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# NUMERICAL SIMULATIONS OF COHERENT STRUCTURES IN A JET FLAME WITH A NONCIRCULAR CROSS SECTION

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<p>► The presence of coherent structures in turbulent shear flows and their importance in enhancing mixing and entrainment of chemical species has been established in recent years through extensive experimental and numerical studies. When non-premixed combustion is considered, the combustion processes could be enhanced by enhancing the fuel-air mixing and entrainment processes associated with these large coherent structures. In recent experimental studies, the entrainment characteristics of jets with different cross sections were studied, and it was determined that an elliptical jet with a certain cross-sectional shape was more efficient in entraining fluid than a circular jet with the same jet area. This increase was attributed to the complex self-induction process and the subsequent three-dimensional deformation of the elliptical vortex ring during its propagation. To understand the complex flow features associated with elliptical jets with and without heat release, a numerical study was undertaken. A new three-dimensional hybrid Navier-Stokes code was developed using spectral techniques and compact schemes to study the spatial evolution of elliptical jets. The simulation code is now ready for carrying out a detailed study of the effect of jet geometry on the mixing and combustion processes.</p>						
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# TABLE OF CONTENTS

	<u>Page</u>
INTRODUCTION	1
TECHNICAL OBJECTIVES OF THIS STUDY	2
SIGNIFICANT RESULTS IN THE PAST YEAR	2
COMPACT SCHEMES	3
THREE-DIMENSIONAL NAVIER-STOKES CODE DEVELOPMENT	4
RECENT RESULTS	5
RECOMMENDATIONS FOR FUTURE EFFORT	6
REFERENCES	7
FIGURES	8



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## INTRODUCTION

Ever since their discovery (e.g., Brown and Roshko, 1974), coherent structures in turbulent shear flows have proven to be important in enhancing the mixing and entrainment of chemical species into the turbulent region. An understanding of the evolution of coherent structures is necessary to predict the mixing rates in turbulent jets accurately. Furthermore, their importance in reacting flows becomes apparent if the large-scale structures could be enhanced to increase mixing. In the past, both active and passive techniques aimed at controlling the evolution of coherent structures have been used. By enhancing the spreading rate in the shear layer, high mixing rates between the fuel and the air can be achieved. This is owing to the simple observation that entrainment into the jet cannot occur faster than the jet growth. Obviously, increased mixing between the fuel and the air streams would also result in enhanced combustion.

Of the active methods, acoustic forcing of the shear layer at various frequencies has been shown to enhance the generation of highly coherent large-scale structures (e.g., Ho and Huang, 1982; Oster and Wagnanski, 1982). Studies have shown that the spreading rate can be dramatically increased when acoustic forcing is applied at the subharmonic of the most unstable frequency. This can result in the simultaneous merging of several vortices, even when the forcing amplitude is small. Experiments by Winant and Browand (1974) have shown that the vortex rollup and pairing process is the dominant mechanism of shear layer growth. Combustion enhancement in coaxial jets of fuel and air was demonstrated by Gutmark et al. (1989) by forcing both the jets at prescribed frequencies that were related to the most unstable modes.

Passive control techniques have also been extensively studied. Ho and Gutmark (1987), Gutmark and Ho (1985), Hussain and Husain (1989) and Schadow et al. (1986) have experimentally studied the entrainment characteristics of jets with different cross sections. It was observed (Ho and Gutmark, 1987) that an elliptical jet with an aspect ratio of 2:1 was about 3 to 8 times more effective in entraining fluid than a circular jet with the same cross-sectional area. The reason for this mixing enhancement was attributed to a complex series of distortions of the coherent elliptical vortex rings due to their self-induced flow and to their mutual interactions. These nonlinear interactions result in the phenomenon of "axis switching," where the orientation of the major and minor axes of the elliptical vortex ring appears to switch during its propagation. The number of switchings and the locations are strongly dependent upon initial conditions, the aspect ratio and, when excited, the Strouhal number and the excitation level (Hussain and Husain, 1989). The deformation and axis switching of the elliptical jets appear to play a major role in the increased entrainment observed with elliptical jets (Hussain and Husain, 1989). How this entrainment process is modified when there is heat release is not clearly known at present. In a chemically reacting flow when heat is released the gas density is lower in the

reacting zone. The dynamics of these elliptical structures can be affected by this density variation.

To understand the complex flow features associated with the propagation and breakdown of elliptical jets with and without heat release, a numerical study was undertaken. Due to the change in affiliation of the principal investigator, Dr. Wen-Huei Jou, this research was terminated after 6 months of study. This report documents the findings of the research in that period and presents some preliminary results of a study that was carried out subsequent to the termination of the contract.

### **TECHNICAL OBJECTIVES OF THIS STUDY**

A research effort involving numerical simulations was undertaken in order to understand the details of the mixing processes associated with elliptical jets with and without heat release. The effort was intended to study the details, using full three-dimensional simulations, of the development of the nonlinear instability waves (Koshigoe et al., 1988), the interaction (merging) of elliptical vortex rings and the associated entrainment process. The effect of heat release on the evolution of the mixing region was also to be investigated. Flow field statistics were to be computed throughout the development of the jet to characterize the mixing properties of the simulated flow field.

### **SIGNIFICANT RESULTS IN THE PAST YEAR**

In the past year, the research effort was entirely directed towards constructing a fourth-order accurate, compact finite-difference scheme for chemically reacting flows. Earlier studies of chemically reacting flows have employed numerical schemes using pseudospectral techniques (McMurtry et al., 1986, 1989). These simulations were restricted to spatially periodic flows. The study of more realistic flows, such as in an elliptical jet, requires a numerical simulation of spatially evolving flows, due to the decomposition of the initial disturbance into a set of complex modes with varying dispersive properties. In addition, to resolve the shear layer regions, a stretched nonuniform grid in the cross-sectional plane is required to prevent boundary effects in simulating axis switching.

For these reasons, a compact higher-order scheme is more flexible in treating the boundary conditions. There are many advantages of a compact scheme. First, a higher order of accuracy (fourth order in this case) can be achieved using a compact stencil of only three grid points. This high accuracy is obtained by solving for the derivatives simultaneously at three points using a tridiagonal solver. The compact scheme also has a smaller truncation error and

smaller phase error than conventional centered, fourth-order finite-difference approximations. These properties are very important when performing simulations of the spatial development of unsteady flows. In the following, we briefly describe a simple test problem that was used to study the effectiveness of the compact scheme to resolve wave motion without significant phase error.

### COMPACT SCHEMES

Consider a one-dimensional unsteady wave equation of the form

$$\partial u / \partial t = \partial u / \partial x \quad (1)$$

which is to be solved subject to some specified initial condition at  $t = 0$ . A fourth-order compact scheme approximation of the first differential spatial operator can be written down as

$$du/dx = [1 + \delta^2/6]^{-1} [(u_{i+1} - u_{i-1})/2\Delta x] \quad (2)$$

where  $\delta^2$  is the central second difference spatial operator, and the discretization is on a uniform grid. Extension to a nonuniform grid is straightforward. This spatial discretization can be combined with time-accurate schemes, such as the second-order Adams-Bashforth scheme or the Runge-Kutta scheme, to obtain a high-order spatially and temporally accurate numerical algorithm.

A detailed study using the one-dimensional wave equation (1) subject to an initial disturbance of the form  $\sin(kx)$  at  $t = 0$  was carried out to evaluate the various compact schemes. The length of the one-dimensional duct  $L$  was chosen to be unity, and 256 grid points were used to discretize the flow field. Periodic boundary conditions were used at  $x = 0$  and  $x = L$ . The nondimensional wavenumber  $k$  of the initial disturbance was varied to study the effect of resolution of the wave. Note that an increase in the wavenumber implies a decrease in the wavelength of the disturbance. Thus, for a fixed number of grid points, an increase in  $k$  results in a waveform that is resolved using a lesser number of grid points. For example, for a wavenumber of  $k = 40$ , the wave is resolved using around six grid points.

The primary objective of this numerical experiment was to determine the error in the phase speed of the initial disturbance during the temporal evolution of the wave. The fourth-order and sixth-order compact schemes were evaluated using time-marching methods such as Adams-Bashforth and Runge-Kutta. The higher-order accuracy of the compact scheme in predicting the phase speed of a simple wave was demonstrated in this study. Some pertinent results are shown here.

Figure 1 shows the error in the phase as a function of wavenumber for various time-marching schemes for the fourth-order compact scheme with third-order boundary conditions. It can be seen that the Adams-Bashforth scheme with a CFL of 0.1 can predict the phase speed of the wave within 0.1 percent for the high wavenumber  $k = 40$ . Although Runge-Kutta schemes could be used with a higher CFL, the overall error in the phase speed exceeds 0.1 percent by  $k \approx 30$ . The wave motion in a portion of the duct can be seen in Figure 2, which shows the shape of the wave for the wavenumber  $k = 40$  at three different times. It can be seen that the wave is adequately resolved using only six grid points.

Figure 3 shows a comparison of the fourth-order [O(4)] and the sixth-order [O(6)] compact schemes using the Adams-Bashforth time-stepping scheme. It appears that, for the same wavenumber, the fourth-order compact scheme is superior to the sixth-order scheme. Based on this study, the decision was made to implement a fourth-order compact scheme in the three-dimensional solver.

### THREE-DIMENSIONAL NAVIER-STOKES CODE DEVELOPMENT

A new hybrid code was developed in this study that uses a fourth-order compact scheme in the streamwise direction and pseudospectral methods in the other two directions. In spectral methods, the solution of a differential equation is represented as a truncated series of known orthogonal functions. If the solution to a problem is infinitely differentiable, the error in a properly implemented spectral method can be shown to go to zero faster than any finite power of  $N$  as  $N$  gets larger, where  $N$  is the number of modes retained in the series expansion. Other advantages of spectral methods over more commonly used finite-difference techniques are that the numerical diffusion and dispersion (phase) errors are very small. In applications to reacting flows, where steep gradients of the chemical reactants can result and where reaction rates are diffusion controlled, numerical diffusion and dispersion can be major sources of error.

The main shortcoming of the spectral method is due to its limited application in problems with complex geometries. The choice of the expansion function is determined by two factors: (1) the physical boundary conditions of the problem and (2) the existence of fast transform techniques to sum the truncated series efficiently. In a spectral method, the boundary conditions of the series expansion must be consistent with the physical boundary conditions. In the application of Fourier series (the most common expansion functions used in spectral methods), we are limited to studying problems with periodic, even or odd symmetries at the boundaries.

In this study we are interested in the spatial development of the elliptical jet. Thus, the inflow and outflow boundary conditions associated with streamwise development must be implemented. This is very difficult using spectral methods but can be accomplished relatively

easily using the compact scheme described above. As shown above, the phase errors associated with the fourth-order compact scheme are quite low, and extension of the method to a nonuniform grid is straightforward.

A three-dimensional Navier-Stokes solver using spectral methods in the transverse and spanwise directions and the fourth-order compact scheme in the streamwise direction has been developed. All the subroutines for this code are written in FORTRAN, allowing it to be portable to any machine with minimal modifications. The development of the basic code was completed, and the debugging of most of its components has also been completed.

## RECENT RESULTS

Subsequent to the termination of this study, the development of the numerical code was continued by Dr. Patrick McMurtry, who was involved in the earlier development work. Some recent results of the initial tests are described here.

The basic issue in implementing the compact scheme in a three-dimensional solver is the proper implementation of the inflow and outflow boundary conditions. To study this feature, the three-dimensional code was reduced to a two-dimensional solver that used spectral techniques in the normal direction and the fourth-order compact scheme in the streamwise direction. A two-dimensional planar jet has been simulated using this technique.

The flow field was initialized with a free-stream velocity in the top half of the domain ( $U_1$ ) with a value of 1 and in the bottom half ( $U_2$ ) with a value of zero. The Reynolds number based on the velocity difference across the layer was 200, and the grid resolution was  $100 \times 32$  ( $x, y$ ). At the inlet, a periodic perturbation was added. This perturbation corresponds to the most unstable wavelength of a hyperbolic tangent mean velocity profile. At the outflow, a convective condition was applied. Mathematically, this condition can be expressed as

$$\partial\phi/\partial t + U_c \partial\phi/\partial x = 0 \quad (3)$$

where  $U_c$  is a convective velocity and is taken to be  $(U_1 + U_2)/2$ .

Figure 4 shows the evolution of the spatially developing shear layer for the case when only the fundamental perturbation was used to initialize the flow. As expected, after the shear layer rolls up and the fundamental reaches a maximum amplitude, the vortex is convected out without any further growth.

Figure 5 shows the case in which the subharmonic perturbation was also added. The development of the unstable modes is clearly evident. A pairing process between the two neighboring vortices is beginning near the outflow. A much larger computational domain will

be needed to simulate the complete pairing process. Note that at the outflow, the structures are convected out without affecting the internal flow field.

These simulations clearly demonstrate that the basic issues involved in implementing the compact scheme in a full Navier-Stokes solver have been successfully resolved. Making the current two-dimensional solver into a full three-dimensional solver should not pose any major problems, since all the elements of the three-dimensional solver are already present and were merely being suppressed to simulate the two-dimensional flow.

#### **RECOMMENDATIONS FOR FUTURE EFFORT**

At this stage, the three-dimensional code development is mostly completed with the resolution of the issues related to the outflow and inflow boundary conditions. With some minor effort, this code can be made ready to carry out a serious investigation of the instability of jets with and without external excitation. In particular, the evolution of an elliptical jet subject to initial disturbance can be simulated. Subsequently, the effects of heat release can be included to evaluate how the mixing and entrainment processes enhance combustion efficiency. Comparisons with experimental data and other numerical studies could be made to validate and demonstrate the capability of this code which is now in a near-operational status.

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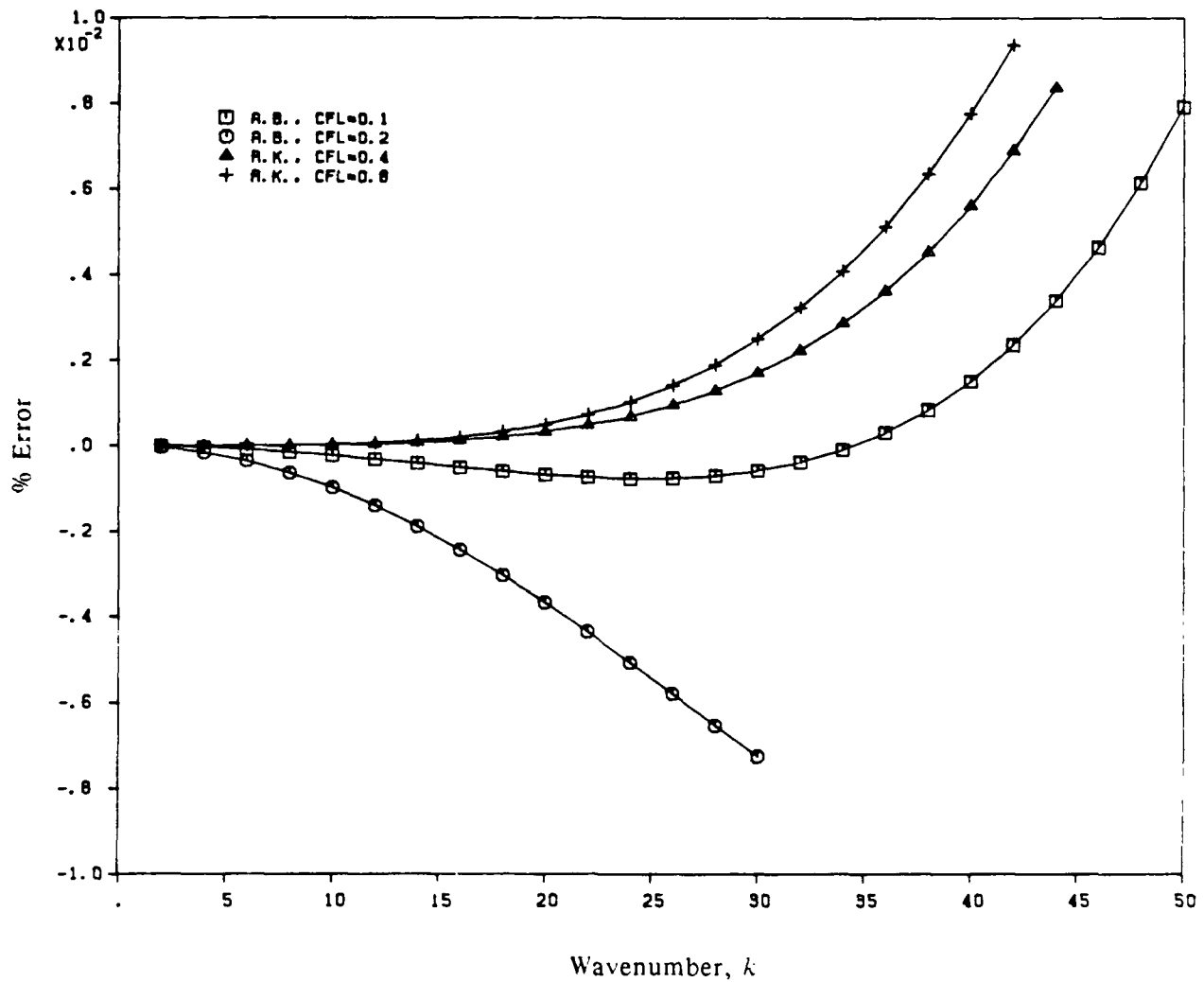


Figure 1. Phase error during wave motion in a one-dimensional duct as a function of wavenumber using different time-stepping schemes and the fourth-order compact scheme.

A•B: Adams-Bashforth scheme  $O(\Delta t^2)$   
 R•K: Runge-Kutta scheme  $O(\Delta t^4)$

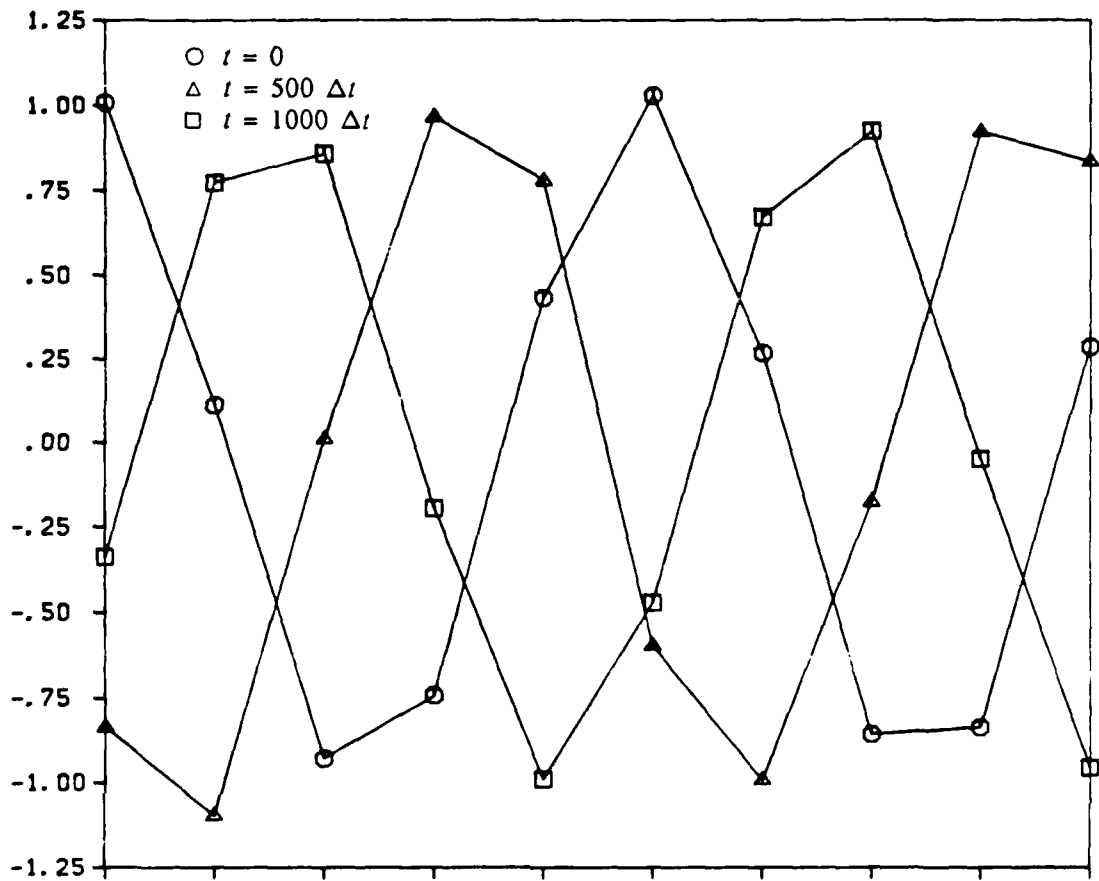


Figure 2. The waveform in the duct at three different times. The wave is resolved by six grid points using the fourth-order compact scheme.

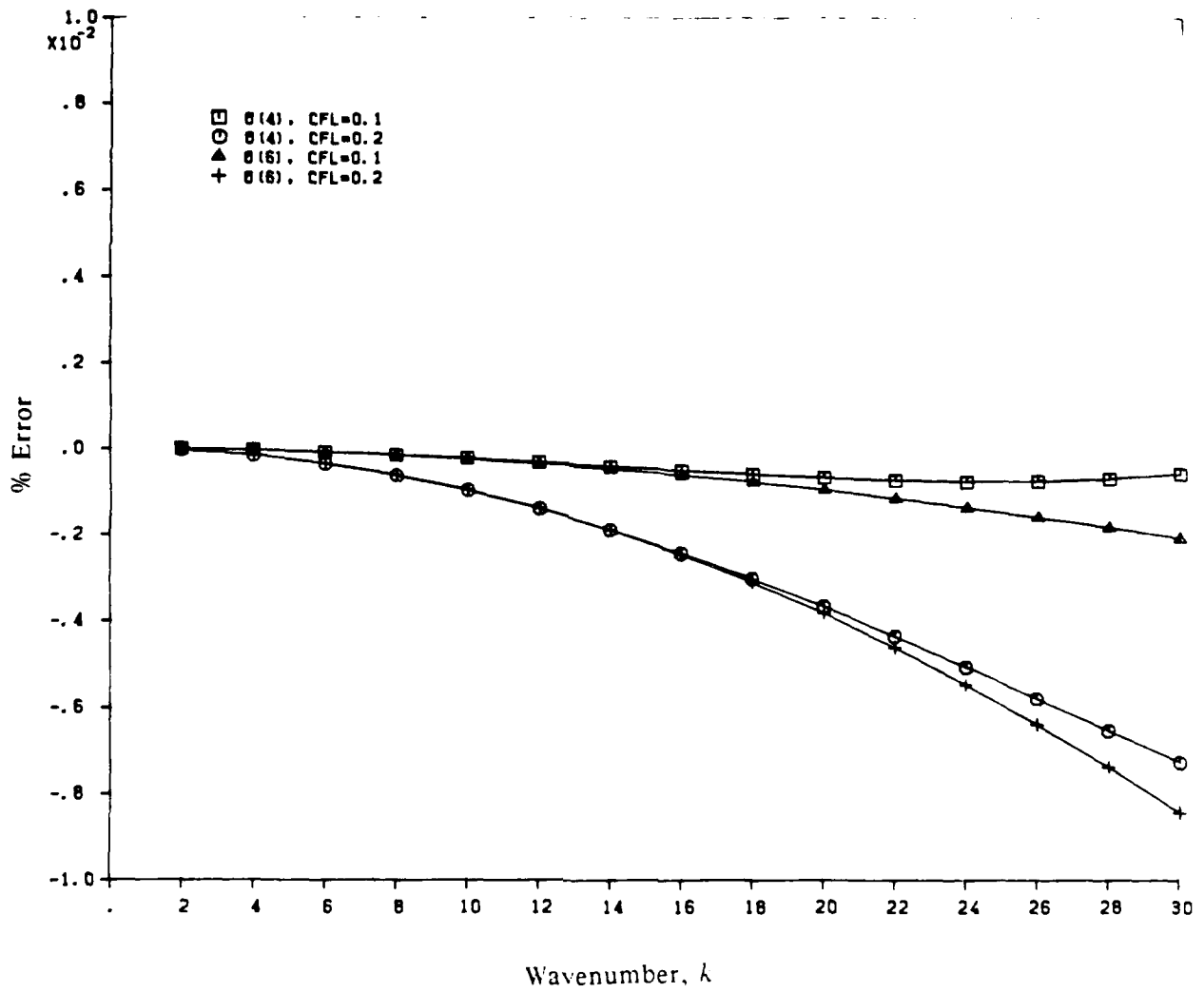


Figure 3. Phase error during wave motion in a one-dimensional duct as a function of wavenumber. Comparison of the fourth-order and the sixth-order compact schemes.

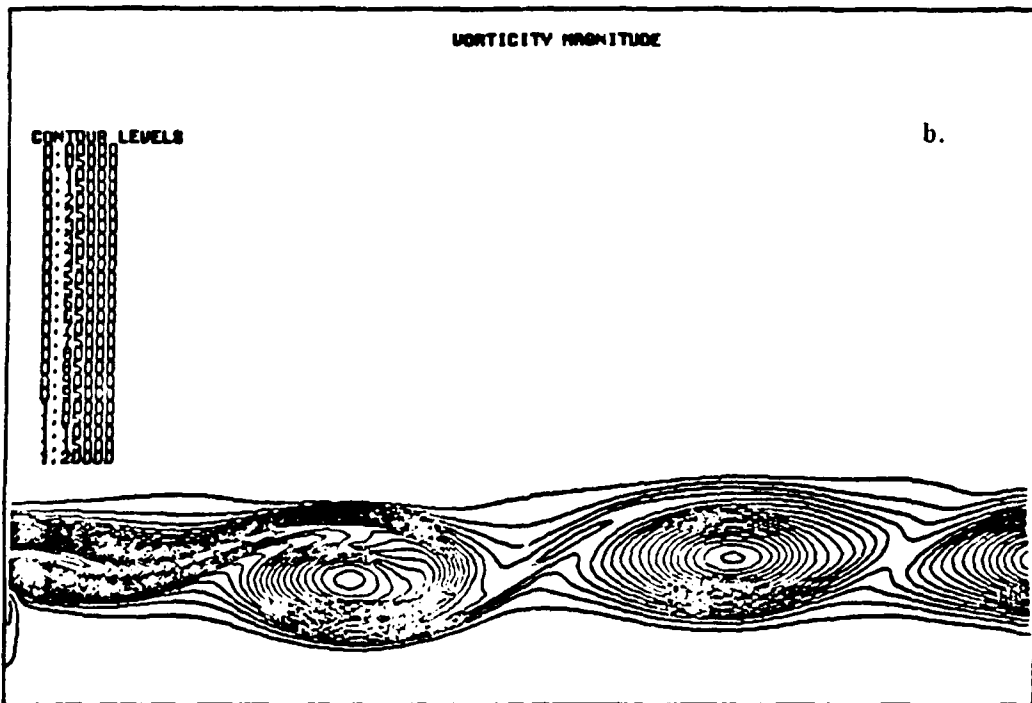
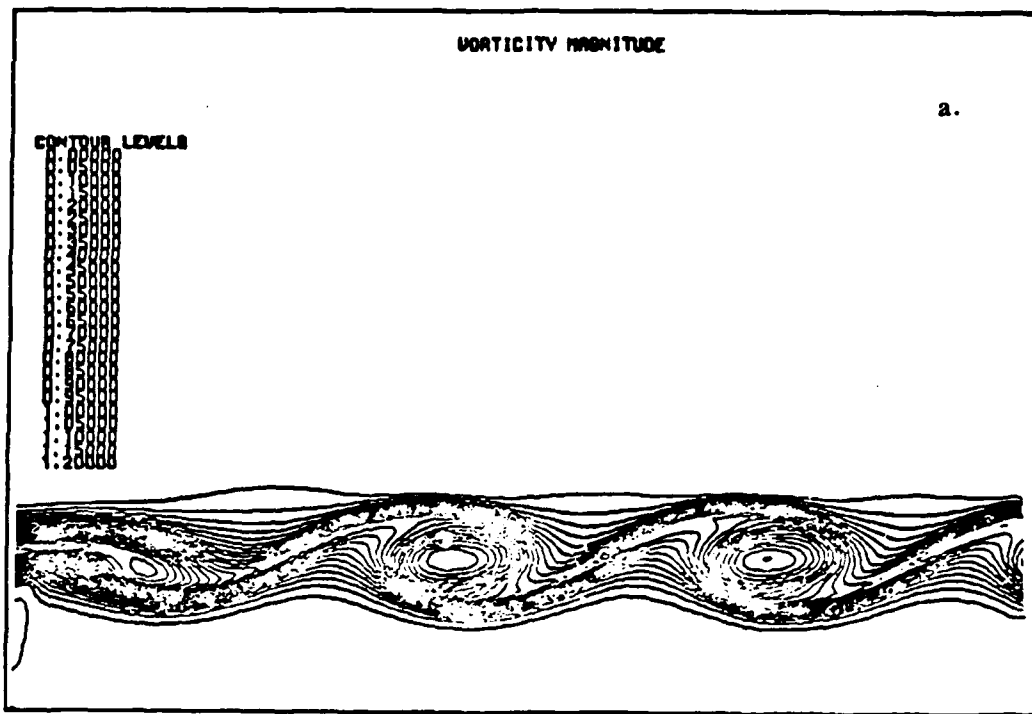
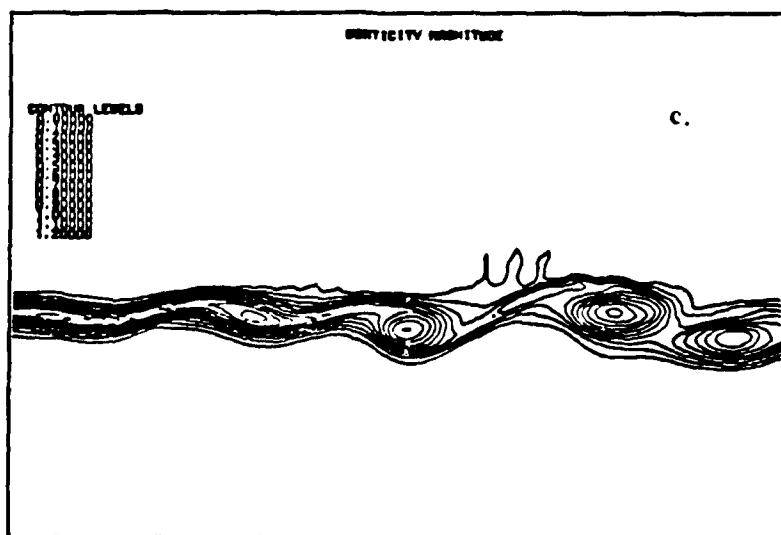
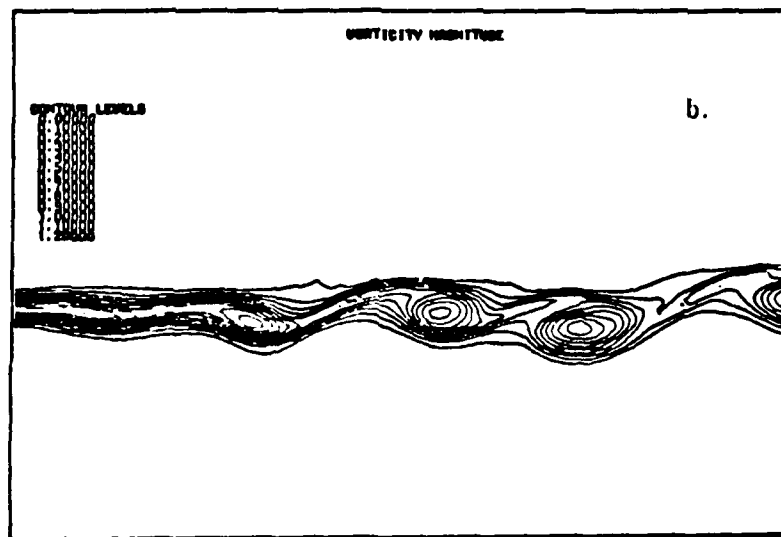
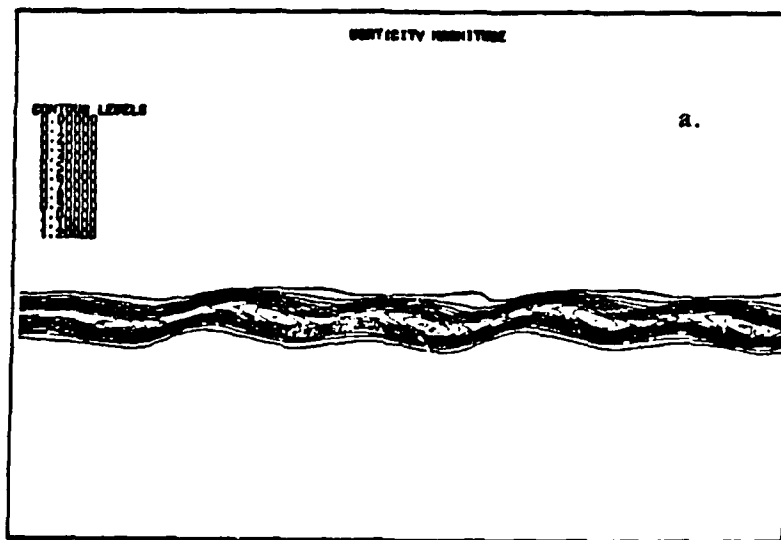


Figure 4. Vortex rollup in a spatially developing two-dimensional shear layer using the hybrid scheme (spectral in the transverse direction and fourth-order compact in the streamwise direction). Shear layer perturbed by the fundamental mode only.



**Figure 5.** Vortex rollup and pairing in a spatially developing two-dimensional shear layer using the hybrid scheme. Shear layer perturbed by the fundamental and subharmonic modes.