LA-5426-MS

INFORMAL REPORT

Dr. 454

200
12-6-73
uc-37 + 36

A Method for Increased Accuracy in Eulerian Fluid Dynamics Calculations

los alamos
scientific laboratory

of the University of California

LOS ALAMOS, NEW MEXICO 87544

MASTER

UNITED STATES
ATOMIC ENERGY COMMISSION
CONTRACT W-7405-ENG. 36

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

In the interest of prompt distribution, this LAMS report was not edited by the Technical Information staff.

Printed in the United States of America. Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151
Price: Printed Copy \$4.00; Microfiche \$1.45

LA-5426-MS
Informal Report
UC-32 & 34

ISSUED: October 1973

A Method for Increased Accuracy in Eulerian Fluid Dynamics Calculations

by

W. C. Rivard
O. A. Farmer
T. D. Butler
P. J. O'Rourke

This work partially supported by the US Air Force under Project Orders AFWL 72-067 and 73-103.

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

MASTER

UNLIMITED

fy

CONTENTS

	Page
Abstract -----	1
I. Introduction -----	1
II. Theory of the Truncation Error Cancellation (TEC) Method -----	2
III. Application of the TEC Method -----	4
A. Diffusional Truncation Errors for the RICE Equations -----	4
B. Stabilization of the RICE Equations -----	7
IV. Diffusional Limits -----	9
V. Numerical Examples -----	9
VI. Summary -----	13
Appendix A. Derivation of the TEC Method -----	14
Appendix B. Truncation Errors for the RICE flow Equations -----	15

A METHOD FOR INCREASED ACCURACY
IN EULERIAN FLUID DYNAMICS CALCULATIONS

by

W. C. Rivard
T. D. Butler
O. A. Farmer
P. J. O'Rourke

ABSTRACT

A method for increased accuracy in Eulerian fluid dynamics calculations is described. The essence of the method is local cancellation of low-order, diffusional truncation errors. These errors are the source of nonlinear numerical instabilities. The methodology is described in general and specific application is made to the transient, two-dimensional flow equations for chemically reacting mixtures. Two example problems are solved to illustrate the method. For comparison, the same problems are solved with an artificial viscosity technique.

I. INTRODUCTION

Computer calculations of time-dependent fluid flows often require the solution of finite difference equations that are inherently unstable. An unstable solution oscillates or grows unbounded in time and in no way resembles the physical flow. Considerable attention has been given to understanding and controlling these instabilities. The Fourier analysis of Von Neumann¹ is successful for analyzing linear equations. This method, however, yields only limited information when applied to the nonlinear equations of fluid dynamics. The nonlinear stability properties have been successfully investigated by Hirt.² Hirt examines the low order truncation errors that lead to diffusion of the dependent variable, e.g., density in the continuity equation. He concludes that the solution will be unstable (i.e., exponentially growing in time) when the algebraic sign of the diffusion coefficient is negative.

It is well known that the inclusion of an artificial viscosity in the momentum equation is an

effective means of maintaining the stability of that equation. A properly chosen amount of artificial viscosity can counter any negative diffusion arising from the truncation errors. One must be extremely careful, however, in the use of artificial viscosity for calculations in more than one space dimension. For example if the same coefficient is used, say to diffuse ρu -momentum in the x and y directions, excessive diffusion can result in one direction. This will occur when the diffusional truncation errors yield vastly different diffusion coefficients in the two directions, a situation that is quite common. It occurs in flows where the motion is largely directed in a single coordinate direction, since the truncation error diffusion coefficient in the x -direction depends upon the x -component of velocity, u , and $\partial u/\partial x$, whereas the coefficient in the y -direction depends upon the y -component of velocity, v , and $\partial v/\partial y$.

The purpose of this paper is to describe and illustrate a general method to stabilize the finite

difference equations of Eulerian fluid dynamics by locally computing and canceling the diffusion-like truncation errors. Lagrangian equations are essentially free of these errors since they arise from the convective acceleration terms, but have other problems of their own when distortions are large.

A significant increase in accuracy is achieved with the Truncation Error Cancellation (TEC) method over usual artificial viscosity schemes because excessive artificial diffusion is eliminated. The order of the finite difference equations generally remains unchanged since all the low order errors, other than those of diffusion, are still present. In this study, no attempt has been made to eliminate the low order dispersion-like errors arising from the difference equations. Such errors can significantly detract from the accuracy of a given flow calculation. This aspect is discussed in Section II, which presents the essential ideas of the TEC method.

The method is particularly powerful for the computation of flows with transverse shears, e.g., in boundary layers and mixing layers, and flows where large Reynolds number effects are important. The computational results demonstrate a greatly increased sensitivity to the Reynolds number in comparison to ordinary artificial viscosity techniques. As presented herein, the method is appropriate for calculating shock flows providing the shocks are sufficiently weak. For strong shocks, the addition of an artificial viscosity applied in the region of the shock is necessary to provide the required kinetic energy dissipation.

To indicate the relative ease of applying this method in complex fluid dynamics codes and to illustrate its effectiveness, a specific application is made to the RICE³ code. This code is used to solve transient, two-dimensional, compressible flows with species mixing and chemical reactions. Details of the application are presented in Section III. RICE uses the ICE⁴ solution technique, an implicit Eulerian scheme for flows at arbitrary Mach number. The difference equations are fully stabilized with the TEC method by locally computing and canceling the low order diffusional truncation errors. The stability theory of Hirt is used to determine the truncation errors and the form of the diffusion coefficients.

By eliminating excessive diffusion, this method usually allows a significant increase in the computational time step. This is particularly true for high Mach number (> 5) flows when the time step in a typical artificial viscosity scheme is dictated by the diffusional limit obtained from Fourier analysis. In this case a reduction in diffusion results directly in an increase in time step. Section IV discusses this aspect.

Finally, solution of example problems are presented and compared in Section V. The solutions are obtained first using the TEC method and then using an artificial viscosity treatment. The increased accuracy of the method is demonstrated by the comparisons.

II. THEORY OF THE TRUNCATION ERROR CANCELLATION (TEC) METHOD

The effects of truncation errors on the stability of finite difference equations have been described in Ref. 2. These effects are briefly reviewed here to the extent that they are preliminary for the stability method proposed. The method is completely general; the description, however, centers on the continuity equation as a specific illustration. A simplified derivation is given here to indicate the general idea of the scheme. A more comprehensive derivation is presented in Appendix A.

In one dimension, the continuity equation is

$$DE(\rho) \equiv \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} \quad (2.1)$$

$$DE(\rho) = 0$$

where $DE(\rho)$ represents the partial differential equation, ρ is the mass density, t is the time, and u is the velocity component in the x -direction. The finite difference approximation $FD(\rho)$ is used for $DE(\rho)$ so that

$$FD(\rho) = DE(\rho) + t.e. \quad (2.2)$$

The truncation errors, t.e., are the higher order terms in a Taylor series expansion of $FD(\rho)$ about the point, $x = i \delta x$ and $t = n \delta t$; the zeroth order terms in the expansion yield $DE(\rho)$.

For consideration of stability, we need only those truncation errors that lead to diffusion of ρ , i.e., errors of the form $\epsilon \frac{\partial^2 \rho}{\partial x^2}$ where ϵ is the diffusion coefficient. Thus we may rewrite Eq. (2.2) in the form

$$DE(\rho) = FD(\rho) + \epsilon \frac{\partial^2 \rho}{\partial x^2} + \text{o.t.e.} \quad (2.3)$$

where we have transposed the truncation error terms, with the last term on the right hand side representing the other truncation errors. Hirt's stability theory states that $FD(\rho) = 0$ is numerically unstable, having an exponentially growing solution, when ϵ is negative. This can be seen from Eq. (2.3) when neglecting the other truncation error terms,

$$DE(\rho) = \epsilon \frac{\partial^2 \rho}{\partial x^2} \quad (2.4)$$

where a negative value of ϵ leads to exponential growth in the solution of the partial differential equation.

The task then is to obtain numerical stability in the calculations by locally sensing the algebraic sign and magnitude of ϵ and, providing the conditions warrant it, to include an explicit diffusion term in the finite difference equation to cancel the negative diffusion. This term is written symbolically as

$$FD \left(A \frac{\partial^2 \rho}{\partial x^2} \right) = A \frac{\partial^2 \rho}{\partial x^2} + \text{o.t.e} \quad (2.5)$$

as in Eq. (2.2) where A is a diffusion coefficient to be defined later. Inserting this into Eq. (2.3) yields

$$DE(\rho) = FD(\rho) - FD \left(A \frac{\partial^2 \rho}{\partial x^2} \right) + (A+\epsilon) \frac{\partial^2 \rho}{\partial x^2} + \text{o.t.e.} \quad (2.6)$$

and the new difference equation to be solved is

$$FD(\rho) - FD \left(A \frac{\partial^2 \rho}{\partial x^2} \right) = 0 \quad (2.7)$$

which results in

$$DE(\rho) = (A+\epsilon) \frac{\partial^2 \rho}{\partial x^2} + \text{o.t.e.} \quad (2.8)$$

The coefficient A is chosen such that $A+\epsilon > 0$. This inequality is necessary in accord with Hirt's stability theory since we solve Eq. (2.7) instead of $FD(\rho) = 0$.

Choosing A such that the inequality is satisfied is necessary for the stability of Eq. (2.7). Negative values of ϵ , which are a source of instability, are countered with positive values of A . Positive values of ϵ are stabilizing and negative values of A can reduce the effective diffusion coefficient. With respect to this latter point, we have found in practice that negative values of A tend to enhance local curvatures in the density field, i.e., local peaks and troughs, until balanced by contributions from the convective term $\frac{\partial \rho u}{\partial x}$. The effect of this is to give rise to dispersive errors since they are proportional to the rate of change of curvature. These errors, although not destabilizing per se, can cause a significant loss of accuracy.

It is frequently desired to cast the finite difference form of the diffusion term into conservation form. This is accomplished with no additional complication when $\frac{\partial A}{\partial x}$ does not contain terms leading to further ρ diffusion. In this case the conservative and non-conservative forms are interchangeable so that we can write

$$FD(\rho) - FD \left[\frac{\partial}{\partial x} \left(A \frac{\partial \rho}{\partial x} \right) \right] = 0 \quad (2.9)$$

in place of Eq. (2.7).

In the event that $\frac{\partial A}{\partial x}$ does lead to ρ diffusion, we introduce a second diffusion coefficient A' and rewrite Eq. (2.9) as

$$FD(\rho) - FD \left\{ \frac{\partial}{\partial x} \left[(A+A') \frac{\partial \rho}{\partial x} \right] \right\} = 0 \quad (2.10)$$

where A' is determined from the differential equation

$$\left(\frac{\partial A}{\partial x} \right)_D \frac{\partial \rho}{\partial x} + \frac{\partial}{\partial x} \left(A' \frac{\partial \rho}{\partial x} \right) = 0 \quad (2.11)$$

The factor $\left(\frac{\partial A}{\partial x} \right)_D$ refers to that portion of $\frac{\partial A}{\partial x}$ leading to ρ diffusion. The solution of Eq. (2.11) is

$$A' = \left(\frac{\partial \rho}{\partial x} \right)^{-1} \left[\int \left(\frac{\partial A}{\partial x} \right)_D \left(\frac{\partial \rho}{\partial x} \right) dx + C \right] \quad (2.12)$$

where C is the constant of integration. The constant has no effect in Eq. (2.10) since we want $\partial[A' \partial \rho / \partial x] / \partial x$; hence it is set to zero and the expression for A' becomes

$$A' = \left(\frac{\partial \rho}{\partial x} \right)^{-1} \int \left(\frac{\partial A}{\partial x} \right) \frac{\partial \rho}{\partial x} dx, \quad (2.13)$$

evaluated locally in the computing mesh.

In summary, we propose to solve Eq. (2.10) as an approximation to

$$DE(\rho) = 0,$$

where A' is given in Eq. (2.13) and A satisfies the inequality $A + \epsilon > 0$.

III. APPLICATION OF THE TEC METHOD

A. Diffusional Truncation Errors for the RICE Equations

The preceding section described, by means of a simple example, the general approach to applying this technique. In the remainder of the report, we shall show in detail how the technique is applied to the difference equations in the RICE³ computer code and the increased accuracy attained with it. RICE was chosen because of its general applicability for solving a broad spectrum of transient, two-dimensional, mixing and chemically reacting flow problems and because its difference equations are typical of other Eulerian fluid dynamics programs. In this section, we derive the relevant truncation error diffusion terms from the finite difference approximations to the mass, momenta, specific internal energy and species transport equations. In addition to the diffusive errors given here, a complete listing of the low order errors in the absence of transport effects is presented in Appendix B.

For the RICE difference equations, the fluid variables are located as shown in Figure 1. Q_i^j represents the density ρ_i^j , pressure p_i^j , specific internal energy I_i^j , and species density $(\rho_\alpha)_i^j$ for species α , which are stored at the cell center. Velocity components $u_{i+1/2}^j$ and $v_{i+1/2}^j$ in the x and y directions are stored at the center of the right and top boundaries respectively. The indices, i and j correspond to the i^{th} column and j^{th} row of computational cells.

Figure 1. Location of variables in the computational mesh. Q_i^j represents the density ρ_i^j , pressure p_i^j , specific internal energy I_i^j , and species density $(\rho_\alpha)_i^j$ for species α which are stored at the cell center. The velocity components $u_{i+1/2}^j$ and $v_{i+1/2}^j$ in the x and y directions are stored on the cell boundaries.

The finite difference expression for the RICE mass equation in Cartesian coordinates is

$$\begin{aligned} FD(\rho) = & \left[\rho_1^{j+1} - \rho_1^j \right] / \delta t + \theta \left\{ \left(\rho_1^j + \rho_{i+1}^j \right) u_{i+1/2}^j \right. \\ & - \left(\rho_1^j + \rho_{i-1}^j \right) u_{i-1/2}^j \left. \right\} / 2\delta x + \left\{ \left(\rho_1^j + \rho_1^{j+1} \right) v_{i+1/2}^{j+1/2} \right. \\ & - \left(\rho_1^j + \rho_1^{j-1} \right) v_{i+1/2}^{j-1/2} \left. \right\} / 2\delta y \left\{ \right. \\ & + (1 - \theta) \left\{ \left(\rho_1^j + \rho_{i+1}^j \right) u_{i+1/2}^j \right. \\ & - \left(\rho_1^j + \rho_{i-1}^j \right) u_{i-1/2}^j \left. \right\} / 2\delta x + \left\{ \left(\rho_1^j + \rho_1^{j+1} \right) v_{i+1/2}^{j+1/2} \right. \\ & - \left(\rho_1^j + \rho_1^{j-1} \right) v_{i+1/2}^{j-1/2} \left. \right\} / 2\delta y \left. \right\}. \quad (3.1) \end{aligned}$$

The parameter θ ranges from 0.0 to 1.0 and is a measure of the implicitness of the calculation, i.e., $\theta = 0.0$ is fully explicit and $\theta = 1.0$ is fully implicit. The time level superscript $(n+1)$ refers to quantities evaluated at the advanced time. When the time level superscript is omitted, time level n is implied.

We expand the finite difference approximation to the mass conservation equation about the point (i, j, n) . Typical expansions are

$$\begin{aligned} n+1 \rho_i^j &= n \rho_i^j + \frac{\partial \rho}{\partial t} \delta t + \frac{\partial^2 \rho}{\partial t^2} \frac{\delta t^2}{2} + \dots, \\ \rho_{i+1}^j &= \rho_i^j + \frac{\partial \rho}{\partial x} \delta x + \frac{\partial^2 \rho}{\partial x^2} \frac{\delta x^2}{2} + \frac{\partial^3 \rho}{\partial x^3} \frac{\delta x^3}{6} + \dots, \\ \rho_i^{j+1} &= \rho_i^j + \frac{\partial \rho}{\partial y} \delta y + \frac{\partial^2 \rho}{\partial y^2} \frac{\delta y^2}{2} + \frac{\partial^3 \rho}{\partial y^3} \frac{\delta y^3}{6} + \dots, \\ u_{i+\frac{1}{2}}^j &= u_i^j + \frac{\partial u}{\partial x} \frac{\delta x}{2} + \frac{\partial^2 u}{\partial x^2} \frac{\delta x^2}{8} + \frac{\partial^3 u}{\partial x^3} \frac{\delta x^3}{48} + \dots, \\ v_i^{j+\frac{1}{2}} &= v_i^j + \frac{\partial v}{\partial y} \frac{\delta y}{2} + \frac{\partial^2 v}{\partial y^2} \frac{\delta y^2}{8} + \frac{\partial^3 v}{\partial y^3} \frac{\delta y^3}{48} + \dots \end{aligned} \quad (3.2)$$

Inserting these expressions into Eq. (3.1) and retaining only the lowest order time and space errors in the diffusion coefficients results in

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} &= FD(\rho) + (2\theta - 1) \frac{\delta t}{2} \left[(u^2 + c^2) \frac{\partial^2 \rho}{\partial x^2} + (v^2 + c^2) \frac{\partial^2 \rho}{\partial y^2} \right] \\ &\quad - \frac{\delta x^2}{4} \frac{\partial u}{\partial x} \frac{\partial^2 \rho}{\partial x^2} - \frac{\delta y^2}{4} \frac{\partial v}{\partial y} \frac{\partial^2 \rho}{\partial y^2} \\ &\quad + \text{o.t.e.} \end{aligned} \quad (3.3)$$

in which c^2 is the square of the adiabatic sound speed. Note that the choice of $\theta = 0.5$ eliminates the first order time error in the equation.

The finite difference approximation to the x-direction momentum equation is given by

$$\begin{aligned} FD(\rho u) &= \left[n+1 (\rho u)_{i+\frac{1}{2}}^j - (\rho u)_{i+\frac{1}{2}}^j \right] / \delta t \\ &\quad + \left[(\rho u^2)_{i+1}^j - (\rho u^2)_i^j \right] / \delta x + \left[(\rho uv)_{i+\frac{1}{2}}^{j+\frac{1}{2}} - (\rho uv)_{i+\frac{1}{2}}^{j-\frac{1}{2}} \right] / \delta y \\ &\quad + \left[\phi (\bar{p}_{i+1}^j - \bar{p}_i^j) + (1 - \phi) (\bar{p}_{i+1}^j - \bar{p}_i^j) \right] / \delta x + \left[(\sigma_{xx})_i^j - (\sigma_{xx})_{i+1}^j \right] / \delta x \\ &\quad + \left[(\sigma_{xy})_{i+\frac{1}{2}}^{j+\frac{1}{2}} - (\sigma_{xy})_{i+\frac{1}{2}}^{j-\frac{1}{2}} \right] / \delta y. \end{aligned} \quad (3.4)$$

The quantity $\bar{p}_i^j$ is a partially, time-advanced pressure

$$\bar{p}_i^j = p_i^j + (c^2)_i^j \left(n+1 \rho_i^j - \rho_i^j \right), \quad (3.5)$$

and the parameter ϕ is similar to θ in Eq. (3.1).

The momentum flux terms are given by

$$\begin{aligned} (\rho u^2)_i^j &= \rho_i^j \left(u_{i+\frac{1}{2}}^j + u_{i-\frac{1}{2}}^j \right)^2 / 4, \\ (\rho uv)_{i+\frac{1}{2}}^{j+\frac{1}{2}} &= \left(\rho_i^j + \rho_{i+1}^j + \rho_{i+1}^{j+1} + \rho_i^{j+1} \right) \\ &\quad \left(u_{i+\frac{1}{2}}^j + u_{i+\frac{1}{2}}^{j+1} \right) \left(v_i^{j+\frac{1}{2}} + v_{i+1}^{j+\frac{1}{2}} \right) / 16, \end{aligned} \quad (3.6)$$

and σ_{xx} and σ_{xy} are the viscous stress tensor components given by

$$\begin{aligned} (\sigma_{xx})_i^j &= 2 \mu_i^j \left(u_{i+\frac{1}{2}}^j - u_{i-\frac{1}{2}}^j \right) / \delta x + \lambda_i^j \left[\left(u_{i+\frac{1}{2}}^j - u_{i-\frac{1}{2}}^j \right) / \delta x + \left(v_i^{j+\frac{1}{2}} - v_i^{j-\frac{1}{2}} \right) / \delta y \right], \\ (\sigma_{xy})_{i+\frac{1}{2}}^{j+\frac{1}{2}} &= \frac{1}{4} \left(\mu_i^j + \mu_{i+1}^j + \mu_{i+1}^{j+1} + \mu_i^{j+1} \right) \left[\left(u_{i+\frac{1}{2}}^j - u_{i+\frac{1}{2}}^{j+1} \right) / \delta y + \left(v_{i+1}^{j+\frac{1}{2}} - v_i^{j+\frac{1}{2}} \right) / \delta x \right], \end{aligned} \quad (3.7)$$

where μ and λ are the coefficients of shear and bulk viscosity and are stored at the cell center.

Substituting the appropriate expansions about the point $(i+\frac{1}{2}, j, n)$ into Eq. (3.4), we obtain

$$\begin{aligned} \frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho uv}{\partial y} + \frac{\partial p}{\partial x} - \frac{\partial \sigma_{xx}}{\partial x} - \frac{\partial \sigma_{xy}}{\partial y} &= FD(\rho u) \\ &\quad + \frac{\delta t}{2} \left\{ \rho \left[(2\phi - 1) c^2 - 3u^2 \right] \frac{\partial^2 u}{\partial x^2} - \rho v^2 \frac{\partial^2 u}{\partial y^2} \right\} - \frac{\delta x^2}{2} \left(\frac{\partial \rho u}{\partial x} \right) \frac{\partial^2 u}{\partial x^2} \\ &\quad - \frac{\delta y^2}{4} \left(\frac{\partial \rho v}{\partial y} \right) \frac{\partial^2 u}{\partial y^2} + \text{o.t.e.}, \end{aligned} \quad (3.8)$$

where we have neglected the low order diffusional errors that arise from the spatial variation of the viscosity coefficients since these are generally small compared to the diffusional terms retained. For stability, we consider only u diffusion, since subtraction of the mass conservation equation from the left hand side of Eq. (3.8) removes the density time derivative.

An equation similar to Eq. (3.8) is derived for the y-direction momentum by expanding $FD(\rho v)$ about the point $(i, j+\frac{1}{2}, n)$:

$$\begin{aligned} \frac{\partial \rho v}{\partial t} + \frac{\partial \rho u v}{\partial x} + \frac{\partial \rho v^2}{\partial y} + \frac{\partial p}{\partial y} - \frac{\partial \sigma_{xy}}{\partial x} - \frac{\partial \sigma_{yy}}{\partial y} = FD(\rho v) \\ + \frac{\delta t}{2} \left\{ -\rho u^2 \frac{\partial^2 v}{\partial x^2} + \rho \left[(2\phi - 1) c^2 - 3v^2 \right] \frac{\partial^2 v}{\partial y^2} \right\} \\ - \frac{\delta x^2}{4} \left(\frac{\partial \rho u}{\partial x} \right) \frac{\partial^2 v}{\partial x^2} - \frac{\delta y^2}{2} \left(\frac{\partial \rho v}{\partial y} \right) \frac{\partial^2 v}{\partial y^2} + o.t.e \end{aligned} \quad (3.9)$$

In the absence of enthalpy diffusion and chemistry, the finite difference equation for the internal energy density, ρI , is

$$\begin{aligned} FD(\rho I) = \left[\rho I_{i+1}^j - \rho I_i^j \right] / \delta t + \left[\rho I_{i+\frac{1}{2}}^j \left(\rho I_{i+1}^j \right. \right. \\ \left. \left. + \rho I_{i+1}^j \right) - \rho I_{i-\frac{1}{2}}^j \left(\rho I_i^j + \rho I_{i-1}^j \right) \right] / 2\delta x \\ + \left[\rho I_{i+1}^{j+\frac{1}{2}} \left(\rho I_i^j + \rho I_{i+1}^{j+1} \right) - \rho I_{i+1}^{j-\frac{1}{2}} \left(\rho I_i^j \right. \right. \\ \left. \left. + \rho I_{i+1}^{j-1} \right) \right] / 2\delta y + \left[\bar{p}_i^j - \left(\sigma_{xx} \right)_i^j \right] \left[\left(\rho I_{i+\frac{1}{2}}^j \right. \right. \right. \\ \left. \left. - \rho I_{i-\frac{1}{2}}^j \right) / \delta x \right] + \left[\bar{p}_i^j - \left(\sigma_{yy} \right)_i^j \right] \left[\left(\rho I_{i+1}^{j+\frac{1}{2}} \right. \right. \right. \\ \left. \left. - \rho I_{i+1}^{j-\frac{1}{2}} \right) / \delta y \right] - \left(\sigma_{xy} \right)_i^j \left[\left(\rho I_{i+\frac{1}{2}}^{j+1} \right. \right. \right. \\ \left. \left. + \rho I_{i-\frac{1}{2}}^{j+1} - \rho I_{i+\frac{1}{2}}^{j-1} - \rho I_{i-\frac{1}{2}}^{j-1} \right) / 4\delta y \right] \\ + \left(\rho I_{i+1}^{j+\frac{1}{2}} + \rho I_{i+1}^{j-\frac{1}{2}} - \rho I_{i-1}^{j+\frac{1}{2}} - \rho I_{i-1}^{j-\frac{1}{2}} \right) \\ \left. / 4\delta x \right] - \left[k_{i+\frac{1}{2}}^j \left(I_{i+1}^j - I_i^j \right) - k_{i-\frac{1}{2}}^j \left(I_i^j \right. \right. \\ \left. \left. - I_{i-1}^j \right) \right] / \delta x^2 - \left[k_{i+\frac{1}{2}}^{j+\frac{1}{2}} \left(I_{i+1}^{j+1} - I_i^j \right) \right. \\ \left. - k_{i-\frac{1}{2}}^{j-\frac{1}{2}} \left(I_i^j - I_{i-1}^{j-1} \right) \right] / \delta y^2, \end{aligned} \quad (3.10)$$

where k is related to the thermal conductivity coefficient and is stored at the cell center. The solution for ρI_i^j is purely explicit using the time advanced density and velocity fields.

A Taylor series expansion of Eq. (3.10) about the point (i, j, n) yields

$$\begin{aligned} \frac{\partial \rho I}{\partial t} + \frac{\partial \rho u I}{\partial x} + \frac{\partial \rho v I}{\partial y} + \left(p - \sigma_{xx} \right) \frac{\partial u}{\partial x} + \left(p - \sigma_{yy} \right) \frac{\partial v}{\partial y} \\ - \sigma_{xy} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) - \frac{\partial}{\partial x} \left(k \frac{\partial I}{\partial x} \right) - \frac{\partial}{\partial y} \left(k \frac{\partial I}{\partial y} \right) = FD(\rho I) \\ + \frac{\delta t}{2} \left(-\rho u^2 \frac{\partial^2 I}{\partial x^2} - \rho v^2 \frac{\partial^2 I}{\partial y^2} \right) - \frac{\delta x^2}{4} \left(\rho \frac{\partial u}{\partial x} \right. \\ \left. + 2u \frac{\partial \rho}{\partial x} \right) \frac{\partial^2 I}{\partial x^2} - \frac{\delta y^2}{4} \left(\rho \frac{\partial v}{\partial y} + 2v \frac{\partial \rho}{\partial y} \right) \frac{\partial^2 I}{\partial y^2} \\ + o.t.e., \end{aligned} \quad (3.11)$$

where analogous to the treatment of the variations in viscosity coefficients in Eq. (3.8), we have neglected the low order diffusional errors that arise from the spatial variation of the coefficient k .

The finite difference approximation to the species transport equation neglecting molecular diffusion is

$$\begin{aligned} FD(\rho_\alpha) = \left[\rho_\alpha^j_{i+1} - \rho_\alpha^j_i \right] / \delta t + \left\{ \left[\rho_\alpha^j_i \right. \right. \\ \left. \left. + \rho_\alpha^j_{i+1} \right] \rho_{i+\frac{1}{2}}^j - \left[\rho_\alpha^j_{i+1} - \rho_\alpha^j_i \right] \right. \\ \left. \left(\rho_{i+\frac{1}{2}}^j \right)^2 \delta t / \delta x - \left[\rho_\alpha^j_i + \rho_\alpha^j_{i-1} \right] \right. \\ \left. \rho_{i-\frac{1}{2}}^j + \left[\rho_\alpha^j_i - \rho_\alpha^j_{i-1} \right] \left(\rho_{i-\frac{1}{2}}^j \right)^2 \right. \\ \left. \delta t / \delta x \right\} / 2\delta x + \left\{ \left[\rho_\alpha^j_i + \rho_\alpha^j_{i+1} \right] \rho_{i+1}^{j+\frac{1}{2}} \right. \\ \left. - \left[\rho_\alpha^j_{i+1} - \rho_\alpha^j_i \right] \left(\rho_{i+1}^{j+\frac{1}{2}} \right)^2 \delta t / \delta y \right. \\ \left. - \left[\rho_\alpha^j_i + \rho_\alpha^j_{i-1} \right] \rho_{i+1}^{j-\frac{1}{2}} + \left[\rho_\alpha^j_i \right. \right. \\ \left. \left. - \rho_\alpha^j_{i-1} \right] \left(\rho_{i+1}^{j-\frac{1}{2}} \right)^2 \delta t / \delta y \right\} / 2\delta y. \end{aligned} \quad (3.12)$$

Here, the subscript α refers to the species α and the solution for $\rho_\alpha^j_i$, just as in the preceding case for the internal energy, is purely explicit. Taylor series expansions for this equation result in

$$\begin{aligned} \frac{\partial \rho_\alpha}{\partial t} + \frac{\partial \rho_\alpha u}{\partial x} + \frac{\partial \rho_\alpha v}{\partial y} = FD(\rho_\alpha) - \frac{\delta x^2}{4} \frac{\partial u}{\partial x} \frac{\partial^2 \rho_\alpha}{\partial x^2} \\ - \frac{\delta y^2}{4} \frac{\partial v}{\partial y} \frac{\partial^2 \rho_\alpha}{\partial y^2} + o.t.e. \end{aligned} \quad (3.13)$$

Because of the time-centering of the convection terms in Eq. (3.12), the lowest time error is of second order and is not specified here because it is usually negligible in comparison to the spatial errors.

B. Stabilization of the RICE Equations

The scheme for stabilizing the RICE equations is presented here in detail. For each equation the conditions $(A+\epsilon_x) \geq 0$ and $(B+\epsilon_y) \geq 0$ are satisfied by choosing A and B according to

$$A = \begin{cases} -(1 - \xi)\epsilon_x & \epsilon_x \geq 0 \\ -(1 + \xi)\epsilon_x & \epsilon_x < 0 \end{cases} \quad (3.14)$$

$$B = \begin{cases} -(1 - \xi)\epsilon_y & \epsilon_y \geq 0 \\ -(1 + \xi)\epsilon_y & \epsilon_y < 0 \end{cases} \quad (3.15)$$

where ϵ_x and ϵ_y are approximated by the low order truncation error diffusion coefficients for the x and y directions and B is the y-counterpart of A. The ϵ 's are calculated as $\epsilon = \text{FD}(\epsilon)$ consistent with our finite difference approximations. The parameter ξ has the range $0 \leq \xi \leq 1$ and is used to control the amount of effective diffusion after the low order diffusional truncation errors are exactly cancelled.

The additional terms to be added to the finite difference equations presented in Sec. IIIA are summarized as follows.

1. Mass equation.

The coefficients ϵ_x and ϵ_y are given by

$$\epsilon_{x_{i+\frac{1}{2}}}^j = (2\theta - 1) \delta t / 2 \left\{ \left(u_{i+\frac{1}{2}}^j \right)^2 + 1/2 \left[\left(c^2 \right)_{i+1}^j + \left(c^2 \right)_i^j \right] \right\} - \left(u_{i+3/2}^j - u_{i-\frac{1}{2}}^j \right) \delta x / 8 \quad (3.16)$$

$$\epsilon_{y_i}^{j+\frac{1}{2}} = (2\theta - 1) \delta t / 2 \left\{ \left(v_i^{j+\frac{1}{2}} \right)^2 + 1/2 \left[\left(c^2 \right)_i^j + \left(c^2 \right)_i^{j+1} \right] \right\} - \left(v_i^{j+3/2} - v_i^{j-\frac{1}{2}} \right) \delta x / 8 \quad (3.17)$$

The equation to be solved for the mass density is

$$\text{FD}(\rho) = \left[A_{i+\frac{1}{2}}^j \left(\rho_{i+1}^j - \rho_i^j \right) - A_{i-\frac{1}{2}}^j \left(\rho_i^j - \rho_{i-1}^j \right) \right] / \delta x^2 - \left[B_i^{j+\frac{1}{2}} \left(\rho_i^{j+1} - \rho_i^j \right) - B_i^{j-\frac{1}{2}} \left(\rho_i^j - \rho_i^{j-1} \right) \right] / \delta y^2 = 0 \quad (3.18)$$

where $\text{FD}(\rho)$ is given by Eq. (3.1), and the coefficients A and B are determined by using Eqs. (3.16) and (3.17) in Eqs. (3.14) and (3.15).

2. Momentum equations.

For the x-component, we have

$$\epsilon_{x_{i+\frac{1}{2}}}^j = \rho_{i+1}^j \left\{ (2\theta - 1) \left(c^2 \right)_{i+1}^j - 3 \left(u_{i+3/2}^j + u_{i+\frac{1}{2}}^j \right)^2 / 4 \delta t / 2 - \left(\rho u_{i+3/2}^j - \rho u_{i+\frac{1}{2}}^j \right) \delta x / 2 \right\} \quad (3.19)$$

$$\epsilon_{y_{i+\frac{1}{2}}}^{j+\frac{1}{2}} = - \left(\rho_i^j + \rho_{i+1}^j + \rho_{i+1}^{j+1} + \rho_i^{j+1} \right) \left(v_i^{j+\frac{1}{2}} + v_{i+\frac{1}{2}}^{j+\frac{1}{2}} \right)^2 \delta t / 32 - \left(\rho v_i^{j+3/2} + \rho v_{i+1}^{j+3/2} - \rho v_i^{j-\frac{1}{2}} - \rho v_{i+1}^{j-\frac{1}{2}} \right) \delta y / 16 \quad (3.20)$$

The x-component of the momentum density is calculated from

$$\text{FD}(\rho u) = \left\{ \left[A_{i+1}^j + (A')_{i+1}^j \right] \left(u_{i+3/2}^j - u_{i+\frac{1}{2}}^j \right) - \left[A_i^j + (A')_i^j \right] \left(u_{i+\frac{1}{2}}^j - u_{i-\frac{1}{2}}^j \right) \right\} / \delta x^2 + \left[B_{i+\frac{1}{2}}^{j+\frac{1}{2}} \left(u_{i+\frac{1}{2}}^{j+1} - u_{i+\frac{1}{2}}^j \right) - B_{i+\frac{1}{2}}^{j-\frac{1}{2}} \left(u_{i+\frac{1}{2}}^j - u_{i+\frac{1}{2}}^{j-1} \right) \right] / \delta y^2 = 0 \quad (3.21)$$

in which $\text{FD}(\rho u)$ is given by Eq. (3.4). In this equation, $\frac{\partial A}{\partial x}$ itself leads to diffusion of u velocity and hence, $A' \neq 0$ as described in Section II. A' is determined from an integral analogous to Eq. (2.13). The integrand is

$$\left(\frac{\partial A}{\partial x} \right)_D \left(\frac{\partial u}{\partial x} \right) = - (1 \pm \xi) \frac{\partial}{\partial x} \left[\rho \left(\frac{\partial u}{\partial x} \right)^2 \right] \frac{\delta x^2}{4} \quad (3.22)$$

where the choice of algebraic signs is governed by Eq. (3.14). The solution for A' yields

$$A' = (1 \pm \xi) \left(\frac{\partial u}{\partial x} \right) \rho \frac{\delta x^2}{4} . \quad (3.23)$$

Similar to the computation of ϵ_x , A' is computed as

$$(A')_i^j = - (1 \pm \xi) \left(u_{i+1/2}^j - u_{i-1/2}^j \right) \rho_i^j \frac{\delta x}{4} \quad (3.24)$$

For the y-component, we have

$$\begin{aligned} \epsilon_{x_{i+1/2}}^{j+1/2} = & - \left(\rho_i^j + \rho_{i+1}^j + \rho_{i+1}^{j+1} + \rho_i^{j+1} \right) \left(u_{i+1/2}^j \right. \\ & \left. + u_{i+1/2}^{j+1} \right)^2 \delta t / 32 - \left(\rho u_{i+3/2}^j + \rho u_{i+3/2}^{j+1} \right. \\ & \left. - \rho u_{i-1/2}^j - \rho u_{i-1/2}^{j+1} \right) \delta x / 16, \end{aligned} \quad (3.25)$$

$$\begin{aligned} \epsilon_{y_i}^{j+1} = & \rho_i^{j+1} \left[(2\phi - 1) (c^2)_i^{j+1} - 3 \left(v_i^{j+1/2} \right. \right. \\ & \left. \left. + v_i^{j+3/2} \right)^2 / 4 \right] \delta t / 2 - \left(\rho v_i^{j+3/2} \right. \\ & \left. - \rho v_i^{j+1/2} \right) \delta y / 2 . \end{aligned} \quad (3.26)$$

The y-component of the momentum density is calculated from

$$\begin{aligned} FD(\rho v) = & \left[A_{i+1/2}^{j+1/2} \left(v_{i+1}^{j+1/2} - v_i^{j+1/2} \right) - A_{i-1/2}^{j+1/2} \left(v_i^{j+1/2} \right. \right. \\ & \left. \left. - v_{i-1}^{j+1/2} \right) \right] / \delta x^2 - \left\{ \left[B_i^{j+1} + (B')_i^{j+1} \right] \left(v_i^{j+3/2} \right. \right. \\ & \left. \left. - v_{i-1}^{j+1/2} \right) - \left[B_i^j + (B')_i^j \right] \left(v_i^{j+1/2} - v_{i-1}^{j-1/2} \right) \right\} \\ & / \delta y^2 = 0 , \end{aligned} \quad (3.27)$$

where analogous to Eq. (3.21), $B' \neq 0$. Similar to the expression for A' , B' is computed as

$$(B')_i^j = - (1 \pm \xi) \left(v_i^{j+1/2} - v_i^{j-1/2} \right) \rho_i^j \frac{\delta y}{4} , \quad (3.28)$$

and the algebraic sign choice is governed by Eq. (3.15).

3. Specific internal energy equation.

The expressions for ϵ_x and ϵ_y are

$$\begin{aligned} \epsilon_{x_{i+1/2}}^j = & - \left(u_{i+1/2}^j \right)^2 \left(\rho_i^j + \rho_{i+1}^j \right) \delta t / 4 - \left[\left(\rho_i^j \right. \right. \\ & \left. \left. + \rho_{i+1}^j \right) \left(u_{i+3/2}^j - u_{i-1/2}^j \right) / 8 + u_{i+1/2}^j \left(\rho_{i+1}^j \right. \right. \\ & \left. \left. - \rho_i^j \right) \right] \delta x / 2 , \end{aligned} \quad (3.29)$$

$$\begin{aligned} \epsilon_{y_i}^{j+1/2} = & - \left(v_i^{j+1/2} \right)^2 \left(\rho_i^j + \rho_i^{j+1} \right) \delta t / 4 - \left[\left(\rho_i^j \right. \right. \\ & \left. \left. + \rho_i^{j+1} \right) \left(v_i^{j+3/2} - v_i^{j-1/2} \right) / 8 + v_i^{j+1/2} \left(\rho_i^{j+1} \right. \right. \\ & \left. \left. - \rho_i^j \right) \right] \delta y / 2 , \end{aligned} \quad (3.30)$$

and the finite difference equation for ρI is

$$\begin{aligned} FD(\rho I) = & \left[A_{i+1/2}^j \left(I_{i+1}^j - I_i^j \right) - A_{i-1/2}^j \left(I_i^j - I_{i-1}^j \right) \right] \\ & / \delta x^2 - \left[B_i^{j+1/2} \left(I_i^{j+1} - I_i^j \right) - B_i^{j-1/2} \left(I_i^j \right. \right. \\ & \left. \left. - I_{i-1}^{j-1} \right) \right] / \delta y^2 = 0 , \end{aligned} \quad (3.31)$$

where $FD(\rho I)$ is given by Eq. (3.10).

4. Species transport equation.

The species transport equation spatial diffusion terms are given in Eq. (3.13) and are computed as

$$\epsilon_{x_{i+1/2}}^j = - \left(n+1 u_{i+3/2}^j - n+1 u_{i-1/2}^j \right) \delta x / 8 , \quad (3.32)$$

$$\epsilon_{y_i}^{j+1/2} = - \left(n+1 v_i^{j+3/2} - n+1 v_i^{j-1/2} \right) \delta y / 8 , \quad (3.33)$$

The finite difference equation to be solved for the species density is

$$\begin{aligned} FD(\rho_\alpha) = & \left\{ A_{i+1/2}^j \left[(\rho_\alpha)_i^j - (\rho_\alpha)_{i+1}^j \right] - A_{i-1/2}^j \left[(\rho_\alpha)_i^j \right. \right. \\ & \left. \left. - (\rho_\alpha)_{i-1}^j \right] \right\} / \delta x^2 - \left\{ B_i^{j+1/2} \left[(\rho_\alpha)_i^{j+1} \right. \right. \\ & \left. \left. - (\rho_\alpha)_i^j \right] - B_i^{j-1/2} \left[(\rho_\alpha)_i^j - (\rho_\alpha)_i^{j-1} \right] \right\} / \delta y^2 \\ & = 0 , \end{aligned} \quad (3.34)$$

where $FD(\rho_\alpha)$ is given by Eq. (3.12).

IV. DIFFUSIONAL LIMITS

In this section the diffusional limits imposed on the time step are established for the TEC method. The method usually allows a larger time step than typical artificial viscosity schemes and the reasons for this are discussed.

The effective diffusion coefficients introduced into the conservation equations after the low order, diffusional truncation errors are exactly cancelled are

$$A_{\text{eff}} = \xi |\epsilon_x| \quad \text{and} \quad B_{\text{eff}} = \xi |\epsilon_y|, \quad (4.1)$$

according to Eqs. (3.14) and (3.15). The diffusion terms added for numerical stability are computed explicitly in Sec. IIIB for each conservation equation so that a Fourier analysis yields the requirement

$$\delta t < \frac{(1/2)\delta x^2 \delta y^2}{(\xi/\rho) [|\epsilon_y| \delta x^2 + |\epsilon_x| \delta y^2]}, \quad (4.2)$$

in the absence of transport effects. A typical artificial viscosity scheme requires

$$\delta t < \frac{(1/2)\delta x^2 \delta y^2}{(4\mu/3\rho) [3\delta x^2/4 + \delta y^2]}, \quad (4.3)$$

for the momentum equation, in which $\lambda = -2/3\mu$.

The TEC method usually allows a larger time step than the artificial viscosity scheme because the effective diffusion is less. The TEC method applies diffusion according to the local needs rather than uniformly in an amount sufficient to counter the largest destabilizing truncation errors in the flow.

A further increase in time step can be achieved for flows directed primarily in one coordinate direction because of the independence of ϵ_x and ϵ_y .

For example, a flow directed in the x-direction with $\delta x = \delta y$ would have $\epsilon_y \ll \epsilon_x$ and would only require

$$\delta t < \frac{(1/2)\delta x^2}{(\xi/\rho) |\epsilon_x|},$$

from Eq. (4.2) as compared to

$$\delta t < \frac{(4/7)(1/2)\delta x^2}{(4\mu/3\rho)},$$

from Eq. (4.3) for an artificial viscosity scheme. With equivalent diffusion coefficients, the TEC method would allow a 75% increase in δt for this

simple example.

V. NUMERICAL EXAMPLES

In this section we present the solutions to two fluid dynamics problems to show the accuracy of the TEC method in comparison with an artificial viscosity technique for stabilizing the calculations. For the first example, we calculate a problem with known solution, the channel flow problem shown schematically in Fig. 2. A perfect gas, with specific heat ratio $\gamma = 1.4$, enters on the left with the piecewise-linear velocity profile shown which ranges from $u = 1.0$ at the free-slip, adiabatic walls to $u = .2$ at the center. The inflow density and specific internal energy are constant at 1.0 and .018 in non-dimensional units. The right boundary is a continuous outflow boundary. The computational mesh consists of 31 columns and 9 rows of cells with $\delta x = \delta y = 1$. The time step is $\delta t = 0.2$. Initially we set $u = 1.0$, $v = 0.$, $\rho = 1.0$, and $I = .018$ in the channel.

Figure 2. Schematic of the channel flow problem.

The exact solution has no x-dependence at steady state so that at any position x the solution corresponds to the inflow conditions. The computed steady state velocity fields and contours of Mach number, M , are shown in Figs. 3a and 3b. Figure 3a shows the results obtained with the TEC method. Figure 3b shows the results obtained with artificial viscosity. These latter results were obtained by solving the Navier-Stokes equations with $\mu/\rho = \lambda/\rho = .1$ and $k = 2.5 \mu/\rho$ where μ and λ are the shear and bulk viscosities used in Eq. (3.7) and k is the thermal conductivity. These values are essentially the minima necessary for stability and are compared to a choice of μ , λ , and $k = 0$ for the TEC method. For both calculations, the continuity equation was stabilized using the truncation error approach.

$H = 9.16, L = 2.79, \text{Interval} = 0.80$

Contours of Mach Number M

(3a)

$H = 9.22, L = 2.80, \text{Interval} = 0.80$

Contours of Mach Number M

(3b)

Figure 3. Comparison of results obtained by the TEC method (a) with results obtained by an artificial viscosity method (b). The figure shows the velocity fields with the vector lengths proportional to the speed (upper) and contours of Mach number, M , (lower). The maximum contour lines are labeled with an H and the minimum contour lines with an L .

The stabilization of the equations in this example and in the one following, was accomplished with $\xi = 1.0$. This choice for ξ has proven satisfactory in a wide variety of applications and does not lead to excessive enhancement of the dispersion errors since A and B are always ≥ 0 .

The velocity field and Mach number distribution in Fig. 3a correspond everywhere to the inflow conditions to within less than 0.2% and less than 0.4% respectively. In Fig. 3b the velocity field is accelerated along the centerline and decelerated near the boundaries as a consequence of the viscosity acting in the transverse direction. Since the diffusional truncation errors in the y -direction are very small compared to those in the x -direction, the use of μ to diffuse u in the y -direction results in very excessive diffusion.

For a more comprehensive illustration of the method, we consider a flow problem associated with continuous flow chemical lasers. The intent here is to show the enhanced detail that can be achieved and still retain a stable solution. As in the previous example, this problem is also solved by an artificial viscosity method for comparison.

The flow configuration is shown schematically in Fig. 4. The lower fluorine nozzle admits F , He , and DF into the lasing cavity at Mach 3.5 while the upper hydrogen nozzle admits H_2 and He at Mach 3.7.

The hydrogen and fluorine mix and react exothermally to produce vibrationally excited HF molecules, which serve as the lasing medium. The calculation begins at the nozzle exit plane and extends downstream. The upper and lower boundaries of the computing region are symmetry boundaries. The right boundary is a continuous outflow boundary.

Figure 4. Fluorine and hydrogen nozzle configuration and computing region.

The distributions of velocity, density, and specific internal energy at the exit plane of the fluorine and hydrogen nozzles are shown in Fig. 5.

Figure 5. Boundary layer profiles at the exit plane of the fluorine and hydrogen nozzles.

The coordinates (a) and (b) refer to the centerline and wall of the fluorine nozzle while the coordinates (c) and (d) refer to the wall and splitter boundary for the hydrogen nozzle. These exit plane distributions furnish the input values for the calculations when scaled by $\rho_0 = 10^{-5} \text{ g/cm}^3$, $u_0 = 10^5 \text{ cm/sec}$, and $I_0 = 239 \text{ cal/g}$. The computational mesh consists of 29 columns and 30 rows of cells with $\delta x = .075$ and $\delta y = .0331$. The time steps for the two calculations are $\delta t = .004$ and $\delta t = .002$. The smaller time step is used in the artificial viscosity calculation to reduce the amount of viscosity necessary for stability.

For the artificial viscosity calculation, the mixture continuity and species transport equations are stabilized by canceling their low order, diffusional truncation errors. The momentum and energy equations, which include the full viscous stress tensor, are stabilized through the viscosity and thermal conductivity. For this purpose we set $\mu/\rho = \lambda/\rho = .01$ and $k = 3\mu/\rho$. These values are essentially the minima necessary for stability.

The steady state solutions are shown in Fig. 6. The results obtained with the TEC method are shown in Fig. 6a for zero physical viscosity and thermal conductivity. The results obtained with artificial viscosity are shown in Fig. 6b.

$H = 2.72, L = 0.53, \text{ Interval} = 0.27$

Contours of I/I_0

(6a)

$H = 1.69, L = 0.48, \text{ Interval} = 0.15$

Contours of I/I_0

(6b)

Figure 6. Comparison of results obtained by the TEC method (a) with results obtained by an artificial viscosity method (b). The figure shows the velocity fields with the vector lengths proportional to the speed (upper) and contours of specific internal energy, I , (lower). The maximum contour lines are labeled with an H and the minimum contour lines with an L .

The figure shows the velocity fields with the vector lengths proportional to the speed, and contours of specific internal energy. The maximum contour lines are designated with an H and the minimum contour lines with an L . The values of H , L , and the interval between contour lines are given below each contour plot.

The velocity fields obtained in the two calculations are much different. The inflow velocity profiles are rapidly smoothed in (b) but retained in (a). This is because the transverse gradients, in particular $\partial u/\partial y$, are smoothed by the large diffusion coefficient, μ , in (b) as compared to the small diffusion coefficient, $B = -(1 \pm \xi)(\rho v^2 \delta t/2 + (\partial \rho v/\partial y)\delta y^2/4)$, in (a). The much higher flow speeds in (a) result from the lack of kinetic energy dissipation by the artificial viscosity. In (a), a

twin vortex can be seen in the wake region separating the fluorine and hydrogen nozzles. The vortex residing in the upper left corner for both calculations has been enhanced in (a). A shock has appeared in the upper right corner in (a), as a result of the collision of the hydrogen stream with the upper symmetry boundary.

The contours of specific internal energy are considerably different. The maximum values of I/I_0 reside in the wake region between the hydrogen and fluorine nozzles for both calculations. The maximum value in (a) is greater than in (b) due to the enhanced mixing of reactants by the twin vortex and consequent heat release from the chemical reaction. The steeper gradients in (a) reflect the absence of thermal conductivity. Downstream in (a), the high values of I/I_0 reside in the region where the

exothermic chemical reaction is occurring. This structure of the reaction zone is lost in (b) due to the viscous dissipation. This is clearly shown in Fig. 7.

Figure 7. Distributions of specific internal energy at $x = 4.7h$ downstream of the nozzle exit plane. The dashed curve is a result of the artificial viscosity calculation. The two solid curves are results obtained by the TEC method. The curve labeled inviscid corresponds to the results presented in Fig. 6a for zero physical viscosity and thermal conductivity. The curve labeled $Re_h = 1000$ shows the sensitivity of I to the physical viscosity.

Figure 7 shows distributions of specific internal energy at $x = 4.7h$ downstream of the nozzle exit plane. The length scale h is the half-width of the fluorine nozzle.

The dashed curve is a result of the artificial viscosity calculation. The two solid curves are results obtained with the TEC method. The curve labeled inviscid corresponds to the results presented in Fig. 6a. The additional curve corresponds to a Reynolds number of 1000 based on the fluorine nozzle half-width and core-flow conditions. This curve shows the sensitivity of the specific internal energy to the physical viscosity. The

enhanced detail in these curves, particularly in the region of chemical reaction, is apparent. This detail is lost in the artificial viscosity calculation due to the excessive kinetic energy dissipation.

VII. SUMMARY

A method of general applicability has been described for stabilizing Eulerian fluid dynamics calculations. It produces a significant increase in accuracy and, in many instances, allows for a larger computational time step over methods using an artificial viscosity scheme to achieve stability. The essence of the method is the local cancellation of the diffusional truncation errors arising from the finite difference equations. The applicability of the method has been demonstrated by applying it in the RICE code, which calculates the transient, two-dimensional flows of chemically reacting mixtures. The effectiveness of the method is demonstrated in the results of two numerical examples.

REFERENCES

1. R. D. Richtmeyer and K. W. Morton, "Difference Methods for Initial Value Problems," 2nd edition, Interscience, New York, 1967.
2. C. W. Hirt, J. Comp. Phys. 2, 339 (1968).
3. O. A. Farmer, T. D. Butler, W. C. Rivard, Los Alamos Scientific Laboratory Report (To be published).
4. F. H. Harlow and A. A. Amsden, J. Comp. Phys. 8, 197 (1971).

APPENDIX A

DERIVATION OF THE TEC METHOD

A more comprehensive derivation of the method is given here to show specifically the implications of the simple derivation presented in Sec. II. We begin with Eq. (2.2) which is

$$DE(\rho) = FD(\rho) + \epsilon \frac{\partial^2 \rho}{\partial x^2} + \text{o.t.e.} \quad (\text{A-1})$$

The stability of $FD(\rho) = 0$ depends upon the algebraic sign of ϵ . To insure a positive diffusion coefficient which is necessary for stability, we introduce into Eq. (A-1) the diffusive term

$$FD\left(A \frac{\partial^2 \rho}{\partial x^2}\right) = A \frac{\partial^2 \rho}{\partial x^2} + \epsilon_1 \frac{\partial^2 \rho}{\partial x^2} + \text{o.t.e.}, \quad (\text{A-2})$$

where $FD(A\partial^2\rho/\partial x^2)$ is the finite difference approximation of $A\partial^2\rho/\partial x^2$, A is a diffusion coefficient to be defined later, and the truncation errors are denoted by $\epsilon_1\partial^2\rho/\partial x^2$ for the diffusive errors and o.t.e. for the others. The value of ϵ_1 depends upon the form of the finite difference approximation of $A\partial^2\rho/\partial x^2$. For $FD(A\partial^2\rho/\partial x^2) = A_1 (\rho_{i+1} - 2\rho_i + \rho_{i-1})/\delta x^2$, ϵ_1 would be zero; whereas for $FD(A\partial^2\rho/\partial x^2) = \frac{1}{2}(A_{i+\frac{1}{2}} + A_{i-\frac{1}{2}}) (\rho_{i+1} - 2\rho_i + \rho_{i-1})/\delta x^2$, ϵ_1 would be equal to $(\partial^2 A/\partial x^2)\delta x^2/8$ + higher order terms. Inclusion of Eq. (A-2) in Eq. (A-1) yields

$$DE(\rho) = FD(\rho) - FD(A\partial^2\rho/\partial x^2) + (A + \epsilon + \epsilon_1) \partial^2\rho/\partial x^2 + \text{o.t.e.} \quad (\text{A-3})$$

The coefficient A is chosen such that $A + \epsilon + \epsilon_1 > 0$ in accord with Hirt's theory since we solve

$$FD(\rho) = FD(A\partial^2\rho/\partial x^2), \quad (\text{A-4})$$

in place of $FD(\rho) = 0$. Negative values of $(\epsilon + \epsilon_1)$, which are a source of instability, are countered with a positive value of A . Positive values of $(\epsilon + \epsilon_1)$ are stabilizing and are reduced by inclusion of a negative value of A .

Equation (A-4) is a non-conservative difference equation. It can be replaced with a conservative equation as follows. Equation (A-3) is written as

$$\begin{aligned} DE(\rho) &= FD(\rho) - FD\left\{\left[\frac{\partial(A + A')}{\partial x}\right] \frac{\partial\rho}{\partial x}\right\} \\ &+ FD\left\{\left(\frac{\partial A}{\partial x}\right) \left(\frac{\partial\rho}{\partial x}\right) + \frac{\partial(A'\partial\rho/\partial x)}{\partial x}\right\} \\ &+ (A + \epsilon + \epsilon_1) \partial^2\rho/\partial x^2 \\ &+ \text{o.t.e.}, \end{aligned} \quad (\text{A-5})$$

by adding and subtracting $FD\left\{\left(\frac{\partial A}{\partial x}\right) \left(\frac{\partial\rho}{\partial x}\right) + \frac{\partial(A'\partial\rho/\partial x)}{\partial x}\right\}$ where A' is determined such that

$$FD\left\{\left(\frac{\partial A}{\partial x}\right) \left(\frac{\partial\rho}{\partial x}\right) + \frac{\partial(A'\partial\rho/\partial x)}{\partial x}\right\} = \text{o.t.e.} \quad (\text{A-6})$$

We can write Eq. (A-6) as a differential equation

$$\begin{aligned} \left(\frac{\partial A}{\partial x}\right) \left(\frac{\partial\rho}{\partial x}\right) + \frac{\partial(A'\partial\rho/\partial x)}{\partial x} \\ + (\epsilon_2 + \epsilon_3) \partial^2\rho/\partial x^2 = 0, \end{aligned} \quad (\text{A-7})$$

by noting that

$$\begin{aligned} FD\left\{\left(\frac{\partial A}{\partial x}\right) \left(\frac{\partial\rho}{\partial x}\right)\right\} &= \left(\frac{\partial A}{\partial x}\right) \left(\frac{\partial\rho}{\partial x}\right) + \epsilon_2 \partial^2\rho/\partial x^2 \\ &+ \text{o.t.e.}, \end{aligned} \quad (\text{A-8})$$

and

$$\begin{aligned} FD\left\{\frac{\partial(A'\partial\rho/\partial x)}{\partial x}\right\} &= \frac{\partial(A'\partial\rho/\partial x)}{\partial x} + \epsilon_3 \partial^2\rho/\partial x^2 \\ &+ \text{o.t.e.}, \end{aligned}$$

where ϵ_2 and ϵ_3 are the coefficients of diffusion arising from truncation errors. These coefficients generally involve derivatives of A and A' so that Eq. (A-7) cannot be easily integrated.

We obtain the results given in Sec. II. by neglecting ϵ_1 , ϵ_2 , and ϵ_3 in comparison to ϵ . These diffusion coefficients are higher order than ϵ when A and its derivatives are the order of ϵ . Neglect of ϵ_1 which generally involves derivatives of A times, say δt or δx^2 , results in an algebraic equation for A , i.e., $A + \epsilon > 0$. Neglect of ϵ_2 and ϵ_3 reduces Eq. (A-7) to Eq. (2.11) with solution for A' given by Eq. (2.13).

TRUNCATION ERRORS FOR THE RICE FLOW EQUATIONS

In this appendix a complete list of the low order truncation errors is given for the RICE flow equations neglecting the molecular transport terms. The RICE finite-difference equations are given in Sec. IIIA and are not repeated here. The low order truncation errors including the diffusional errors are as follows.

1. Mass Equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = FD(\rho) + (2\theta - 1) \frac{\delta t}{2} \left\{ (u^2 + v^2) \right.$$

$$\begin{aligned} & \left. \frac{\partial^2 \rho}{\partial x^2} + (v^2 + c^2) \frac{\partial^2 \rho}{\partial y^2} + 4u \frac{\partial \rho}{\partial x} \frac{\partial u}{\partial x} + 2\rho \frac{\partial}{\partial x} \left(u \frac{\partial u}{\partial x} \right) \right. \\ & + \frac{\partial \rho}{\partial x} \frac{\partial c^2}{\partial x} + 2 \frac{\partial^2 \rho u v}{\partial x \partial y} + 4v \frac{\partial \rho}{\partial y} \frac{\partial v}{\partial y} + 2\rho \frac{\partial}{\partial y} \left(v \frac{\partial v}{\partial y} \right) \\ & + \frac{\partial \rho}{\partial y} \frac{\partial c^2}{\partial y} \left. \right\} - \frac{\delta x^2}{24} \left\{ 6 \frac{\partial u}{\partial x} \frac{\partial^2 \rho}{\partial x^2} + 4u \frac{\partial^3 \rho}{\partial x^3} + 3 \frac{\partial \rho}{\partial x} \right. \\ & \left. \frac{\partial^2 u}{\partial x^2} + \rho \frac{\partial^3 u}{\partial x^3} \right\} - \frac{\delta y^2}{24} \left\{ 6 \frac{\partial v}{\partial y} \frac{\partial^2 \rho}{\partial y^2} + 4v \frac{\partial^3 \rho}{\partial y^3} \right. \\ & \left. + 3 \frac{\partial \rho}{\partial y} \frac{\partial^2 v}{\partial y^2} + \rho \frac{\partial^3 v}{\partial y^3} \right\} + o.t.e., \quad (B-1) \end{aligned}$$

where $FD(\rho)$ is given by Eq. (3.1).

2. Momentum Equations

For the x-component, we have

$$\begin{aligned} & \frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho u v}{\partial y} + \frac{\partial p}{\partial x} - \frac{\partial \sigma_{xx}}{\partial x} - \frac{\partial \sigma_{xy}}{\partial y} = FD(\rho u) \\ & + \frac{\delta t}{2} \left\{ \rho \left[(2\theta - 1)c^2 - 3u^2 \right] \frac{\partial^2 u}{\partial x^2} - \rho v^2 \frac{\partial^2 u}{\partial y^2} \right. \\ & + c^2 \left(2 \frac{\partial \rho}{\partial x} \frac{\partial u}{\partial x} + u \frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho v}{\partial x \partial y} \right) + 2 \frac{\partial c^2}{\partial x} \left(\frac{\partial \rho u}{\partial x} \right. \\ & \left. + \frac{\partial \rho v}{\partial y} \right) - 3 \frac{\partial u^2}{\partial x} \frac{\partial \rho u}{\partial x} - u^3 \frac{\partial^2 \rho}{\partial x^2} - 2 \frac{\partial}{\partial x} \left(\frac{\partial \rho u^2 v}{\partial y} \right. \\ & \left. + u \frac{\partial p}{\partial x} \right) - \frac{\partial}{\partial y} \left(v \frac{\partial p}{\partial x} + u \frac{\partial p}{\partial y} \right) - 2 \frac{\partial u}{\partial y} \frac{\partial \rho v^2}{\partial y} \\ & \left. - u \frac{\partial^2 \rho v^2}{\partial y^2} \right\} - \frac{\delta x^2}{24} \left\{ 12 \frac{\partial \rho u}{\partial x} \frac{\partial^2 u}{\partial x^2} + 8\rho u \frac{\partial^3 u}{\partial x^3} \right. \end{aligned}$$

$$\begin{aligned} & + 12 \frac{\partial u^2}{\partial x} \frac{\partial^2 \rho}{\partial x^2} + u^2 \frac{\partial^3 \rho}{\partial x^3} + 24 \frac{\partial \rho}{\partial x} \left(\frac{\partial u}{\partial x} \right)^2 \\ & + 3 \frac{\partial}{\partial y} \left\{ u v \frac{\partial^2 \rho}{\partial x^2} + \rho u \frac{\partial^2 v}{\partial x^2} \right\} + \frac{\partial^3 \rho}{\partial x^3} \left. \right\} \\ & - \frac{\delta y^2}{24} \left\{ 6 \frac{\partial \rho v}{\partial y} \frac{\partial^2 u}{\partial y^2} + 4\rho v \frac{\partial^3 u}{\partial y^3} + 6 \frac{\partial u v}{\partial y} \frac{\partial^2 \rho}{\partial y^2} \right. \\ & + 4u v \frac{\partial^3 \rho}{\partial y^3} + 6 \frac{\partial v}{\partial y} \frac{\partial \rho}{\partial y} \frac{\partial u}{\partial y} + 3 \frac{\partial \rho u}{\partial y} \frac{\partial^2 v}{\partial y^2} + \rho u \frac{\partial^3 v}{\partial y^3} \left. \right\} \\ & + o.t.e. \quad (B-2) \end{aligned}$$

where $FD(\rho u)$ is given by Eq. (3.4).

For the y-component, the appropriate equation is obtained by substituting v and y for u and x respectively in Eq. (B-2).

3. Specific Internal Energy Equation

$$\begin{aligned} & \frac{\partial \rho I}{\partial t} + \frac{\partial \rho u I}{\partial x} + \frac{\partial \rho v I}{\partial y} + (p - \sigma_{xx}) \frac{\partial u}{\partial x} + (p - \sigma_{yy}) \frac{\partial v}{\partial y} + \sigma_{xy} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\ & - \frac{\partial}{\partial x} \left(k \frac{\partial I}{\partial x} \right) - \frac{\partial}{\partial y} \left(k \frac{\partial I}{\partial y} \right) = FD(\rho I) + \frac{\delta t}{2} \left\{ -\rho u^2 \frac{\partial^2 I}{\partial x^2} \right. \\ & - \rho v^2 \frac{\partial^2 I}{\partial y^2} - u \left[2 \frac{\partial I}{\partial x} \frac{\partial \rho u}{\partial x} + I \frac{\partial^2 \rho u}{\partial x^2} \right] + \frac{u \partial}{\partial x} \left[\frac{\partial \rho v I}{\partial y} \right. \\ & + p \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \left. \right] - v \left[2 \frac{\partial I}{\partial y} \frac{\partial \rho v}{\partial y} + I \frac{\partial^2 \rho v}{\partial y^2} \right] \\ & + \frac{v \partial}{\partial y} \left[\frac{\partial \rho u I}{\partial x} + p \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] + \frac{\partial}{\partial t} \left[\gamma \rho I \left(\frac{\partial u}{\partial x} \right. \right. \\ & \left. \left. + \frac{\partial v}{\partial y} \right) \right] - 2c^2 \frac{\partial \rho}{\partial t} \frac{\partial u}{\partial x} - \frac{\partial \rho I}{\partial x} \frac{\partial u}{\partial t} - \frac{\partial \rho I}{\partial y} \frac{\partial v}{\partial t} \\ & - 2\gamma \rho I \frac{\partial}{\partial t} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \left. \right\} - \frac{\delta x^2}{24} \left\{ \left(6\rho \frac{\partial u}{\partial x} + 12u \frac{\partial \rho}{\partial x} \right) \right. \\ & \frac{\partial^2 I}{\partial x^2} + 4\rho u \frac{\partial^3 I}{\partial x^3} + 3 \frac{\partial \rho I}{\partial x} \frac{\partial^2 u}{\partial x^2} + \gamma \rho I \frac{\partial^3 u}{\partial x^3} \\ & + \left(12u \frac{\partial I}{\partial x} + 6I \frac{\partial u}{\partial x} \right) \frac{\partial^2 \rho}{\partial x^2} + 4u I \frac{\partial^3 \rho}{\partial x^3} + 12 \frac{\partial u}{\partial x} \\ & \frac{\partial \rho}{\partial x} \frac{\partial I}{\partial x} \left. \right\} - \frac{\delta y^2}{24} \left\{ \left(6\rho \frac{\partial v}{\partial y} + 12v \frac{\partial \rho}{\partial y} \right) \frac{\partial^2 I}{\partial y^2} \right. \\ & + 4\rho v \frac{\partial^3 I}{\partial y^3} + 3 \frac{\partial \rho I}{\partial y} \frac{\partial^2 v}{\partial y^2} + \gamma \rho I \frac{\partial^3 v}{\partial y^3} + \left(12v \frac{\partial I}{\partial y} \right. \end{aligned}$$

$$+ 6I \frac{\partial v}{\partial y} \left\{ \frac{\partial^2 \rho}{\partial y^2} + 4vI \frac{\partial^3 \rho}{\partial y^3} + 12 \frac{\partial v}{\partial y} \frac{\partial \rho}{\partial y} \frac{\partial I}{\partial y} \right\}$$

$$+ \text{h.o.t.}, \quad (\text{B-3})$$

where $FD(\rho I)$ is given by Eq. (3.10).

4. Species Transport Equations

For species α , we have

$$\begin{aligned} \frac{\partial \rho_\alpha}{\partial t} + \frac{\partial u \rho_\alpha}{\partial x} + \frac{\partial v \rho_\alpha}{\partial y} = FD(\rho_\alpha) + \frac{\delta t}{2} \left[\frac{\partial u}{\partial x} \frac{\partial \rho_\alpha}{\partial t} \right. \\ \left. - \rho_\alpha u \frac{\partial^2 u}{\partial x^2} + \rho_\alpha \frac{\partial^2 u}{\partial x \partial t} + \frac{\partial u}{\partial t} \frac{\partial \rho_\alpha}{\partial x} + u \frac{\partial u}{\partial x} \frac{\partial \rho_\alpha}{\partial x} \right. \end{aligned}$$

$$- u \frac{\partial^2 \rho_\alpha v}{\partial x \partial y} + \frac{\partial v}{\partial y} \frac{\partial \rho_\alpha}{\partial t} - \rho_\alpha v \frac{\partial^2 v}{\partial y^2} + \rho_\alpha \frac{\partial^2 v}{\partial y \partial t}$$

$$+ \frac{\partial v}{\partial t} \frac{\partial \rho_\alpha}{\partial y} + v \frac{\partial v}{\partial y} \frac{\partial \rho_\alpha}{\partial y} - v \frac{\partial^2 \rho_\alpha u}{\partial x \partial y} \left. \right] - \frac{\delta x^2}{24}$$

$$\left[6 \frac{\partial u}{\partial x} \frac{\partial^2 \rho_\alpha}{\partial x^2} + 4u \frac{\partial^3 \rho_\alpha}{\partial x^3} + 3 \frac{\partial \rho_\alpha}{\partial x} \frac{\partial^2 u}{\partial x^2} + \rho_\alpha \frac{\partial^3 u}{\partial x^3} \right]$$

$$- \frac{\delta y^2}{24} \left[6 \frac{\partial v}{\partial y} \frac{\partial^2 \rho_\alpha}{\partial y^2} + 4v \frac{\partial^3 \rho_\alpha}{\partial y^3} + 3 \frac{\partial \rho_\alpha}{\partial y} \frac{\partial^2 v}{\partial y^2} \right.$$

$$\left. + \rho_\alpha \frac{\partial^3 v}{\partial y^3} \right] + \text{h.o.t.}, \quad (\text{B-4})$$

where $FD(\rho_\alpha)$ is given by Eq. (3.12).