diffusion, evaluated for different values of $\alpha$. 
Growth Rate for the Most Unstable Mode
TIME = 0.00 | ELEMENTS = 572
TIME = 24.00 | ELEMENTS = 891

TIME = 8.00 | ELEMENTS = 572
TIME = 30.0 | ELEMENTS = 1623

TIME = 16.00 | ELEMENTS = 595
TIME = 37.50 | ELEMENTS = 3257

ORDER OF INTEGRATION=2
ORDER OF CORE=2

LAYER=13 ELOB/LAYER=44 SIGB=0.375 THICKNESS=3.500 AMPL.=0.0010 U.LENGTH=10.20
TIME = 0.00  ELEMENTS = 440  TIME = 18.00  ELEMENTS = 980

TIME = 6.00  ELEMENTS = 440  TIME = 24.00  ELEMENTS = 1778

TIME = 12.00  ELEMENTS = 574  TIME = 28.5  ELEMENTS = 2747

ORDER OF INTEGRATION = 2  ORDER OF CORE = 2  MESH = 21x21  STATION = 22
LAYER = 1  BLOB/LAYER = 40  SIGB = 0.100  THICKNESS = 0.300  WPL = -0.0100  U LENGTH = 13.20
\[ \varepsilon = 0.01\lambda \\]
\[ \varepsilon = 0.1\lambda \\]
\[ \varepsilon = 0.001\lambda \]
TIME = 0.00 ELEMENTS = 455

TIME = 12.00 ELEMENTS = 593

TIME = 4.00 ELEMENTS = 455

TIME = 16.00 ELEMENTS = 893

TIME = 8.00 ELEMENTS = 501

TIME = 20.00 ELEMENTS = 1315

ORDER OF INTEGRATION-2 ORDER OF CORE-2

LAYER-13 BLOB/LAYER-35 SIGB=0.375 THICKNESS=3.600 WPL.=0.0100 U-LENGTH=10.50
ORDER OF INTEGRATION=2  ORDER OF CORE=2

LAYER= 9  BLOB/LAYER=0.0  SIGB=0.500  THICKNESS=0.520  NPL.-0.0100  U.LENGTH=28.40
TIME = 0.00 ELEMENTS = 810  TIME = 24.00 ELEMENTS = 1123

TIME = 8.00 ELEMENTS = 810  TIME = 32.00 ELEMENTS = 2143

TIME = 16.00 ELEMENTS = 810  TIME = 34.00 ELEMENTS = 2556

ORDER OF INTEGRATION=2  ORDER OF CORE=2
LAYER=9  ELOB/LAYER=90  SIGB=0.500  THICKNESS=3.520  WPL+=0.0100  U LENGTH=39.60
ORDER OF INTEGRATION-2
ORDER OF CORE-2

LAYER-9  BLOB/LAYER-90  SIGB-0.500  THICKNESS-2.520  AMPL.-0.1000  U.LENGTH-39.00
TIME = 0.00 ELEMENTS = 336

TIME = 5.00 ELEMENTS = 483

TIME = 10.00 ELEMENTS = 796

TIME = 15.00 ELEMENTS = 1237

TIME = 20.00 ELEMENTS = 1891

TIME = 25.00 ELEMENTS = 2914

ORDER OF INTEGRATION = 4
ORDER OF CORE = 2

LAYER = 7 BLOB/LAYER = 48 SIGOB = 0.000 THICKNESS = 3.300 AMP = 0.1000 U_LENGTH = 13.20
ORDER OF INTEGRATION=1
ORDER OF CORE=2

LAYER=13      BLOB/LAYER=445  SIGB=0.375  THICKNESS=3.000  AMPL.=-0.0010  W.LENGTH=12.20
ORDER OF INTEGRATION = 2    ORDER OF CORE = 2

LAYER = 11  BLOB/LAYER = 40  SIG submission = 0.400  THICKNESS = 3.300  AMPL = 0.81000  U LENGTH = 13.20
ORDER OF INTEGRATION = 2  ORDER OF CORE = 2  MESH = 21x21  STATION = 22

LAYER = 11  BLOB/LAYER = 40  SIGB = 0.400  THICKNESS = 3.300  AMPL. = 0.1000  U.LENGTH = 10 20
ORDER OF INTEGRATION=2    ORDER OF CORE=2

LAYER=11    BLOB/LAYER=40    SIGB=0.400    THICKNESS=3.300    AMPL.=0.1000    W.LENGTH=10 20
Appendix II

The paper on "Numerical simulation of a reacting shear layer using the transport element method" describes the formulation of the vortex element method and the transport element method for a chemically reacting flow with finite rate of heat release governed by Arrhenius chemical kinetics. The application of the method to a non-reacting spatially developing shear layer and a reacting temporally evolving shear layer are presented.
AIAA-87-1718
Numerical Simulation of a Reacting Shear Layer Using the Transport Element Method
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ABSTRACT

The transport element method is a numerical scheme that couples the vortex model with the Lagrangian transport of scalar gradients, used to study the evolution of concentration in a reacting shear layer. The method was adapted to the transport of scalar gradients distribution in a number of Lagrangian finite elements. The elements move along material lines, and change their shape or configuration to accommodate the distortion induced by the stream fields. Their volumes strength vary with the chemical reaction rate.

Premixed combustion at finite activation energy, moderate chemical kinetic rate and finite diffusion coefficients is considered. Processes that lead to burning enhancement or flame extinction were analyzed. It is found that the result of shear mixing in the flame is the reaction surface, and increasing the mass diffusional fluxes into the burning zone, resulting in burning rates which are proportional to the square of the strain rate. However, at high strain rate, strain leads to fuel transport through external heat release cannot compensate for the total flux out of the reaction zone and mass flux into the reaction zone.

INTRODUCTION

Turbulent combustion is governed by the complex interaction between convective and diffusive transport processes, chemical reactions and heat release. Chemical reactions are strongly nonlinear functions of temperature and species concentrations, and thus their rates are critically dependent on transport fluxes. Meanwhile, rates and magnitudes of heat release, associated with the chemical oxidation of practical fuels, are large enough to affect the transport phenomena. Understanding the role of these interactions is important to achieve better control of burning processes in practical systems. It is the objective of this work to develop numerical models suitable of predicting turbulent combustion processes, identify the most important factors of turbulent combustion.

...interactions and evaluate the influence of some of these interactions. We confine our attention to shear layers since they are relatively simple to analyze, and since they represent a general model for many reacting flows. Turbulent combustion has been the subject of extensive experimental, theoretical, and numerical investigations over the years. However, only a few fundamental processes remain understood. On one hand, progress in phenomenological turbulence combustion models, based on the closure of the system of average transport equations which describe the statistical behavior of the aerothermal parameters, has made it possible to produce results which agree with experimental measurements. On the other hand, since most of the interesting dynamics of turbulence-combustion interactions are modeled as generic in these models, solutions do not provide a better understanding of the phenomena and are difficult to reproduce for particular systems.

Two problems have been identified as most challenging in the study of turbulence in reactive flow: the source of the statistical correlations between fluctuating quantities, and the nature of the source terms in the energy and species conservation equations. In turbulent shear layers, the first problem is complicated by the presence of large scale turbulence structures which cannot be modeled by gradient-diffusion type terms. In second problem stems from the fact that chemical reactions are strongly affected by fluctuations in local variables and relatively large Reynolds numbers. In the following, the two issues are discussed in more detail...

Time-resolved flow visualization and instantaneous point measurements in nonreacting and reacting shear layers have revealed the existence of large scale periodic turbulent structures for a long distance downstream the separation point. It has been shown experimentally and supported by numerical studies, that these structures appear via the Kelvin-Helmholtz instability of the vorticity layer which forms between the initially-separate streams. By a different mechanism, the sub-synchronous instability, these structures persist through successive pairings, thus maintaining the periodicity downstream though at different frequency level. Qualitatively, it is known that the role these structures play in the mixing process is as follows: thin, stretched layers of fluid may be stretched by the Kelvin-Helmholtz instability and entrain...
The equations of motion for an inviscid fluid are the Navier-Stokes equations. 

In the context of investigating turbulent combustion, these equations must be solved numerically. Existing numerical techniques do not yield adequate results. Even though there exist different models which are designed to mimic the actual conditions of turbulent combustion, these models do not provide an adequate description of the flow. Moreover, they do not contain enough information about the chemical reactions. Therefore, the solution to the Navier-Stokes equations alone is not sufficient to predict the combustion process. Even in the case of a homogeneous, isothermal medium, the solution to the equations does not provide an adequate description of the combustion phenomena.

Since chemical reaction depends on the rate of molecular mixing within, as previously described, it is a combination of large-scale mixing by turbulence and the small-scale mixing by molecular diffusion. The importance of chemical reactions in the presence of large-scale convective structures is as important as the mass of the fluid. Most of the reaction occurs at the interface, but molecular reaction is not caused. One way to represent the interface is by using an accurate numerical solution to the Navier-Stokes equations. However, the equations are not accurate enough. A new numerical solution to the Navier-Stokes equations is needed. The new solution should be able to represent the interface accurately.

Vortex methods, which have been successful in Lagrangian schemes, are used to obtain solutions at high Reynolds numbers. Eulerian methods are used to obtain solutions at low Reynolds numbers. However, these methods are not realistic enough to be used in practice. In this paper, the purpose of using vortex methods is to simulate the hydrodynamics of the flow.

In this article, we will introduce the transport element method, which is a new method for simulating the vorticity field. When applied to obtain a solution of the vorticity transport equation, the method becomes the vortex element method. The method is based on the Lagrangian formulation of the conservation equations, which preserve its nature. A new numerical solution should be able to represent the interface accurately and to provide a more accurate result. If the interface is not represented accurately, the results will be useless. Therefore, we propose a new numerical solution that is based on an understanding of the interface phenomena.
identify different number of turbulent combustion interactions in a single system and to study the behavior of these interactions in different regimes of the governing parameters. Proceeding in the next section with our first extraction for the effect on the reaction kinetics and relationship in the context of the present work.

II. EQUATIONS

The non-dimensional form of the conservation equations governing a two-dimensional, unsteady reacting flow in a supersonic wind tunnel is of the following form that initially approximated by

\[ \frac{\partial u}{\partial t} + \frac{\partial (u^2)}{\partial x} + \frac{\partial (uv)}{\partial y} = \frac{1}{Re} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \]

and

\[ \frac{\partial v}{\partial t} + \frac{\partial (uv)}{\partial x} + \frac{\partial (v^2)}{\partial y} = \frac{1}{Re} \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \]

for gas velocities in the x and y directions respectively. The rate of formation of products per unit mass and time is also represented with respect to the approximate combustion of a stoichiometric fuel-air mixture at the exit of the fuel-air mixer. The free stream temperature of the reactants at \( \infty \), \( T_\infty \), and the activation energy of the gas mixture is the mass of hydrocarbon fuel per unit fuel. The mass of fuel per unit fuel is given by

\[ E = \frac{1}{RT_\infty} \left( \frac{\partial P}{\partial T} \right) \]

for the fuel-air mixture. The mass of fuel per unit fuel is given by

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\[ E = \frac{1}{RT_\infty} \left( \frac{\partial P}{\partial T} \right) \]
III. NUMERICAL METHOD

THE VORTEX ELEMENT METHOD

An important step in improving the accuracy and extending the application of vortex schemes to flow fields that develop large strain rates, such as shear layers, is the vortex element method. In this method, the vorticity field is accurately discretized among finite elements that move along particle trajectories and participate in the transport of finite vortices. The strain field is used to redistribute the vorticity among the computational elements at time progressions. Small vortices generated by planar shear layers have been stretched to very small scales, and these lead to fast damping and, therefore, to the generation of strong gradients as will be shown in the results. In the following, we summarize the method and show how it can be extended to compute compressible, nonequilibrium flows.

The vorticity field is initially discretized among vortex elements of finite structure. The distribution of vorticity associated with each element is represented by a radially symmetric function, \( f \), with a characteristic radius, \( r_c \), such that: most, or all, of the vorticity is concentrated within \( r < r_c \).\( \) vortex elements are initially distributed in the area where \( r > r_c \) such that the distance between neighboring elements is \( h \) in the two principal directions. The accuracy of the discretization, however, depends on the choice of \( r_c \), the value of \( h \), and the value of \( h \).

The strength of the vortex element located at \( X_1 \), denoted by \( \Omega_1 \), is obtained from the solution of the system of equations:

\[
\Omega = \int f(r) X r \cdot dS
\]

where \( X_1 \) is the vortex distribution at \( t=0 \). Using a Taylor series expansion, it can be shown that the effect of the element is an interaction term given by:

\[
\Delta \Omega = \int f(r) X r \cdot dS
\]

where \( \Delta \Omega \) is the mutual interaction between vortex elements, \( f(r) \) is the weight function, \( X(r) \) is the vorticity distribution, and \( dS \) is the area element. This method is exact, and \( \Delta \Omega \) must be evaluated at each time step.

For compressible, barotropic flows, \( \Omega \) is the local vorticity that is constant along a particle path, \( \Omega = \omega \). Using the definition of the vorticity \( \Omega = \omega \), and \( \omega = -\nabla \times u \), where \( u \) is the velocity vector, the vorticity can be written as:

\[
\omega = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j} \right)
\]

where \( x_i \) and \( x_j \) denote spatial coordinates. The vorticity field is obtained from the solution of the system of equations:

\[
\frac{\partial \omega}{\partial t} + \nabla \cdot (u \times \omega) = 0
\]

where \( \omega \) is the vorticity, \( u \) is the velocity, and \( \nabla \) is the gradient operator.

To obtain the velocity field of a collection of vortex elements in the form of Eq. (11), we note that the stream function of a single vortex element is obtained by integrating Eq. (11). Using polar coordinates, the equation for a vortex element located at \( r = \rho_0, \theta = \theta_0 \), is:

\[
\frac{\partial \psi}{\partial r} + \frac{1}{r} \frac{\partial \psi}{\partial \theta} = 0
\]

where \( \psi \) is the stream function, \( r \) is the radius, and \( \theta \) is the angle. The velocity field of a single element is then:

\[
\psi = \int f(r) r \cdot dS
\]

where \( f(r) \) is the weight function, \( r \) is the radius, and \( dS \) is the area element.

According to Eq. (12), vortices are located at the local velocity at their centers. As the vortex element progresses, the distance between neighboring elements increases in the direction of maximum strain rate such that the distance in the direction of maximum strain is defined as \( \Delta s = \lambda_\omega \Delta r / \Delta \theta \), where \( \lambda_\omega \) is the time increment. The circulation of the new element, and that of the original two neighboring elements, is then obtained by integrating the circulation of the original two elements:

\[
\Gamma = \int \omega \cdot dS
\]

where \( \Gamma \) is the circulation, \( \omega \) is the vorticity, and \( dS \) is the area element. The circulation can be computed by using the vortex element method. In the next section, we shall use this method to compute the circulation of vortex elements.
\[
\frac{\partial V_a}{\partial t} = - \frac{V_a}{x} x + \frac{\partial V_a}{\partial x} \frac{\partial x}{\partial t}
\]

where \( f \) and \( g \) are the same definitions as before, and \( \gamma \) should be chosen to satisfy the same requirements. To see how to transport the scalar gradient in a Lagrangian form, we start by the non-diffusive case. If \( s \) is a passive, non-diffusive scalar, the conservation equations for \( s \) are:

\[
\frac{\partial s}{\partial t} = 0
\]

Furthermore, the flux initialized by Eq. (17) becomes:

\[
g'(x,t) = \sum_{i=1}^{N} g_i(t) n_i f_i(x - x_i(t))
\]

where

\[
g_i(t) = \frac{\partial \gamma_i(t)}{\partial n_i}
\]

From Eqs. (17) and (20), it can be shown that the gradient is a function of \( \gamma \), where \( \gamma = |\mathbf{g}| \). Thus, the gradient transported by an element that follows a particle path can be written as \( \gamma \) (Eq. (21)).

Figure 1. Schematic sketch showing the evolution of a material layer separating two values of the conserved scalar, \( s \) and the associated scalar gradient, \( g \), under the effect of stretch.
\[ \frac{\partial i}{\partial t} = -u \cdot \frac{\partial i}{\partial x} \]

where \( i, x, u \) are updated according to Eq. (1) and \( n = i, j \). Equation (1) is equivalent to updating \( i \), according to Eq. (2).

However, the expression in Eq. (1) conserves the value of \( i \). Moreover, instead of integrating Eq. (1), one can save computational effort by noticing that \( i_2 = i_1 \). Thus, it is sufficient to save the motion of the transport elements, and to move the neighboring elements to update \( i_1 \). If this is done, these elements are assumed to move as straight lines.

Given the location and strengths of the transport elements, the linear concentration can be computed as follows. When \( V_s = g \), one can take the gradient \( \nabla T = \mathbf{g.v} \). The equation of the gradient in an infinite domain can be written as:

\[ \mathbf{a} \cdot \nabla \mathbf{v} = \mathbf{g.v} \times \mathbf{x} \]

where \( \mathbf{a} = \frac{\nabla \mathbf{v}}{\nabla T} \) is.

The final equation is the divergence of the curl of the gradient. Integrating by parts, one gets:

\[ \mathbf{v} \times \mathbf{x} = \mathbf{g.v} \times \mathbf{x} \]

Using Eqs. (1) and (2) for \( g \), one gets:

\[ \mathbf{v} \times \mathbf{x} = \mathbf{g.v} \times \mathbf{x} \]

where \( \mathbf{x} = \frac{n+1}{n} \mathbf{v} \times \mathbf{x} \).

If the distance between neighboring elements in the direction of principle strain exceeds a maximum distance \( d \), then one element is inserted halfway between the two elements and the value of \( i \) is updated for the three elements. A recombination procedure can also be implemented to double the growth in the number of computational elements. The need for this insertion procedure is more apparent here since the magnitude of the gradient increases where the strain field is high, and to maintain the accuracy, more elements must be used to transport this gradient.

With finite diffusivity, the first term on the right hand side of Eqs. (6-8) should be eliminated in the solution. In gradient form, the conservation equation can be written as:

\[ \frac{\partial g}{\partial t} = \mathbf{g.v} \times \mathbf{x} \]

where \( a \) is the molecular diffusivity, or the inverse of the Peclet number. At high speed flow, \( a \) is typically \( 10^{-15} \). To solve Eq. (12) using the scheme that we have developed so far, each element \( g \) must be updated according to the diffusion equation:

\[ \frac{\partial g}{\partial t} = a \mathbf{g.v} \]
The vortex element scheme and the transport element scheme were applied to simulate the initial stages of development of a spatially developing two-stream shear layer. On the left boundary of the domain, it is assumed that the wake region behind the splitter plate, where the two incoming boundary layers merge to form the shear layer, is very small. Thus, at \( x = 0 \) for \( y > y_x ; \) \( y = -1, -1/3 \), and for \( y < -y_x ;\) \( y = 0.33 \),

\[ \text{and } y = 0, \text{ where } \mp \text{ means "approaches asymptotically"}. \]

Here, the normalized temperature is defined as \( T^* = \left( T - T_w \right) / \left( T_h - T_w \right), \)

\[ T_y^* = 2T_y, \]

where \( \sigma \) is the standard deviation of the Gaussian distribution that describes the vorticity and the scalar gradients, and \( 2y_x \) is the nominal shear layer thickness. For the results in Figure 1, \( y_x \) \( = 1/26.4 \), leading to a most unstable wavelength, as predicted by the linear theory, of 1.1. Within the shear layer, the velocity and temperature distribution are represented by functions that are computed by using conformal mapping and image vortices. At the downstream side of the computational window, at \( x = b \), vortex elements are deleted. This induces a strong perturbation which ensures that the rollup and first pairing will always take place within the computational window. Since this perturbation is not applied in an organized manner, the resulting shear layer will be considered as an unforced layer.

Figure 2 shows the location and velocity of all vortex elements used in the computations for five time steps. The time step of the computations is \( \Delta t = 0.015 \). The plots exhibit a very clear and accurate portrait of the rollup. During rollup, the vorticity within the shear layer is attracted towards the center of a large eddy, entraining fluid from both sides, and forming what appears to be a moving focal point of a spiral. Between neighboring large eddies, a zone of strong strain is developing where the vorticity is depleted and the gradients are growing. This "braided" zone can be described as a moving saddle point where locally the fluid flow experiences a separation into two streams; one moving towards the left and the other moving towards the right with respect to the saddle-stagnation point. Downstream, the process of rollup continues until a stronger perturbation forces two neighboring eddies to interact in a pairing process. It is important to stress that the algorithms of inserting elements at the strain field develops are responsible for maintaining the organization of the calculation for a long time.

Quantitatively, the natural frequency of shedding, \( f_n \), is defined as \( f_n = \omega_n / \pi \), where \( \omega_n = \left( U_1 + U_2 \right) / 2 \), and \( \lambda \) is the wavelength of the large eddy. The corresponding Strouhal number is \( S_t = f_n \lambda / U_1 \). This is the same value as the frequency of the most unstable mode computed from the linear stability theory of a spatially developing shear layer under the conditions described above. Preliminary results for the rollup rate, average velocity and turbulent statistics were presented in study of Gontier and Ng for the forced shear layer.

The high resolution of the transport element method demands the use of a large number of transport elements. Moreover, the number of elements grows rapidly with time due to the evaporation towards the saddle-stagnation point of downstream, the process of rollup continues until a stronger perturbation forces two neighboring eddies to interact in a pairing process. It is important to stress that the algorithms of inserting elements at the strain field develops are responsible for maintaining the organization of the calculation for a long time.
V. TEMPORALLY-DEVELOPING, REACTING SHEAR LAYER

Computational results showing the evolution of a large eddy in a temporal, shear layer are presented in Figure 3. In this case, the boundary conditions are periodic, i.e., \( w(x,y,t) = w(x+L,y,t) \) and \( u(x,y,t) = u(x+L,y,t) \), where \( L \) is the wavelength of the perturbation. Since the flow is unconfined, the wavelength \( \lambda \) is used instead of \( H \) to non-dimensionalize the length.

The temperature profile across the midsection of the large eddy is exhibited in Figure 4. The rollup brings fluid from one side to the opposite side, while stretch increases the gradient across each layer. The profiles show that after the relaxation of the first rollup, a secondary instability develops which forces the core through another turn, thus creating a more ragged temperature distribution. Moreover, it can be seen that the rollup of the shear layer is the mechanism of entrainment that leads to strong mixing enhancement as the two fluids diffuse across the stretched interface. Since rollup is associated with strong stretch that reduces the thickness of the material layers, it increases the gradients across these intertwining layers, thus enhancing the diffusion fluxes. Quantitatively, the rate of mixing can be expressed as \( \dot{\theta} = \dot{q} \cdot n \) da, where \( q \) is the diffusion flux, \( n \) is the unit vector normal to the material surface, and \( da \) is the surface area element. Since for two-dimensional flow, \( da = dl \), and since \( q \cdot n \) is constant, then \( \dot{\theta} \) is proportional to \( (\dot{q})^2 \). The net result is that stretch by a factor \( \xi \) enhances mixing by a factor \( \xi^2 \). The quadratic rise in mixing during rollup will have a significant effect on the rate of reaction.

In the reacting layer calculations, the full system of equations is integrated using particles that transport vortex elements, temperature gradient elements, reactant and product gradient elements. At time \( t = 0 \), the flame front coincides with the vorticity layer and the thickness of the vorticity layer as well as the temperature and species concentration within the layer are taken to be equal. A small sinusoidal perturbation with amplitude \( 0.05 \lambda \) is imposed on both distributions. The first case to be computed corresponds to the following set of parameters:

- \( P_e = 200 \), \( L_e = 1 \), \( A_e = 1 \), \( C = 4 \), and \( T_a = 10 \), and \( n = 1 \).
The corresponding laminar number, measured at the condition of maximum reaction rate is around \( 0.2 \), and the temperature ratio across the layer is \( T_{\infty}/T_0 \).

Figure 5 shows the reacting shear layer at rollup proceeds along with the chemical reaction. At the early stages, the eddy strongly resembles that of the nonreacting flow shown in Figure 5. However, as rollup starts, the following is observed: (1) a swelling, due to the concomitant increase in the rate of heat release, continues as more reactants are entrained into the burning core; (2) the growth of the instability, as measured by the angle between the major axis of the elliptical structure and the main stream direction, is encumbered because the volumetric expansion causes the vorticity intensity to decrease and the eddy to become weaker and less coherent; and (3) the eddy loses its symmetry and becomes eccentric due to the asymmetric expansion and the generation of a non-baroclinic torque associated with heat release. As the initial core is burnt, the fluid inside the eddy ceases to spin, contrary to the nonreacting case. Meanwhile reactants move through the side to enter the reaction region. These results agree qualitatively with the experimental results of Keller and Daily on the reacting mixing layer at high equivalence ratios.

On the same figure, a solid line is plotted through points of maximum reaction rate. The line indicates where the flame front, or the maximum heat release rate, is within the shear layer. Below this line, the product concentration approaches unity and the temperature reaches \( T_{\infty} \).

During the early stages of rollup, the line of maximum reaction rate follows one of the material lines closely, i.e., the growth of perturbation initially changes the topology of the flame front. At later stages, this line, while staying near another material line, forms a solution of products where the reactants are entrained by burn. Below this line, the product flux, core almost stops its rotation. At the last stage of burning of the eddy, the two sides of the flame front close, and the flame moves out of the eddy and becomes a ordinary laminar flame.

The effect of heat release on the structure of the eddy, which is generated by the roll-up of the shear layer, can be seen from the temperature profiles across the midsection of the wavelength. Figure 6. Since the Lamé number is \( 0.2 \), \( T_{\infty}/T_0 = 17 - T_0/\lambda_0 \). As reactants are entrained into the core of the growing eddy from the right side, a Z-shaped flame is formed. At the initial stages where the rate of entrainment is faster than the rate of burning, the flame extends deeper into the lower stream. As the reactants within this zone burn, heat is released within the core of the rotating eddy, causing the eddy to swell, while maintaining its elliptical shape. The non-baroclinic vorticity generated around this zone causes the observed eccentricity of the large eddy. The temperature profiles show that the higher order instabilities observed in the nonreacting case are suppressed by the heat release, and that the core of the eddy stops its rotation. As the reactants within the eddy burn, the flame leaves the structure and moves into the reactants. This results in the formation of a temperature profile which is very similar to the temperature profile at two.

To study the effect of the shear layer on the chemical reaction, we compare the rate of burning
for a flame moving through a shear layer, i.e., a reacting shear layer, with the same flame moving into a quenched environment, i.e., a laminar flame. Results for the laminar flame are obtained using the same method but with \( \lambda \rightarrow 0 \). The rate of burning is defined in terms of the total mass of products generated since \( t = 0 \). Figure 7 depicts the total mass burn, \( M_p \), for both cases.

![Figure 7](image)

**Figure 7.** Total mass of products \( M_p \) formed since \( t = 0 \) in the reacting shear layer, labelled as RSL, and in the laminar flame, labelled as LF, at the same conditions, and the total length of the flame in the reacting shear layer of Figure 5.

showing clearly the different stages of burning in the reacting shear layer. At the early stages, during the linear phase of development where the stretch is negligibly small, the rate of burning is linear and identical to that of a laminar flame. As the layer starts to roll up, the area of the reaction surface increases and the flame is convoluted around the growing eddy. The increase in the flame area due to convolution is nearly linear, as shown in Figure 7. However, as indicated by the Figure 7, the products form at almost a quadratic rate during this stage. This phenomenon can only be explained by recalling that mixing is enhanced as the square of the stretch, and that in this case of fast chemistry, the rate of burning is governed by mixing.

At later stages, around \( t = 20 \), the amount of products forming is almost nine times that which forms in the laminar flame. Due to flame convolution, the reacting surface area has increased by three folds. Since stretching a layer of material by three times its initial length decreases its thickness by the same amount, and the fluxes across it increase by three fold as well, this augments the rate of mixing by nine times over the non stretching case. When the chemical reaction is fast, as in this case, the material mixed reacts and the rate of reaction increases by the same rate as the mixing. This is what has been labelled "mixing-controlled reaction" in the turbulent combustion literature.

To further analyze the results, we plot the temperature \( T \), the strain rate \( \dot{s} \), and rate of expansion \( \dot{e} \) along layer 7 in the reacting eddy.

![Figure 8](image)

**Figure 8.** The temperature \( T \), strain rate \( \dot{s} \), and rate of expansion \( \dot{e} \) along layer 7 in the reacting eddy.

![Figure 9](image)

**Figure 9.** The temperature \( T \), strain rate \( \dot{s} \), and rate of expansion \( \dot{e} \) along layer 8 in the reacting eddy.
Figure 10. Layers 7 and 8 in the reacting eddy of Figure 9.

show these plots for layers 7 and 8, respectively, which are shown in Figure 10. Figures 6 and 9 show a positive correlation between the temperature and the strain rate; each temperature peak corresponds to a maximum in the strain rate.

VORTICITY LOCATION
STEP: 350 TIME: 17.57 LE: 1.0

Figure 11. The eddy in a reacting temporal shear layer at the same conditions as in Figure 5 but with \( A_f = 0.5 \), \( t = 17.57 \).

As the layer stretches, the diffusion flux of the reactants into the flame increases and, since chemistry is fast, the rate of burning increases. Under compression, the reactants diffusion flux is reduced and the amount of burnt mixture, and hence the rate of expansion, is reduced.

Decreasing the frequency factor to \( A_f = 0.25 \), which reduces the Damköhler number \( D_l \), the eddy factor, yields another characteristic parameter of development of the large eddies, as is shown in Figure 11. The eddies in the regions reduced since the rate of chemical reactions is less than in the case of \( A_f = 0.5 \). At the earlier stages, the reaction proceeds in the manner of Figure 9. However, at \( t = 18.51 \), the reaction suddenly stops, as shown in Figure 12 for the mass of products \( M_p \). The laminar flame was too eman.
Figure 14. The temperature $T$, strain rate $\dot{\epsilon}$, and expansion rate $\dot{\epsilon}$ along layer 3 in the reacting eddy in Figure 11.

Figure 15. The temperature $T$, strain rate $\dot{\epsilon}$, and expansion rate $\dot{\epsilon}$ along layer 5 in the reacting eddy in Figure 11.

Advanced numerical methods enable one to integrate elaborate and detailed models, which cannot be done analytically, so that complex mechanisms may be revealed and analyzed; and to provide detailed information about the flow field which may not be possible using traditional, experimental techniques. Computer output, rich in data, offers a challenge in how to extract valuable information about the phenomena under investigation, and how to present these information in compact form. Finding out the appropriate diagnostics to probe computational results is half the way to reaching the conclusions.

In this article, we have introduced the transport element method: a Lagrangian particle scheme based on the discretization of the vorticity and the gradients of the scalars into finite elements. The particles move along material lines, in accordance with their transport equations. As strong strains develop in the dynamic field, the finite elements may change their shape or configuration to accommodate the distortion which is produced by these strain fields. In case of chemical reaction: (1) the strength of the elements, i.e. the source strength, changes according to the rate of reaction; and (2) the chemical heat release induces volumetric expansion and non-baroclinic vorticity into the dynamic field.

The simplest model which can be proposed to study turbulence-combustion interactions contain five parameters: (1) the Peclet number which defines the ratio between the rate of convective and diffusive heating; (2) the Lewis number which represents the ratio between the rate of heat and mass diffusion; (3) the frequency factor which defines the ratio between the rate of chemical reaction and mass convection; (4) the activation energy of the reaction; and (5) the enthalpy of reaction. The outcome of these interactions can, thus, be presented on a five dimensions space or...
The jet flame was found to result from the interaction of the fuel diffusion field with the mixing layer.

At values larger than $A = 0.1$, combustion is intermittent under strong structure. At smaller values of $A$, the flame is extinguishing.

Thus, due to the fact that the fuel and air mix into the reaction zone is not balanced by an increasing in heat release, the reaction zone within this zone. The reaction zone is thus obscured, followed by the extinction of the flame.

Work is underway to vary the rest of the controlling parameters and study their effects on the flame stability.

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REFERENCES


Appendix III

The paper on "Vortex-scalar element calculations of diffusion flame stabilized on a plane mixing layer" describes the scalar element method and its application to a diffusion flame with low heat release.
AIAA-87-0225
Vortex-Scalar Element Calculations of a Diffusion Flame
A. F. Ghoniem, Massachusetts Institute of Technology, Cambridge, MA; and
P. Givi, Flow Research Company, Kent, WA

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ABSTRACT

The vortex-scalar element method, a scheme which utilizes vortex elements to discretize the region of high vorticity and scalar elements to represent species or temperature fields, is utilized in the numerical simulations of a twodimensional reacting mixing layer. Computations are performed for a diffusion flame at high Reynolds and Froude numbers without resorting to turbulence models. In the non-reacting flow, the mean and fluctuation profiles of a conserved scalar show good agreement with experimental measurements. Results for the reacting flow indicate that for temperature-independent kinetics, the chemical reaction begins immediately downstream of the splitter plate where mixing starts. Results for the reacting flow with Arrhenius kinetics show an ignition delay, which depends on the reaction temperature, before significant chemical reaction to occurs. Harmonic forcing changes the structure of the layer, and concomitantly the rates of mixing and reaction, in accordance with experimental results. Strong stretch within the braids in the non-equilibrium kinetics case causes local flame quenching due to the temperature drop associated with the large convective fluxes.

I INTRODUCTION

Turbulent diffusion flames have been the subject of extensive experimental and theoretical investigations during recent years [for a review, see Bilger [1]]. In most of the theoretical work, turbulence models are used to close a system of averaged transport equations which describes the statistical behavior of the aerothermodynamical variables. Moment methods [2], eddy break-up and mixing controlled models [3], flame sheet approximation [4], assumed probability density function (PDF) shape methods [5], solutions based on modelled joint PDF of scalar and velocity [6,7], and based on modelled joint PDF of scalar and velocity [8] are examples in which turbulence modelling have been used for the closure of equations governing the statistical quantities. Much effort has gone into constructing accurate models and in obtaining results that are in agreements with experimental measurements. However, in complex systems, modelling is difficult because of our lack of knowledge on the detailed dynamics of the flow. Furthermore, since most of the interesting dynamical behavior of the flow is modelled a priori, such features are not exhibited from the results of numerical computations based on turbulence models, and thus can not advance our understanding of turbulent combustion.

The progress in numerical methods and the availability of supercomputers have had a major impact on turbulence research. Improved accuracy of the numerics and increased storage and computational speed have made it possible to solve the appropriate transport equations governing turbulent combustion directly without the need for modelling for some limited parameter range. Such model-free "simulations," in comparison with calculations utilizing turbulence models, have the advantage that the physics of the problem is not modelled a priori, but is recovered directly from the computed results. Their results can be used to understand many important mechanisms of turbulent transport and its direct influence on chemical reactions. Furthermore, since the instantaneous behavior of the variables are known at all points and at all times, accurate simulations offer a good method of probing the flow when experimental techniques may fail. Ultimately, by validating the results of the simulation against experimental measurements, ab initio predictions will be a reality.

Numerical methods have been used in a variety of forms for the simulation of turbulent flows in complex configurations. A recent survey can be found in review articles [9,10]. In reacting flow, three approaches are used: (1) finite difference methods, (2) spectral methods; and, (3) vortex methods. In the first approach, the variables are defined on a grid and the transport equations are approximated by discretizing the derivatives on the grid nodes. Examples of this approach can be found in the work of Corcos and Sherman [11] who used a projection method to study the temporal evolution of a periodic shear layer, and in Grinstein et al. [12] who used a flux-corrected transport scheme to simulate the development of coherent structures in a two-dimensional spatially evolving shear layer and examined their effect on mixing.

In spectral methods, the variables are expanded in series of harmonic functions that satisfy the differential equations on a number of collocation points. Riley et al. [13] used a pseudo-spectral scheme to study a three-dimensional temporally-evolving reacting mixing layer assuming a constant reaction rate, constant
density and no heat release. McMenemy et al. [18] considered the effects of thermal heat release on the flow dynamics of a two-dimensional mixing layer for a constant reaction rate. The interaction between fluid dynamics and the chemical reaction is investigated under these conditions. McMenemy et al. [18] also used the same method to compute a two-dimensional mixing layer with an Arrhenius-type reaction and constant density to assess the effects of large coherent structure on the local extinction of the flame. Extension to spatially evolving layers was initiated by Civi and Dukowicz using a hybrid pseudo-spectral second-order finite difference scheme. In all cases, the Reynolds number was kept at small values, 0.0001, limited by the grid resolution and the number of harmonic modes.

In the third approach, vortex methods are used. These schemes are grid-free, the transport of the variables take place in a Lagrangian form, and the solution is not restricted by the geometry of the confinement. Therefore they can provide accurate simulations for high Reynolds number, spatially evolving flows. Moreover, vortex methods allow to optimize the computational efforts by distributing computational elements around regions of high vorticity. The application of the method in thin premixed flame calculations with a finite density jet has been reported by Gnish et al. [17] and Settles [18], among others. In these calculations, the vortex method was employed to simulate the flow field, and the result presents the mixing of species at the laminar burning velocity as a volumetric source. Vortex methods were also used in simulating diffusion flames in connection with a finite-difference approach for the treatment of the scalar variables. Ashurst and Barr [19] used the vortex method to compute the hydrodynamic field and the Eulerian flux-corrected transport algorithm to compute the diffusion and convection of a conserved Shvab-Zeldovich scalar approximating the shape and convolution of the flame in the limit of infinitely fast chemical reaction. Lin and Pratt [20] used the random vortex method to simulate the large-scale motion and a Lagrangian particle method to calculate the time-dependent probability density function of the scalar quantities for both gaseous and aqueous mixing layers. The PDF transport equation, however, required a closure model for the molecular mixing term.

From this short review, it is clear that numerical simulations have played an important role in elucidating the physics of turbulent reacting flows, and that there is a continuing need for more model-free simulations in order to explain better some of the interesting physical phenomena that have been observed in laboratory experiments.

In this work, we extend the vortex method to study non-premixed chemical reactions. A vortex-scalar element method is developed to treat both the hydrodynamic flow and the scalar field in a Lagrangian sense. The fact that a chemical reaction is truly a Lagrangian process, i.e., it occurs when the particles (or macroscopic elements) interact as they flow, motivate the implementation of Lagrangian methods to simulations of high Reynolds number reacting flows. The method is capable of handling a variety of initial and boundary conditions and is not limited to simple cases.

II FORMULATION AND NUMERICAL SCHEME

A two-dimensional, confined, planar mixing layer is considered. A schematic diagram for the flow field is shown in Fig. 1. Two initially unmixed reactants, fuel \( F \) and oxidant \( O \), are present at small concentrations in the top high-speed stream and bottom low-speed stream, respectively. We make the following assumptions: (1) the heat release is low so that its effect on the dynamics of the flow is negligible; (2) the Mach number is small; (3) the free stream concentrations of \( F \) and \( O \) are equal and constant; (4) the molecular diffusivities are equal and constant; (5) the viscosity is the same in all streams; and (6) the chemical reaction is single step, irreversible, and first order. The density is, therefore,
NUMERICAL SIMULATION OF TURBULENT FLAMES USING VORTEX METHODS

UNCLASSIFIED
the transport equations of the hydrodynamic field and the scalar — temperature or species — fields are decoupled. The equations governing this system are:

\[ \frac{\partial \bar{u}}{\partial t} + \nabla \cdot (\bar{u} \bar{u}) = -\nabla \cdot \bar{p} + \nabla \cdot \left( \nu \nabla \bar{u} \right) + \bar{f} \]

\[ \frac{\partial \bar{T}}{\partial t} + \nabla \cdot (\bar{u} \bar{T}) = \nabla \cdot \left( \kappa \nabla \bar{T} \right) + \bar{Q} \]

where \( \bar{u} \) and \( \bar{T} \) are the velocity and temperature fields, respectively, \( \nabla \cdot \bar{p} \) and \( \nabla \cdot \left( \nu \nabla \bar{u} \right) \) are the pressure forces and viscous stresses, and \( \bar{f} \) is the body force. The finite rate kinetics effects can be taken into account considering the transport equation for the product of chemical reaction, Eq. (6), and Eq. (7) for a conserved scalar. If the Lewis number is unity, another conserved scalar can be introduced, \( \delta_{FP} = \frac{c_p}{T}Q/TQ \), and the solution of Eqs. (6) and (7) for \( c_p \) and \( \delta \) will determine the behavior of all the scalar quantities, \( c_p, c_0, c_0^*, c_p, \) and \( T \).

II.1 THE VORTEX SCHEME

In the vortex method, the vorticity field is represented by a finite number of vortex elements of finite cores:

\[ \omega(x,t) = \int \Gamma_i \delta^2(f(x-x_i)) \]

where \( \Gamma_i \) is the circulation of a vortex element and \( \delta \) is the core radius, while \( x_i \) is the center of the element. \( f \) represents the vorticity distribution associated with a vortex element, or the core function (Chorin [23] and Hald [24]), and Beale and Majda [25].) The velocity field is obtained by solving Eq. (2) using the discrete vorticity distribution:

\[ u = \int \Gamma_i K(x-x_i) \kappa(x-x_i) + u_p \]

where \( K(x) = -\frac{1}{2}(y-x)^2 \) is the kernel of the Poisson equation, \( \kappa(x) = \int \pi f(r) \) is the circulation within \( r \), and \( r = |x| \). \( u_p \) is an irrotational velocity field added to satisfy the potential boundary condition; \( u_p = \nabla \phi \) where \( \nabla \phi = 0 \) and \( u_p \) and \( \phi \) are on solid boundaries while \( u_p = u \) at the inlet, \( n \) is the normal unit vector. For the confined shear layer, the boundary condition at \( x = 0 \) is: \( u = U \) for \( y > 0 \) and \( u = U_2 \) at \( y < 0 \), while \( y = 0 \) is a vortex sheet of strength \( \omega \) at \( U_1 - U_2 \).

In this work, we use Rankine vortex elements, i.e., the vorticity of an element is constant within the core and zero outside, \( f(r) \) is the kernel of the Poisson equation, \( \kappa(x) = \int \pi f(r) \) is the circulation within \( r \), and \( r = |x| \). \( u_p \) is an irrotational velocity field added to satisfy the potential boundary condition; \( u_p = \nabla \phi \) where \( \nabla \phi = 0 \) and \( u_p \) and \( \phi \) are on solid boundaries while \( u_p = u \) at the inlet, \( n \) is the normal unit vector. For the confined shear layer, the boundary condition at \( x = 0 \) is: \( u = U \) for \( y > 0 \) and \( u = U_2 \) at \( y < 0 \), while \( y = 0 \) is a vortex sheet of strength \( \omega \) at \( U_1 - U_2 \).

The motion of the vortex elements must be constructed such that the vorticity field satisfies Eq. (3). This is accomplished by solving this equation in two fractional steps:

Convection:

\[ \frac{\partial \bar{u}}{\partial t} + \nabla \cdot (\bar{u} \bar{u}) = -\nabla \cdot \bar{p} + \nabla \cdot \left( \nu \nabla \bar{u} \right) + \bar{f} \]

Diffusion:

\[ \frac{\partial \bar{T}}{\partial t} + \nabla \cdot (\bar{u} \bar{T}) = \nabla \cdot \left( \kappa \nabla \bar{T} \right) + \bar{Q} \]

In the first step, the convective transport of vorticity is implemented in terms of the Lagrangian displacement of the vortex elements using the current velocity field computed from Eq. (9). In the second step, the solution of the diffusion equation is simulated stochastically by the random walk displacement of the vortex elements according to the appropriate population. Thus:

\[ \chi(t+\Delta t) = \chi(t) + \Delta t \omega \Delta k \]

\[ k \]
for \( i = 1, 2, ..., N \), where \( I_k \) is a \( k \)-th order time-integration scheme and \( \eta_1 \) is a two-dimensional Gaussian random variable with zero mean and standard variation \( \sqrt{2} \sigma_t / \text{Re} \). For more details, see Ghoniem and Ng [22], Ghoniem and Gagnon [26].

The no-slip boundary condition at the walls is satisfied by generating new vortex elements to cancel the induced velocity by the vorticity field. Here, we generate vorticity only at the point of separation, i.e. at the tip of the splitter plate since the growth of the boundary layers along the channel walls at these high Reynolds numbers is small. At each time step, the new vorticity \( \alpha' = -U_m \text{d}t \), where \( U_m = (U1 + U2)/2 \), is consigned to No elements of strength \( \alpha' / \text{No} \) and added to the field at points \( \Delta x = U_m / \text{No} \) apart downstream of \( x = 0 \).

The effect of the numerical parameters on the accuracy of the results was investigated by Ghoniem and Ng [22]. Their results emphasized the importance of using a high order time-integration scheme with \( k = 2 \) to avoid excessive numerical diffusion in the vorticity field. The value of \( \text{No} = 6 \) was also found to be appropriate in order to obtain well-defined eddy structures after the rollup and the first two pairings. The second pairing is accomplished within the domain of \( 0 \leq x \leq \frac{\pi}{2} \), therefore the computational domain was limited to \( \text{Xmax} = 6 \). Downstream of \( \text{Xmax} \), the vorticity was deleted. Varying \( \text{Xmax} \) showed that the effect of deleting the vortex elements propagates about one channel height upstream, hence the results are accurate only for \( 0 \leq x \leq \frac{\pi}{4} \).

II.2 THE SCALAR ELEMENT METHOD

In this scheme, which is a two dimensional extension of the vortex element method of Ghoniem and Oppenheim [27], the scalar field is represented by a set of elements each carrying a finite amount of the scalar field:

\[
s(x, t) = \sum_{i} s_{i} \delta(x-x_{i})
\]

where \( s \) is a scalar field, being the temperature or species concentration, \( s_{i} \) is the strength of an element, defined as the amount of scalar carried by this element and \( \delta(...) \) is the Dirac delta function. \( s_{i} = 1/6A / s(x, t) \Delta A \), where \( \Delta A = 4\pi \Delta x \), and \( \Delta x \) is the distance between the centers of neighboring elements in the streamwise and cross stream directions, respectively, and \( x_{i} \) is the center of the element. If \( s \) is an active scalar, its transport is governed by:

\[
\frac{\partial s}{\partial t} + u \cdot \nabla s = \frac{1}{\text{Se}} \nabla^{2} s + \dot{W}
\]

where \( \text{Se} \) is the ratio between the diffusive and convective time scales of transport of \( s \), \( \dot{W} = \text{Pe} \) for \( s = T \), and \( \dot{W} = \text{Pe} \text{Le} \) if \( s = c \). In the scalar element method, this equation is solved in three fractional steps:

\[
\text{Convection} \quad \frac{\partial s}{\partial t} + u \cdot \nabla s = 0
\]

\[
\text{Diffusion} \quad \frac{\partial s}{\partial t} = \frac{1}{\text{Se}} \nabla^{2} s
\]

III. RESULTS AND DISCUSSION

The computer code, developed by Ghoniem and Ng [22] for vortex simulation of a non-reacting shear layer, was vectorized in order to take advantage of the computational capability of a CRAY-XMP. The scheme, being explicit in time and requiring mostly non recursive computations, can utilize this capability efficiently. The dynamics of the non reacting layer was investigated in detail in the work of Ghoniem and Ng [22]. Here we concentrate on results pertaining to mixing and to a chemically-reacting layer.

III.1 NON-REACTING MIXING LAYER

Results of a typical simulation, presented in terms of the velocity and location of all vortex elements used in the computations, are shown in Figs. 2, 3, and 4 for the cases of \( \text{Re} = 24000 \), \( \text{Re} = 4000 \), and \( \text{Re} = 1000 \), respectively. Each vortex element is depicted by a point, while its velocity relative to the mean velocity is represented by a line vector starting at the center of the vortex element. The velocity ratio across the layer at the inlet is \( U2/U1 = 1/3 \).
Results show the formation of large vortex eddies by the rollup of the vorticity layer emanating at the splitter plate, and the subsequent pairings of these eddies into larger structures. The rollup of the shear layer was investigated in Ghoniem and Ng [22] by analyzing results at a wide range of the Reynolds number and at different boundary conditions. Their analysis showed that: (1) the rollup is due to the growth of perturbations by the Kelvin-Helmholtz instability mechanism, and the shedding frequency corresponds to the most unstable frequency predicted from the linear stability analysis of a spatially growing layer; (2) pairing, which is associated with the local subharmonic perturbations, results in a step-wise increase in the size of the vorticity layer as two eddies merge; (3) the two sources of the subharmonic perturbations are the downward motion of the layer and the monotonic growth in the size of the eddies downstream; (4) the intrinsic dynamics of the instability is not strongly affected by the value of the Reynolds number, except that at the low Reynolds number the eddies are slightly larger due to the dispersion of vorticity by diffusion; and (5) the computed velocity statistics with experimental data, indicating that the fundamental mechanisms of the shear layer are two dimensional and, hence, the numerical scheme is capable of predicting the large scale features accurately.

To study entrainment, a passive conserved scalar with a normalized concentration value equal to zero in the high speed stream and equal to one in the low speed side is introduced at the inlet section. At each time step, 19 elements are introduced in each stream. The initial distance between two neighboring elements in the cross stream direction is taken as $6y = 0.021$. The time step at $t = 0.1$, thus the distance between the elements in the streamwise direction is $6x = 0.05$ on average. Since diffusion is more critical in the cross stream direction, $6y$ is chosen to be smaller than $6x$. A case with $6y = 0.016$, using 25 elements in each stream was computed, showing no significant change in the overall behavior.

Figures 5, 6, and 7 are obtained for Reynolds number, Peclet number and velocity ratio 10,000, 4,000 and 1/2, respectively. Figures 5 and 6 show the velocity and location of all the vortex and scalar elements respectively, while Fig. 7 exhibits the strength of each of the scalar elements at the non-dimensional times of $t = 28$, $29$ and $30$. In Fig. 6, the dots represent the fluid from the high speed side with normalized concentration $c = 0$, and the open circles represent the fluid from the low speed side with $c = 1$. This figure indicates that the rollup of the vortices and their subsequent pairing entrains fluid from both sides of the free streams into the cores of the vorticity layer, which results in the enhancement of mixing between the two streams. Entrainment asymmetry is observed as more fluid from the high speed side is present in the low speed side than the opposite (Koochesfahan [29]).

The instantaneous profiles of the concentration field are averaged over a long-time period and the statistical values are compared with experimental data in Figs. 8 and 9. Figure 8 shows the mean value of the concentration, $C_m$, as
a function of \((y-y_0)/(x-x_0)\). where \(y_0\) is measured at \(x = 0.5\) and \(x_0\) is the virtual origin of the mixing layer based on the mean concentration profile (in the calculation, \(x = 0\)). In this figure, the solid line is the computed mean concentration at \(x = 4\) and the data points are obtained from recent experimental measurements by Masutani and Bowman [30] for a dilute non-reacting mixing layer with the same velocity ratio. Figure 9 shows a comparison between the computed and measured mean concentration, \(\bar{c} - c(\bar{c}_m)^2\).

It is evident from the two figures that both the mean and the second moment of the conserved scalar across the width of the shear layer are accurately predicted by our computations.

![Graph](image_url)
We note that the results in Figs. 8 and 9 are in better agreement with experimental data than those previously predicted by Givi et al. [31]. In these calculations, a k-ε turbulence model and a gradient diffusion model for turbulent transport of the scalar mean, moment and probability density function was utilized. In the k-ε calculations, the concentration fluctuations exhibit a fairly smooth bell-shaped profile with a much less clear double "hump" in the middle region, indicating poor agreement near the high speed stream. The present calculations show the two local maxima in the fluctuation profiles that correspond to the location where the gradient of the mean value is highest. The same behavior is observed by the experimental results of Masutani and Bowman [30] and Batt [32]. It is clear that, in accordance with the findings of Broadwell and Briedenthal [33], the intermittency caused by the large coherent structures contributes greatly to the statistics of turbulent flows.

III.2 REACTING MIXING LAYER

In the calculation of a reacting mixing layer, two reactants F and O are introduced on both sides of the splitter plate. At x = 0, for y > 0, c_F = 1 and c_O = 0, and for y < 0, c_F = 1 and c_O = 0, while c_P = 0. As reactants are entrained into the mixing cores of the layer, they diffuse across the original interface and chemical reaction proceeds. The rollup and pairing increases the original length of the interface by many folds and allow the entrained fluid to diffuse along a larger boundary (Gholien et al. [34]). During this process, if the Lagrangian elements utilized to represent the interaction between chemically reacting species are brought close enough so that the distance between two neighboring elements is smaller than the characteristic diffusion length, they react at the rate defined by Eq. (17).

In Figs. 10, 11 and 12, we present the velocity, location and the strength of the elements in terms of product concentration for the reacting mixing layer with constant rate chemical kinetics and temperature-dependent reaction rate, respectively. The amount of the products formed due to chemical reaction is represented by the diameter of the circles in the figures, i.e. larger circles indicate more products. In both cases, Re = 10000, Pe = 4000, and U_2/U_1 = 1/3 while Le=1. In the constant rate kinetics case, the value of the Damkohler number Da = 1 and in the temperature-dependent kinetics Da = 10 and Q = 5. Note that in both cases the value of the non-dimensional kinetic parameters are low enough so that the effects of heat release on the fluid dynamics can be negligible. The stiffness of Eq. (19) for large values of the Damkohler number imposes a restriction on the time step of integration. In these calculations, we found that at = 0.1 is sufficiently small to accurately integrate the slow chemistry.

A comparison between the two figures reveal that under isothermal conditions, the products are formed as mixing occurs just downstream of the splitter plate, while in the temperature-dependent kinetics calculations, there is an ignition delay before the reactant reach a temperature high enough to allow any significant chemical reaction to occur. Once the reaction begins, the mechanism
of product formation and chemical reaction in both cases are asymptotically the same. Increasing the Damkohler number to Da = 400 results in a shorter ignition delay, and preheating the reactants by increasing the temperature at the inlet to Ti = Q/2 while Da = 200, eliminates the ignition delay as indicated in Figs. 13 and 14, respectively.

In order to examine the effects of chemical reaction on the transport of species, the concentration statistics in the temperature-independent reaction case are presented in Figs. 15 and 16. These figures correspond to the ensemble mean and fluctuation in the bottom-stream species concentration in a reacting mixing layer with Da = 1, U2/U1 = 1/2, Re = 10000, and Pe = 4000. A comparison between figures 15 and 8, and between figures 16 and 9 indicates that near the free stream, the chemistry affects the statistical behavior of the species. Near the reaction zone, however, the mean and the rms values of the concentration are lower under reacting conditions, while the second hump near the high speed stream side of the rms profile in the non-reacting layer is eliminated in the reacting flow due to the local consumption of the species by chemical reaction. The same behavior was also observed in the experiments of Masutani and Bowman [30] in a reacting mixing layer under isothermal conditions. Their results, however, cannot be compared quantitatively with the present calculations since the values of the chemical parameters employed in the numerical simulation are substantially lower than those of the experiment.

III.3 EFFECT OF HARMONIC FORCING

The dynamic effect of oscillating the upstream side of the layer was studied experimentally by several authors, e.g. Oster and Wygnanski [35] and Roberts and Roshko [21] and numerically by Ghoniem and Ng [22]. Their results indicate that in the forced case, eddy interactions follow four stages. In the first stage, the layer rolls up at the harmonic of the forcing frequency closest to the most amplified mode. In the second stage, a process of accelerated pairings yields a large eddy which is in tune with the forcing frequency. This large resonant eddy appears earlier than it would appear in the case of an unforced layer. In the third stage, pairing among resonant eddies, which represents a neutrally stable mode, is disabled and the growth of the vorticity layer is impaired for several eddies downstream. In the fourth stage, the effect of forcing diminishes and pseudo-random pairing is resumed. Moreover, velocity statistics is affected by forcing, and the sign of momentum transfer across the layer is reversed following pairing. Entrainment of passive particles was found to be commensurate with the development of the vorticity layer.

Figure 15. Normalized mean concentration profile as a function of the cross-stream coordinate.

Figure 16. Normalized rms concentration profile as a function of the cross-stream coordinate.
In the recent experiment by Roberts and Roshko [21], it has been observed that periodic forcing has a direct influence on the outcome of chemical reaction across a turbulent shear layer. The results of this experiment indicate that when harmonic forcing is applied, the mixing rate: (1) is increased in the initial stages where the resonant eddy is forming; (2) is decreased in the intermediate stage which corresponds to the resonant or "frequency-locked" region; and, (3) is the same as that of the unforced layer further downstream. In order to characterize these three regions, the Wygnanski-Oster parameter $X_w = \Omega U_0 x/\Omega U_0^2$ is utilized, where $\Omega$ is the forcing frequency [35]. Roberts and Roshko [21] and Browand and Ho [36] show that the three different regions can be classified according to the local value of $X_w$. In region I, $X_w < 1$, the growth rate is enhanced. In region II, $X_w > 1$, the frequency-locked region, the growth rate is inhibited. In region III, the growth rate relaxes to that of the unforced layer.

In order to investigate this phenomenon computationally, the response of the reacting shear layer to the application of low frequency, low amplitude perturbations on the upstream side of the shear layer is computed. Streamwise oscillations are applied on both sides of the layer, hence a pressure perturbation is imposed without changing the vorticity field. The streamwise velocities are taken as $U_1 = 1 + a \sin (2\pi ft)$, and $U_2 = a U_2$, where $a$ is the amplitude of forcing.

The normalized distribution of the product thickness along the mixing layer for three cases, $\Omega = 0$, 0.5 and 1, is shown in Fig. 17. In these calculations, $a = 0.1$, and $Re = 4000$. The figure indicates that for $\Omega = 1$, mixing is enhanced in the initial part of the layer, $1 \leq x \leq 2$. The resonant, frequency-locked region begins at $x = 2$ and ends at $x = 3$. In this region, mixing is reduced and is less than that of the unforced layer. Downstream of this region, $x \geq 3$, mixing rate resumes its natural growth and reaches asymptotically that of the unforced layer. For lower forcing frequency, $\Omega = 0.5$, the same overall behavior is observed. In this case, however, the results of numerical calculations indicate that the resonant, frequency-locked region is approximately in the range $3 \leq x \leq 4$. A comparison between the range of the frequency locked region calculated here with that estimated by Browand and Ho [36] is shown on Table I. Considering the fact that our simulations ignore the effect of small scale three-dimensional turbulence motion, and considering the non-universality of the Browand and Ho's curve due to its independence to experimental conditions and other important non-dimensionalized parameters, this agreement is encouraging.

### Table I

<table>
<thead>
<tr>
<th>Frequency locked region</th>
<th>calculated</th>
<th>measured [36]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Omega = 0.5$</td>
<td>$3 \leq x \leq 4$</td>
<td>$2.66 \leq x \leq 5.33$</td>
</tr>
<tr>
<td>$\Omega = 1.0$</td>
<td>$2 \leq x \leq 3$</td>
<td>$1.33 \leq x \leq 2.66$</td>
</tr>
</tbody>
</table>

![Figure 17. Variation of the product thickness versus the downstream distance.](image)

III.4 EFFECT OF STRAIN RATE

It has been shown experimentally by Tsuji [37], numerically by Liew et al. [38], and analytically by Peters [39], that the strain rate has a major influence on the flame structure, particularly in non-premixed systems. In the counter-flow diffusion flame experiment of Tsuji [37], it was observed that increasing the magnitude of stretch near the flame surface results in an increase of the flow of reactants into the reaction zone. As a result, the chemical reaction is not able to keep pace with the supply of reactants, and the reaction rate is reduced until local flame quenching occurs. The analysis of Peters [39], which is based on the method of matched asymptotic expansion at large activation energy, shows that the mechanism of flame extinction can be addressed by examining the local value of the rate of scalar dissipation. This parameter is viewed by Peters [39] as the inverse of the diffusion time scale. If the local value of dissipation is increased beyond a critical limit, the heat conducted away from the diffusion flame can not be balanced by the heat produced by the chemical reaction. As a result, the maximum value of the temperature decreases, and the reaction eventually ceases.

By increasing the number of scalar elements to 38 in each stream while decreasing the computational domain to $X_{max} = 4$, and by preheating the incoming reactants to $T_i = Q/2$ to start the chemical reaction immediately downstream the splitter plate, we were able to observe this phenomenon. Figures 18 and 19 show the
instantaneous velocity and temperature rise, \( T - T_i \), of the scalar elements at times of \( t = 19 \) and \( t = 21 \), respectively. In this case, the Damkohler number, the normalized enthalpy of reaction, the activation energy and the velocity ratio at the inlet are 50, 8, 20 and 1/3, respectively. The cross stream direction is enlarged by a factor of 2 for the purpose of clarity.

The figures show that the number of scalar elements near the braid, which is the thin link between two neighboring cores, is only a small portion of the total number of elements within the computational domain, which reached more than 5100. This indicates an instantaneous quenching at the stagnation points of the layer. Moreover, the temperature and product concentration in the reaction zone reach a maximum at the core of the eddies where the vorticity concentration is high, while they reach a minimum at the stagnation point within the braid between the neighboring cores where the strain and the scalar gradients reach their maximum values. This is consistent with the results of the pseudo-spectral calculations of Givi et al. [15], and with the experimental observations of Tsuji [37] who showed that the local extinction of diffusion flames occurs mainly at the regions of high dissipation rate. At these regions, the temperature tends to decrease, and if it goes below a critical characteristic value, the flame locally extinguishes.

Quantitative analysis of the effects of stretch on the chemical reaction is rather difficult in the context of present algorithms. This is due to the fact that there are very few scalar elements near the regions of high strain, and as shown by Ghoniem et al. [34], most of the elements tend to be concentrated near the regions with low dissipation. Implementation of a numerical scheme based on the transport of the scalar gradients, as in Ghoniem et al. [34] can improve the accuracy of the analysis substantially, particularly those associated with the effects of stretch. In this method, the elements are concentrated near the regions of large gradients, or high dissipation, and hence a smaller total number of elements have to be considered. The implementation of this method for the numerical simulation of unpremixed reacting flows is presently underway to study the effect of strain rate more accurately.

**IV CONCLUSIONS**

In this work, a numerical scheme based on the transport of computational elements carrying vorticity and scalar quantities has been developed to simulate a reacting planar, two-stream mixing layer with unmixed reactants. The scheme solves the transport equations at high Reynolds and Peclet numbers without using models for turbulence closure. A Lagrangian stochastic model is used to implement the chemical reactions for both constant rate kinetics and variable temperature Arrhenius reactions.

In the non-reacting flow simulations, the calculated statistics of the mixing of a conserved scalar are in good agreement with experimental data. In particular, the numerical results show the presence or two maxima in the fluctuation profile. In the constant rate reacting flow simulation, the effect of chemistry is to smooth out this curve and produce a single maximum, which agrees with the experimental observations. Harmonic forcing enhances the mixing within the accelerated growth zone of the vorticity layer, while it impairs the entrainment of the unmixed fluid into the cores in the resonating region. As a result, the numerical simulation indicates a decrease in the rate of product formation in the frequency-locked region, similar to previous experimental findings.

In the Arrhenius, temperature-dependent kinetics, the mechanism of ignition delay and the effects of reactants preheating on the decrease of the duration of this delay is observed. Also, the
non-equilibrium coupling between the scalar dissipation rate and the flame structure is revealed as quenching frequently appears within the braids. To describe this phenomenon more accurately, work is underway to construct a higher order scheme which can provide better resolution at the regions of strong strain rates.

ACKNOWLEDGEMENT

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The paper on "Three dimensional vortex simulation with application to an axisymmetric shear layer" describes the three dimensional vortex element method and its application to the evolution of the azimuthal instability on a vortex ring and the initial stages of development of a turbulent jet.
Three-Dimensional Vortex Simulation with Application to Axisymmetric Shear Layer
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THREE DIMENSIONAL VORTEX SIMULATION WITH APPLICATION TO AXISYMMETRIC SHEAR LAYERS

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ABSTRACT

A three dimensional vortex element method is developed for the numerical simulation of incompressible flow at high Reynolds number. The method utilizes vortex vector elements with finite point-symmetric cores to discretize the vorticity field. The transport of these elements is done in Lagrangian coordinate by computing the velocity field as a summation over the individual contributions of the elements. The method is used to compute the self-induced velocity of a vortex ring and the stability of a vortex ring with finite core. Results show that vortex rings become unstable to a particular azimuthal perturbation that depends on the core/radius ratio. The mode frequency and shape of the unstable state are in excellent agreement with analytical and experimental results. The method is applied to study the rollup of an axisymmetric shear layer and the generation of large scale vortex ring structures.

I. INTRODUCTION

At high Reynolds numbers, vorticity occupies a small subset of the volume of the flow field. This is exemplified by boundary layers, shear layers, wakes, jets, separation and recirculation zones, etc. These vorticity distributions are unstable to natural perturbations. At small amplitudes, perturbations grow exponentially in time, however, they have a limited effect on the flow. The growth of these perturbations into the non-linear stages is, however, accompanied with severe distortions of the shape of the vorticity field and strong changes in the local concentration of vorticity. Examples for these changes is the formation of large scale structures in shear layers and recirculation zones.

In highly three-dimensional flows, several forms of instability may arise simultaneously. The evolution of spanwise waves on the large scale eddies and the development of azimuthal instability along the axis of vortex rings have been observed experimentally as evidence of multiple forms of instability. In this case, the distortion of the vorticity field occurs faster and the non-linearity is compounded by the interaction between different instability modes. Moreover, the problem is governed by several length and time scales, and multiple states can be expected depending on which mode grows faster (for photographic record of the development of vorticity fields, see Van Dyke [1] and Lugt [2]).

It has been reported experimentally, and observed in numerical studies, that these changes in the vorticity field may not incur strong variations in the mean flow field. This is expected since the velocity is an integral mean of the vorticity field. However, they affect the fluctuations strongly and to the level where the order of magnitude of the fluctuation may change. This is extremely important in mixing and heat release in chemically reacting flows since the rate of mixing, and thus chemical reaction, is a strong function of the fluctuations and depends weakly on the mean field. It has been confirmed that by changing the vorticity field of a shear layer through imposing certain perturbations on the flow, the rate of chemical reaction can be enhanced or slowed and that twodimensional shear stresses can reverse sign during the same process (for a review and some recent results, see Ho and Huerre [3], Robert and Roshko [4] and Ghoniem and Ng [5]).

To capture these changes, numerical simulation of the unaveraged non-linear equations of motion has been utilized. For the success of these simulations, care must be exercised in resolving small variations since they ultimately grow to produce the finite amplitude changes, and hence numerical diffusion should be minimized. Moreover, schemes must adapt to the strong distortion in the flow field without developing numerical instabilities. Thus, Lagrangian schemes seem like natural candidates. A grid-free class of Lagrangian schemes, vortex methods, is utilized in this work to study the evolution of three

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dimensional flow fields dominated by high concentration of vorticity at high Reynolds numbers.

In vortex simulation, vorticity distribution is represented by a finite number of localized vortex elements, or vortex disks in two dimensions (blobs according to Chorin [6]), and vortex balls in three dimensions (vortons according to Saffman and Merian [7], or vortex arrows according to Leonard [8]) which move in an inviscid field with the local particle velocity. A particular flow configuration can be fully described when the appropriate boundary conditions are imposed on the velocity field by adding an extra irrotational field. Two-dimensional vortex simulations have been useful in providing an accurate description of the large-scale structure of turbulence in shear flows (Ashurst [9], Ghomie and Sethian [10], and Ghoniem and Ng [5]). However, they cannot be used to describe phenomena in which streamwise vorticity, or variation along vortex lines, plays an important role. Moreover, they lack the ability to capture small-scale turbulence structures which arise due to vortex stretching and tilting with respect to the main flow plane.

In this work, a three-dimensional vortex element method is developed for the numerical simulation of flow fields with high concentration of vorticity at high Reynolds number. The scheme utilizes vortex vector elements with finite point-symmetric cores to discretize the vorticity field and follows their motion in Lagrangian coordinates. The vortex vector elements change their vorticity according to the local stretch, while their direction is determined by the tilting of the vortex lines. The rotational velocity field is computed by summing over the field of each individual element, which is evaluated from the desingularized Biot-Savart law. The potential velocity field added to satisfy the boundary conditions is computed by using the appropriate image system of the vortices. For recent reviews of vortex calculations in three dimensions, see Leonard [8,11] and Saffman and Baker [12].

To check the accuracy of the vortex method, we use test problems and make comparison with experimental and analytical results. The discretization algorithm is applied to compute the self-induced velocity of a vortex ring and the results are compared with the Saffman’s analytic solution [13]. The stability results of a vortex ring with a finite non-deformable core and a vortex torus with a deformable core are compared with the analytical solutions of Widnail and Sullivan [14] and Widnail et al. [15]. Preliminary results for the rollup of a three-dimensional shear layer subject to an axisymmetric perturbation are compared with the experimental results of Vandauberger et al. [16] and Roquemore et al. [17].

II. FORMULATION AND NUMERICAL SCHEME

In this section, the construction of a three-dimensional scheme for tracking the evolution of a vorticity structure in an arbitrary domain is described. The accuracy of the scheme is checked against theoretical results regarding the motion and stability of a vortex ring and a vortex torus. The scheme is constructed as follows: The vorticity field is first discretized into a finite number of small straight line vortex vector elements and then followed in a Lagrangian frame of reference. Each element has a finite core of vorticity which is point-symmetrically around its center, and hence the nomenclature "vortex ball".

The velocity produced by a distribution of vortex vector elements, or vortex balls, is obtained by the desingularized Biot-Savart law, which amounts to summing the velocity produced by individual vortex elements. The procedure for a consistent discretization and the evaluation of the Biot-Savart law is explained in Section II.2. Its numerical accuracy and convergence under steady state conditions is shown in Section II.3. The comparison between the numerical and analytical results for the stability of a thin vortex ring and a vortex torus, another test for the accuracy of the method under unsteady state, is discussed in Sections II.4 and II.5.

The potential velocity field added to satisfy a particular set of conditions on the boundaries is determined by solving the Laplace equation numerically subject to the appropriate boundary conditions. When the boundary conditions match those of a standard potential solver, i.e. Dirichlet or Neumann conditions, that particular routine can be used to evaluate the potential velocity. In cases when the boundary conditions are neither Dirichlet nor Neumann type, one faces difficulty in satisfying continuity along the boundaries, and a special algorithm must be constructed to handle this difficulty. This is discussed in Section III.

II.1. EQUATIONS OF MOTION

The motion of an incompressible inviscid flow is governed by the Euler equations:

\[ \mathbf{v} \cdot \mathbf{u} = 0 \]  

(1)

\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \mathbf{f} \]  

(2)

expressing the conservation of mass and momentum, respectively. In these equations, \( \mathbf{u} = (u, v, w) \) is the velocity, \( t \) is time, \( \mathbf{V} = (\partial / \partial x, \partial / \partial y, \partial / \partial z) \) is the gradient operator, while \( x = (x, y, z) \), and \( p \) is pressure. Quantities are normalized with respect to the appropriate combination of a characteristic length scale, velocity scale and density. In vortex simulation, the equations are recast in terms of the vorticity \( \omega \):

\[ \omega = \nabla \times \mathbf{u} \]  

(3)

The vortex transport equations are obtained by taking the curl of Eq. (2). Using Eq. (1) and using the fact that \( \nabla \cdot \omega = \nabla \cdot (\nabla \times \mathbf{u}) = 0 \), i.e. the vorticity forms a solenoidal vector field, we get:

\[ \frac{\partial \omega}{\partial t} + (\mathbf{u} \cdot \nabla) \omega = \nabla \times \mathbf{f} \]  

(4)

If the vorticity field is known, the velocity can be evaluated by integrating Eqs. (1) and (3), as shown below, while Eq. (4) is used to transport the vorticity in the form of a number of discrete
By construction, \( u \) is the velocity induced by the vorticity field in an unbounded space, and \( u_p \) is the potential component added to satisfy the potential no-flow condition along the boundary of the domain. Each component will be evaluated separately, satisfying the appropriate boundary conditions, and then added to obtain the total velocity.

To evaluate the velocity field induced by a given vorticity distribution \( \omega \) in an unbounded space, we assume the existence of a vector stream function \( \phi \) such that

\[
u = \nabla \times \phi
\]

(5)

By construction, \( u \) satisfies the continuity equation since \( \nabla \cdot \mathbf{u} = 0 \) identically. Substituting in Eq. (3) and assuming that \( \nabla \phi = 0 \), one obtains:

\[
\nabla^2 \phi = -\omega
\]

(6)

The solution of this Poisson equation in three dimensions is given by:

\[
u(x) = \int V(x-x') \omega(x') \, dx'
\]

(8)

where \( V(x) = 1/(4\pi r) \) is the Green function, and \( r = |x| \). As shown by Batchelor [18], the above expression for \( \phi \) is solenoidal, as previously assumed, if the boundaries of the domain extend to infinity. This is essentially the condition needed to evaluate \( u \).

The solenoidal velocity component, \( u_s \), can be evaluated by substitution in Eq. (6) which yields the well-known Biot-Savart law:

\[
u = \int (K(x-x')) \times \omega(x') \, dx'
\]

(9)

\[
K(x) = -\frac{1}{4\pi} \frac{x}{r^3}
\]

(10)

where \( x' \) is the position of the volume element \( dx' \).

The implications of the equations of motion, Eqs. (3) and (4), regarding the evolution of the vorticity field can be summarized in the following important dynamical statements, as given without proof while used later in the construction of the numerical algorithm (for details, see Batchelor [18]):

1. Kelvin theorem: The circulation around a closed material loop, defined as \( \Gamma = \int A \cdot \omega \, dA \), where \( A \) is the surface area within the loop, is conserved as the loop is deformed;

2. Helmholtz theorem: Vortex lines, parallel everywhere to the local vorticity vector, move as material lines.

Furthermore, the vorticity vector can be written as \( \omega = \omega \mathbf{n} \), where \( \mathbf{n} \) is the direction of the local vortex line, or material lines, while \( dx = d\mathbf{A} \) where \( \mathbf{A} \) is the cross-sectional area normal to the direction \( \mathbf{n} \). The circulation of a vortex line, \( \Gamma \), which is conserved along a particle path according to Kelvin theorem, is expressed in terms of the vorticity \( \omega \) as \( \Gamma = \oint \mathbf{A} \cdot \omega \, dA \).

Since \( u_p \) is an irrotational component, then \( u_p = \nabla \phi \), where \( \phi \) is a velocity potential governed by:

\[
\nabla^2 \phi = 0
\]

(11)

while the total velocity, \( u \), is subject to a potential boundary condition at the boundaries of the domain, i.e. \( u = \nabla \phi \). \( m \) is given on \( \partial \Omega \), where \( m \) is the local normal to \( \partial \Omega \), which denotes the boundary of the domain.

II.2. EVALUATION OF THE ROTATIONAL FIELD

Analytical evaluation of the Biot-Savart integral in Eq. (9) is restricted to simple vorticity distributions, such as rectilinear vortices and circular vortex rings of concentrated vorticity. Therefore, the integration must be performed numerically for an arbitrary vorticity distribution. For that purpose, the continuous vorticity field is discretized into a number of vortex vector elements, each with an assigned vorticity \( \omega_i \). The magnitude of the vorticity associated with each element is distributed over a small spherical volume around its center according to a core function \( f \) with a characteristic core radius \( \delta \). The vorticity field is hence expressed as:

\[
\omega(x,0) = \sum_{i=1}^{N} \omega_i(0) h^3 f_i(x-X_i)
\]

(12)

where \( N \) is the total number of vortex vector elements, and \( X_i \) is the center of the vortex element, while \( h \) is the initial distance between the centers of neighboring elements. The accuracy of this discretization is discussed in Beale and Majda [19,20]. Note that if \( f_i = \delta(x-X_i) \), where \( \delta(.) \) is the Dirac delta function, Eq. (12) represents a distribution of singular vortex lines, or vortons [7]. However, in this representation, vortex balls, while equivalent to vortex disks in two dimensions, are used and \( f_i = 1/4\pi \delta(r/\delta) \), while \( \delta \) is finite. The distribution of the magnitude of the vorticity associated with each element is point symmetrical around its center \( X_i \), while its direction everywhere is \( \omega = \omega_i / \omega_s \), and \( \omega = |\omega| \). \( \delta \) is the core radius of the element where most of its vorticity is concentrated, \( \delta > 0 \) for \( r < \delta \), and \( f \) vanishes rapidly for \( r > \delta \).

A simple intuitively appealing choice for a core function could be the Hill spherical vortex for which \( \omega = \omega_s / r \) for \( r < \delta \) and \( \omega = 0 \) for \( r > \delta \).
where \( a^2 = r^2 + s^2 \), \( r \) being the radial direction in a cylindrical coordinate system. This, however, is a poor choice for the core function since the latter should have a maximum at the center and decay further away. Moreover, \( a \) is not a function of \( r \). A better choice may be the three dimensional analogue of the Rankine vortex, i.e. \( a = \omega_0 \) for \( r < \delta \) and \( a = 0 \) for \( r > \delta \).

For accurate discretization of the continuous vorticity distribution, \( \delta \) should be chosen larger than \( h \), where \( h \) is the initial separation between the elements and \( h^3 \) is the volume element used to construct the vortex balls. This will ensure that the core functions \( f \) associated with neighboring elements are highly overlapping. The introduction of a similar discretization procedure has been widely used in two dimensional simulations to construct stable and accurate vortex algorithms [5,6,8,9,19]. Moreover, \( h \) may take on different values in the three principle directions, and \( h^3 \) is replaced by \( \delta V \), where \( \delta V = h_x h_y h_z \). In this case, the vorticity associated with an element is \( \omega = \frac{1}{\delta V} \oint \omega \cdot dx \), the integration is performed over \( \delta V \).

From Helmholtz theorem, the vorticity associated with a material element changes as it stretches, \( \omega(t) = \omega(0) \int_{\delta \Omega(t)} \partial U / \partial t \), while \( \delta \Omega = [\delta \Omega] \). Moreover, according to Kelvin theorem, the circulation of the vortex vector element remains constant as it moves along particle paths, while due to incompressibility, \( \delta V \) is constant. Thus, Eq. (11) can be written as:

\[
\omega(x,t) = \sum_{i=1}^{N} \Gamma_i \delta \Omega_i(t) \int_i (x - x_i) \}
\] (13)

In this expression, \( \delta \Omega_i \) is the material vector associated with the vortex vector element, and \( x_i \) is the midpoint of this vector, \( x_i(x_i,0) = X_i \).

The velocity field is obtained by substituting Eq. (9) into Eq. (10) and integrating:

\[
u = \frac{1}{\delta V} \sum_{i=1}^{N} \Gamma_i \frac{1}{r_i^3} \frac{(x - x_i) \times \delta \Omega_i}{r_i^3} \}
\] (14)

where \( \kappa(r) = k \int f(r') r'^2 dr' \), and \( r_i = |x - x_i| \). While \( x_i \) is the center of the vortex vector \( \delta \Omega_i \). In this representation, each vortex vector element is described by \( (r, x, \delta \Omega_i) \). Since \( x \) and \( \delta \Omega \) are the position and length of a material particle and a material line, respectively, their variation with time can be obtained from [Truesdell 21]:

\[
\frac{dx}{dt} = u(x(t), t)
\]

\[
\frac{d\delta \Omega}{dt} = \delta \Omega \cdot \nabla u
\]

Thus, using a first-order time integration:

\[
x_i(t+\Delta t) = x_i(t) + u_i \Delta t
\]

and

\[
\delta t_i(t+\Delta t) = \delta t_i(t) + \delta \Omega_i \cdot \nabla u_i \Delta t
\]

The velocity gradient can be evaluated analytically by differentiating Eq. (14), as proposed by Anderson and Greenough [22]. However, since the vorticity moves along particle paths, the material line coinciding with the vortex vector \( \delta \Omega \), can be approximated by its terminal points \( x_1 = x_1 - \delta \Omega/2 \) and \( x_2 = x_1 + \delta \Omega/2 \), and the center of the vortex vector element is approximated by \( x = (x_1 + x_2)/2 \). In this scheme, a vortex vector element is described by \( (r, y_1, y_2) \) and both terminal points are updated each time step. A similar construction was used by Chorin [21]-[26] to study boundary layer stability, the evolution of a turbulent vortex and the properties of developed turbulence. Since the vorticity field is solenoidal, the end of an element is the beginning of the next element if these elements were neighboring elements on the same vortex line at \( t = 0 \). Thus, this scheme can be used to ensure the satisfaction of the condition \( \nabla \cdot W = 0 \) by maintaining the connectivity of vortex tubes no matter how accurate is the discretization of the vorticity field. The same property is utilized in the filament scheme of Leonard [26] (see also Ashurst and McEneaney [27]). A discussion of the relationship between different algorithms is given by Greenough [28]. In our computations, a second-order time integration algorithm is used to move the terminal points, \( (y_1, y_2) \), of the vortex vector elements, e.g., for \( y_1 \):

\[
x_{11}(t+\Delta t) = x_{11}(t) + u_{11} \Delta t
\]

and

\[
x_{12}(t+\Delta t) = x_{12}(t) + (u_{12} + u_{12}^*)/2 \Delta t
\]

where \( u_{12} = u(y_2) \).

The accuracy of the vorticity discretization depends on: the choice of the core function \( f \), the distance between the centers of neighboring elements \( h \), and the ratio between the initial separation between the vorticities and the core radius, \( h/\delta \). In the analysis of Beale and Majda [29], it is shown that a second order scheme is obtained if the following third order Gaussian core function is used:

\[
f(r) = \frac{k}{k^3} e^{-r^2/\delta^2}
\]

and:

\[
\kappa(r) = \frac{k}{k^3} e^{-r^3}
\]

As the flow develops strong stretch along the vortex lines, the effective value of \( \delta \) exceeds \( h \) and the amount of vorticity transported by each
vortex ball grows. To maintain a uniform resolution, if \( \alpha_i > 2h \), a vortex element is split into two elements, each with \( \Delta \alpha = \alpha_i/2 \) and \( f = T \). Effectively, this amounts to redistributing the vorticity field among a larger number of elements to maintain the accuracy of the calculations. The value of \( \alpha \) is kept constant in our calculations.

II.3. SELF-INDUCED VELOCITY OF A RING

To investigate the effect of discretization of the vorticity field on the accuracy of the calculation of the velocity field, the self-induced velocity of a vortex ring with a radius \( R \) and a finite core radius \( \alpha \) is computed and compared with the analytical results for a thin vortex ring. For this purpose, the ring is discretized along its axis into a number \( N \) of vortex vector elements, where the length of each element is \( h = \Delta \alpha < 2 \pi R/N \). Each element is represented by a computational vortex ball with core radius \( \alpha = \alpha_0 \). This is a worst-case analysis, since normally one would use several elements to represent the core, and choose \( \alpha \ll \alpha_0 \) (as will be shown later). However, we start with this case for simplicity and computational convenience.

To distinguish between the two representations of a vortex ring, where the vortex balls are aligned along the ring axis forming a tube of vorticity, is called the thin tube approximation while if several vortex balls are used within the cross section of the ring, it is called a vortex torus. The first approximation is different from the thin filament approximation of Leonard [26]. In the thin filament approximation, the Biot-Savart law is modified to remove the singularity at the center of the filament and the core maintains its vorticity distribution as the filament is deformed. In the thin tube approximation, neighboring elements can move freely with respect to each other, and hence changing the local vorticity distribution of the tube.

In the discretization of the vortex ring using the thin tube approximation, \( \alpha = \alpha_0 h \), where \( \alpha > h \) to insure the overlapping between neighboring elements. Eq. (14) is used to evaluate the self-induced velocity \( V \) by summing the contribution of the elements around the ring, excluding the effect of the element on itself. Results are compared with the analytical expression of Saffman [13] for a thin vortex ring, \( \alpha/R \ll 1 \):

\[
V = \frac{T}{4\pi R} \left( \ln \frac{8R}{\alpha} - C \right)
\]

where \( C = 0.558 \) for a second order Gaussian distribution of vorticity within the core and \( \alpha \) is the effective radius, i.e. it is the standard deviation in the Gaussian.

A comparison between our computations of the self-induced velocity and Eq. (22) is shown in Fig. 1 for different values of \( N \), \( V = V/(4\pi R) \).

Three comments should be made here: (1) since the core function of the vortex elements is a third order Gaussian, Eq. (18), and not a second order Gaussian as in Saffman's calculations, a slight discrepancy in the self-induced velocity is expected (a comparison between the two distributions is presented in Fig. 2): (2) since \( \alpha > h \), and a strong overlap between the cores of neighboring elements is ensured, the vorticity at any point is the contribution of many elements.

\[
V = \frac{T}{4\pi R} \left( \ln \frac{8R}{\alpha} - C \right)
\]

Figure 1. The normalized self-induced velocity of a vortex ring \( V = V/(4\pi R) \) vs. the number of computational vortex balls used to discretize the ring. The analytical results of Saffman is represented by the straight line. \( \alpha/R=0.1 \sim 0; \alpha/R=0.2 \sim 0.5; \alpha/R=0.3 \sim 0.5 \).

Figure 2. A comparison between the vorticity distribution within the core of the thin ring used in the computations of Fig. 1, i.e. a third order Gaussian described by Eq. (18), and that of Saffman ring, i.e. a second order Gaussian. In both cases, \( \alpha/R = 0.25 \).
along the ring axis (the vorticity of a single element and the total ring vorticity at any point is presented in Fig. 3, showing that while the magnitude is strongly affected by neighboring elements, the core size is the same); and, (3) the analytical expression applies for \( \alpha \ll R \), and hence best comparison is expected for \( \alpha / R = 0.1 \), while it deteriorates for thicker rings.

As the ring becomes thinner, i.e., larger \( R / \alpha \), more elements are required to achieve an accurate discretization. This is expected, since by choosing \( \delta \ll \alpha \) and \( \delta = 8 \alpha \), where \( 8 \) is a factor larger than one, the number of elements \( N = 2 \pi R / (8 \alpha) \sim O(\alpha / \alpha) \), which increases as \( \alpha \) decreases. Therefore, for a fixed core size \( \alpha \), the number of elements required to compute the self-induced velocity due to curvature \( R \) grows as \( R \) increases.

II.4. STABILITY OF A THIN VORTEX RING

A more interesting problem, providing a test for the accuracy of the time-dependent computations, is the growth of small perturbations on the vortex ring. There is a rigorous asymptotic linear theory for the stability of vortex rings in two forms: (1) for a ring with a non-deformable core, performed by Widnall and Sullivan [14]; and (2) a more elaborate theory for a ring with a deformable core reported in Widnall et al. [15], Widnall [30] and Widnall and Tsai [31]. We will compare the results of the thin tube approximation to the first case, and results for the vortex torus to the second case.

To study the linear stability of thin vortex rings in the thin tube approximation, i.e., with almost non-deformable cores, a radial perturbation of amplitude \( \epsilon / R = 0.02 \) and a wavenumber \( n \) is imposed on the axis of the ring. The wavenumber is defined here as the number of waves that is fitted along the entire length of the ring axis, thus the size of the perturbation varies in the azimuthal direction as \( \phi = \epsilon \sin(2 \pi n \phi) \). Originally, the ring lies in the \( x-y \) plane, and the streamwise is the \( z \)-direction while \( \phi = R \) for all vortex balls. We start with \( n = 1 \) and increase by an increment of one. The time step used is \( \Delta t = 0.1 \). Similar results were obtained for \( \alpha / R = 0.1, 0.15, 0.2, 0.25 \). In the following, only the first case is discussed in detail.

For \( n < n_n \), where \( n_n \) is the wavenumber of a neutrally stable mode that neither rotates around the ring axis nor grows, the waves rotate, or spin, around the ring axis at a frequency \( \Omega \) that depends on \( n \). As it rotates around the unperturbed axis of the ring, the instantaneous center of the ring draws an ellipse whose major axis is in the radial direction, \( p \), and the minor axis is in the streamwise direction \( z \). Thus, these are bending waves that move around the ring axis, hence the name helical waves (if the ring is opened to form a rectilinear vortex, the waves will like a corkscrew spinning at frequency \( \Omega \)). The sense of rotations of the waves is the same as that of ring vorticity. The frequency of rotation \( \Omega \) starts out low at small \( n \), grows to a maximum and then decreases again. The amplitude in the radial \( p \)-direction and streamwise \( z \)-direction are shown in Fig. 4 for \( n = 2, 4, 6, 8, 10 \) and 12 for
Figure 4. The amplitude of the perturbation in the radial \( \rho \)-direction and the streamwise \( z \)-direction for a vortex ring with \( \sigma / R = 0.1 \), computed using the thin tube approximation. The wavenumber of the perturbation is \( n = 2, 4, 6, 8, 10 \) and 12, arranged from the top figure. Both amplitudes are normalized with respect to the initial perturbation in the radial direction, \( \sigma / R \), 0.02, and time is normalized with respect to \( R^2 / \sigma \). In this figure, the behavior of the modes \( n < n \) is shown.

\( \sigma / R = 0.1 \). Note that the radial perturbation produces a streamwise perturbation of almost the same magnitude. All these modes are characterized as being linearly stable since their amplitudes remain bounded.

At \( n = n \), the waves neither grow nor rotate.

For \( \sigma / R = 0.1 \), at \( n = 13 \) the ring remains in its original plane without bending, as depicted by Fig. 5. The next mode, \( n^* = 14 \), the waves grow in the radial direction, and then in the streamwise direction so that the total amplitude grows exponentially in time, i.e. the ring becomes linearly unstable and streamwise vorticity is produced. Moreover, no wave rotation is observed.

The wave amplitudes are shown in Fig. 6 for \( \sigma / R = 0.1 \).

Figure 5. The amplitude of the perturbation in the radial and streamwise directions for the neutrally stable mode for the same ring as in Fig. 4.

Figure 6. The amplitude of the perturbation in the radial and streamwise directions for the unstable mode \( n^* \) of the ring of Fig. 4.

As \( n > n^* \), the ring is stabilized again and the eigenfunctions behave in a similar way to \( n < n \). However, the major axis of the ellipse is now in the streamwise direction and the frequency of rotation increases indefinitely. Moreover, the sense of rotation is in the opposite to that of the ring vorticity. The wave amplitudes in the \( \rho \) and \( z \) directions are shown in Fig. 7 for \( n = 15, 17 \) and 19.

Similar observations are made for \( \sigma / R = 0.15, 0.2 \) and 0.25. In all cases, the unstable mode \( n^* \) is a bifurcation in the eigenfunction that corresponds to \( \Omega = 0 \). In Fig. 8, the results of
these computations are summarized in terms of $Q$, the rotation frequency of the waves, v.s. the wave number $k = n \omega / R$. In this figure, $Q$ is normalized with respect to $\Omega R^2$. In all cases, the unstable mode $k^2 = n^2 \omega R^2 = 1.25$ corresponds to a non-rotating mode, $Q = 0$. This is in agreement with the theoretical results of Widnall and Sullivan [14]. They observed, similar to what we see in the numerical results, that a mode becomes unstable when the self-induced rotation of the waves balances the rotation induced by the rest of the ring and the energy of the perturbation is utilized in stretching the wave amplitude.

In order to check on the accuracy of the computations, we varied the discretization parameter $\Delta$ by using more elements around the axis of the ring, $h = 2\pi / R$. Figure 9 shows the growth of the amplitude of the perturbation with time using an increasing number of elements for $\epsilon / R = 0.2$ and $n = n^* = 7$. $N = 30$ is the smallest number necessary to satisfy the condition $\epsilon < \Delta$, however, we notice that $N = 90$ is necessary to compute the logarithmic growth rate accurately. It is the same number required to compute $V = 3.1309$ accurately, as seen in Fig. 2. This is not surprising since the stability of the local waves depends strongly on the velocity (or strain field) induced by the ring on the perturbation. The linear growth rate, $\alpha_k = (\log A)/\Delta t = 0.1625$. The analytical value obtained by Widnall and Sullivan [14] for the same value of $V$ is $\alpha_k = 0.157$. 

Figure 8. The computed results for the dispersion relation of a ring using the thin tube approximation. $\epsilon/R = 0.1 - a$; $\epsilon/R = 0.15 - y$; $\epsilon/R = 0.2 - b$; $\epsilon/R = 0.25 - c$. The frequency of rotation of the mode $Q$ is normalized with respect to $R^2/\Omega$ while $k$ is normalized with respect to $R/\omega$.

Figure 9. The growth of the unstable mode $n^* = 7$ for $\epsilon/R = 0.1$, computed using $N = 30-140$, with increments $\Delta N = 10$.

Figure 7. The amplitude of the perturbation in the radial and streamwise directions for the modes $n > n^*$ of the ring described in Figure 4. The wavenumber of the perturbation is $n = 15, 17$, and 19, arranged from the top.
Thus we may write the more elaborate theory for a non-deformable core as:

\[ \omega = \frac{1}{r^2} \left( \frac{d^2 \phi}{dr^2} - \frac{1}{r} \frac{d \phi}{dr} + \frac{2}{r^2} \phi \right) \]

Values of the ring with a non-deformable core, the model is not circulation of the results presented here, nine balls were used across each cross-section of the ring. In the results presented here, nine balls were used across each cross-section of the ring, one at the center and eight distributed along the circumference of a circle with radius \( \rho = 0.74a \), arranged at 45°. This choice for the initial location of the centers of the vortex balls is used to minimize the difference between the total circulation of the vortex torus and the sum of the circulation of the vortex balls. The core radius of each ball was taken as \( \delta = 0.8a \), and the distance between the centers of neighboring elements is \( h = 6/1.1 \). Therefore, the number of elements used along the circumference of the torus depends on its radius. Figure 12 shows the actual vorticity distribution and the numerical vorticity distribution produced by the vortex balls. The motion of these balls throughout the cross-section of the torus allows a substantial deformation of its core at different sections. Thus, higher-order radial modes associated with the instability of vortex rings, which has been observed experimentally and analytically, can be captured.
Figure 12. The actual and discretized vorticity distribution of a vortex torus using nine vortex balls within the core.

Computations were performed for four tori with $a/R = 0.15, 0.20, 0.25,$ and $0.35$. In all cases, the vorticity distribution is the same third-order Gaussian utilized before. The initial amplitude of the perturbation $a/R = 0.02$, and a number $n$ of sinewaves were fitted along the torus to model the initial perturbation. The time step of integration $at = 0.1$, and the computations were performed for 1000, or 2000 time steps to observe the growth of the perturbation. The overall behavior of the vortex torus was the same in all cases. As an example, results for $a/R = 0.2$ are discussed next in detail.

Figure 13 shows two views of the torus after 1000 time steps, when perturbed with $n = 8, 9, 10,$ and $11$. In the first three cases, the core deforms, as seen by the redistribution of the individual rings within the torus, and the waves spin around the unperturbed axis of the ring. However, the perturbation stays bounded. In the last case, the perturbation grows in both the radial and the streamwise directions causing substantial non-uniform deformation around the ring axis, and the generation of streamwise vorticity. The amount of deformation in each case is seen from the total number of elements used at the last time step. In the first three cases, the number of elements remains constant at $N = 1080$ for 1000 steps. In the unstable case, the number of elements grows to 1262. Since from Helmholtz theorem, $w(t)/w(0) = a(t)/a(0)$, where $a(t)$ is the summation over $a_i$ for all the vortex elements, this stretch is accompanied by intensification of the vorticity within the ring at the same ratio of stretch.

Figure 14 shows two views for the torus in the unstable case every 200 computational time steps, starting at $t = 0$. It is clear that, at the unstable mode, waves do not rotate around the axis of the torus while their amplitudes grow.
Figure 14. The growth of the perturbation on a vortex torus with $c/R = 0.2$, $e/R = 0.02$ and $n = 11$. The torus is discretized into 9 rings with 120 vortex balls along each ring. Results are shown every 200 time steps starting with $t = 0$. The plots show that this is an unstable mode in which the amplitude of the waves grow without rotation.

Figure 15. The same vortex ring as in Fig. 14, but with $n = 9$. The plots indicate that this is a stable mode without growth, while the waves rotate around the unperturbed center of the ring. The ring is plotted every 300 steps starting at $t = 0$. 
similar to the results of the thin tube approximation and to the results of Widnall and Tsai [31]. Moreover, the core vorticity is redistributed into a number of sectors equal to the number of waves. The outer portion of each sector stretches forward in the streamwise direction while the inner part elongates backwards. On the other hand, results for \( n = 9 \), which is a stable mode, depicted every 300 steps in Fig. 15, show the rotations of the waves as peaks and valleys exchange their locations while the core vorticity remains uniform in the azimuthal direction.

The average amplitude of the perturbation around the circumference of a torus with \( \sigma/R = 0.15 \) and 0.35 is shown in Figs. 16 and 17, respectively. The exponential growth of small perturbations at the early stages is seen at \( n = 11 \) and 6 for the two cases, respectively. Figure 18 summarizes the results for the four tori, \( \sigma/R = 0.15, 0.2, 0.25 \) and 0.35, showing a very good agreement with the experimental results of Widnall and Sullivan [14]. As before, the value of \( V \) is used to characterize the ring in order to remove any confusion about the definition of the core and the vorticity distribution. The analytical results for a vortex torus with a non-uniform vorticity distribution within the core, the numerical results, and the experimental data are in close agreement, differences can be primarily attributed to the vorticity distribution within the core.

The form of the unstable torus with \( \sigma/R = 0.35 \) at \( n = 6 \), is shown at time steps 1400-2000, every 200 steps in Fig. 19 (it was found that \( n = 7 \) is also an unstable mode for this torus). It is interesting to note that the core deformation is different at different azimuthal locations and that the inner and outer radii do not follow the same pattern (Yule [32]). The figures indicate that the inner and outer edges of the vorticity core of the torus may move in anti-phase and that variations at frequencies different than the perturbation frequency arise at late times. Thus, higher order radial modes form as part of the instability of vortex rings, in accordance with the conclusion of the analytical theory [15]. To quantify these frequencies, we study the energy spectra of two tori. In Figs. 20 and 21, the spectra for \( \sigma/R = 0.20 \) at \( t = 100 \) and for \( \sigma/R = 0.35 \) at \( t = 200 \) are shown. In the stable modes, only the perturbation frequency is present at very small amplitude. In the unstable modes, higher harmonics of the perturbation frequency, which had zero amplitudes at \( t = 0 \) are excited at substantial levels.

Figure 16. The growth of the perturbation with time for a torus with \( \sigma/R = 0.2 \), perturbed with \( n = 8, 9, 10, \) and 11.

Figure 17. The growth of the perturbation with time for a torus with \( \sigma/R = 0.35 \), perturbed with \( n = 5, 6 \).

Figure 18. Comparison between the experimental data, \( x \), of Widnall et al. [15] and of the numerical predictions, \( \phi \), of the unstable modes of a vortex torus. The plots include data from Fig. 10.
Figure 19. The evolution of the unstable mode of a vortex torus with \( \sigma/R = 0.35 \), perturbed at \( t = 0 \) with \( \sigma/R = 0.02 \) and \( n = 6 \). The torus is shown at time steps 1400-200, every 200. The total number of vortex elements at these plots is 810 (as at \( t = 0 \)), 622, 673 and 1092, respectively.

Figure 20. The frequency spectra for the energy of a torus with \( \sigma/R = 0.2 \) measured at \( t = 100 \), for \( n = 8 \) – 9; \( n = 10 \) – 11; and \( n = 11 \) – 0. In the unstable mode, higher harmonics at 22 and 33 are excited.

Figure 21. The frequency spectra for the energy of a torus with \( \sigma/R = 0.35 \), measured at \( t = 200 \), for \( n = 5 \) – 6 and \( n = 6 \) – 0.

Results of this section indicate that the numerical simulation of vortex rings with finite and deformable cores, as represented by a number of vortex balls distributed within the ring core and along its axis, can accurately be used to compute the wavenumber of the unstable modes and their growth. The deformation of the ring into a number of sectors aligned with the unstable standing waves resembles strongly the experimental results. The generation of small scales, accompanied by higher frequencies in the energy spectrum, is due to vortex stretch and leads to the well-known turbulence cascade. Thus, the azimuthal instability of vortex ring may be one mechanism of transition to turbulence.
The ultimate goal of this work is to study, using three-dimensional vortex simulation, the evolution of a turbulent axisymmetric shear layer. Analytical and experimental studies of this configuration indicate that several types of instability can arise and influence the development of the flow field (e.g. Yule [32], Crow and Champagne [33] and Michalke and Hermann [34]). These instabilities include axisymmetric modes, such as the rollup and pairing of ring-like vortex eddies, and the jet-preferred mode, as well as azimuthal modes such as the type which was analyzed in the previous section. The interaction between these modes, which have not been fully understood, govern the flow, and in particular, the velocity fluctuations, entrainment, and mixing between the fluids on both sides of the layer. Chemical reactions, sound generation, combustion instability can be strongly affected by these interactions.

In this section, results for the evolution of an axisymmetric shear layer, subject to an axisymmetric perturbation, and using the three-dimensional vortex scheme developed in the previous section, are presented. The computations are restricted to a periodically excited layer, thus boundary conditions on both sides of the computational domain, i.e. the wavelength, are satisfied. This is accomplished by using image vortices on both sides of the domain and computing their field by summing over the induced velocity of these images. The first image of each vortex on both sides must be considered as a vortex ball with a finite core radius. Beyond that, images can be considered as vortex points with zero cores. The effect of the latter can be arranged as a summation over an infinite series for a two-parameter function. This function is computed, using a large number of terms in the series, and stored as a two-dimensional table of the two parameters. During the computations, an interpolation procedure is used to obtain the value of the function at intermediate points. Details will be published elsewhere.

Results are obtained for an axisymmetric shear layer with the following parameters: The thickness of the vorticity layer \( \epsilon / D = 0.2 \), wavelength of the perturbation \( \lambda / D = 1.32 \), and amplitude of perturbation \( \sigma / D = 0.04 \), where \( \epsilon, \lambda, \) and \( \sigma \) is the standard deviation of the second-order Gaussian vorticity distribution within the layer and \( D \) is the mean diameter of the layer. The layer is discretized into 16 sections in the streamwise direction and 5 sections in the cross-stream direction, resulting in 80 vortex rings. Each ring is represented by 50 vortex balls along its axis. The vorticity of each vortex ball was obtained as before using \( \epsilon / D = 0.0825 \). Figure 22 shows a comparison between the actual and discretized vorticity distribution.

Figure 22 shows the location of the vortex elements in \( p-z \) plane, where \( p \) is the radial direction and \( z \) is the streamwise direction, and their streamwise velocity relative to the mean flow. In Fig. 24, vortex balls which were neighbors in the \( z \)-direction at time \( t = 0 \) are connected using cubic spline curves to show that the flow experiences while vorticity is during the rollup phase. The vorticity field and the material lines are plotted every 20 computational time-steps starting at \( t = 0 \). Although five layers of vortex elements were used to discretize the vorticity in the radial direction, the plots in Fig. 24 show only two layers, the central layer and the next layer to the outside. Plots of vortex elements locations in the radial plane and the \( p-z \) plane show that the elements remain on perfect circles while the radii of these circles increase or decrease as the vorticity layer rolls up.

Results in Fig. 23 indicate that the initial perturbation causes the layer to rollup, forming a large scale ring-like vortex eddy. As time progresses, more of the vorticity becomes concentrated around this eddy, and more irrotational fluid from both streams is entrained into its core. Due to the self-induced velocity of curved vortex lines, the eddy moves in the streamwise direction. However, within the duration of the computation, it maintains perfect azimuthal symmetry. Figure 24 shows that the central layer experiences the strongest stretch within the core as it endures several turns due to secondary instabilities, while the "braids", i.e., the two sleeves connecting neighboring cores, become thinner due to the strain field of the cores.

Since the layer maintains a perfect axisymmetric configuration during rollup, one can make a preliminary conclusion that the growth of the axisymmetric modes during the early stages of development suppresses the azimuthal instability modes of the evolving vortex-ring eddy. This is widely supported by the analytical linear theory of Michalke and Hermann [35] and by the experimental results of Vandsburger et al. [16], Roquemore et al. [17] and Namazian et al. [35]. The analytical study shows that the exponential

![Figure 22. Actual and discretized vorticity within the shear layer. Five vortex balls are used at the indicated location.](image-url)
Figure 23. Rollup of an axisymmetric shear layer due to an axisymmetric perturbation. Vortex balls are represented by circles and their velocity relative to the mean velocity is depicted by a line vector starting at the center of the circle. Results are plotted every 20 time steps starting at $t = 2.0$. The solid line indicates the centerline of the layer.

Figure 24. Lines connecting neighboring vortex balls in the streamwise direction. The figure shows the central layer and the next layer to the outside. The solid line indicates the centerline of the layer.
growth rates of axisymmetric modes are higher than those of azimuthal modes. Moreover, in all the reported experimental results, including those of Yule [32] and Crow and Champagne [33], the layer starts by rolling up into a perfect vortex ring. At later stages, the rings become susceptible to the azimuthal instability discussed in the previous section and the flow loses the azimuthal coherence.

However, this is only a preliminary conclusion since, in the numerical solution, the flow started with a large axisymmetric perturbation and zero azimuthal perturbation. The amplitudes of the perturbations were selected to model most experimental situations, where azimuthal perturbations are inhibited at the onset of the layer by the nozzle. The higher growth rate of the axisymmetric mode could also be a property of the linear range, as shown by the analytical results. To support this result and to study the effect of the azimuthal modes on the growth of the axisymmetric modes, we are planning to run the same case for different ratios of the axisymmetric/azimuthal amplitudes. Another issue to be investigated is at what stage does the azimuthal modes start to grow and what effect does the strain field generated during pairing have on its development.

Apart from the displacement of the ring eddy in the streamwise direction due to the curvature of the vortex lines, this eddy resembles the eddy that forms during the rollup of the planar shear layer (Ghoniem et al. [36]). This similarity has been observed before in the two-dimensional calculations of Davis and Moore [37]. As Fig. 24 indicates, the streamwise strain field, associated with the non-linear stages of rollup, pulls the vortex elements apart so that the distance between the neighboring centers exceeds h by a large factor. In order to maintain the resolution at late times, the vorticity fields must be redistributed between a different set of elements which are organized so that they can accommodate this strain field, as suggested by Ghoniem et al. [36] in the 2D vortex element method.

The stability of this ring eddy, which has an elliptical core, to azimuthal perturbations while it is moving in the strain field of its neighboring eddies is of central importance to the later stages of development of the layer. A numerical study of this problem is underway.

IV CONCLUSIONS

In this work, we have embarked on the task of applying three dimensional vortex methods for the numerical solution of the unsteady Navier-Stokes equations at high Reynolds number. The 3D vortex element method presented here combines the advantages of the vortex filament method of Leonard [8,11], and the vortex stick method of Chorin [23,23] in maintaining the connectivity of the vorticity field, thus satisfying the solenoidality condition. It utilizes the results of the convergence analysis of Beale and Majda [19,20] in selecting the core of the vortex elements. The scheme is Lagrangian, is capable of capturing the effect of strain as well as the vortex stretching along vortex lines by changing the number and strength of the vortex elements. It is readily extendable to flow fields with boundaries.

Results for the stability of a vortex ring with a finite core, which forms as an axisymmetric vorticity layer roll up, show very good agreement with the analytical and experimental results. The results reveal: (1) the breakdown of the azimuthal coherence of the ring due to the growth of radial perturbations along and within the core; (2) the evolution of streamwise vorticity in the non-linear stages of instability in the form of elongated lobes of vorticity along wedges within the expanding core; and (3) the development of an energy cascade to small scales which accompanies the stretch of vorticity during the non-linear growth of instability. Similar configurations were captured in experimental studies on vortex rings and later stages of turbulent jets.

The scheme was used to investigate the initial stages of transition to turbulence in an excited axisymmetric mixing layer, and the results showed good agreement with the recent qualitative results of Vangaburger et al. [16] and Roquemore et al. [17]. Quantitative study will be performed to investigate the interaction between the axisymmetric and the azimuthal instability modes and their effect on the development of the flow.

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