FLUX SPLITTING ALGORITHMS FOR TWO-DIMENSIONAL VISCOUS FLOWS WITH FINITE-RATE CHEMISTRY

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ABSTRACT

The Roe flux-difference splitting method has been extended to treat two-dimensional viscous flows with nonequilibrium chemistry. The derivations have avoided unnecessary assumptions or approximations. For spatial discretization, the second-order Roe upwind differencing is used for the convective terms and central differencing for the viscous terms. An upwind-based TVD scheme is applied to eliminate oscillations and obtain a sharp representation of discontinuities. A two-stage Runge-Kutta method is used to time integrate the discretized Navier-Stokes and species transport equations for the asymptotic steady solutions. The present method is then applied to two types of flows: the shock wave/boundary layer interaction problems and the jet in cross flows.

OBJECTIVES

1. To develop a numerical algorithm for real gases which is robust for high Mach number flows and has the ability to accurately capture strong shocks and other types of discontinuities.

2. To include nonequilibrium chemistry in the formulation.

3. To make the formulation consistent and simple.

GOVERNING EQUATIONS

The 2-D, thin layer Navier-Stokes and species equations for a chemically reacting gas of N species:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F(U)}}{\partial x} + \frac{\partial \mathbf{G(U)}}{\partial y} - \frac{\partial \mathbf{W(U, U_y)}}{\partial y} = \mathbf{S},$$

where

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ C_1 \\ C_2 \\ \cdot \\ \cdot \\ C_{N-1} \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(\rho E + p) \\ uC_1 \\ uC_2 \\ \cdot \\ \cdot \\ uC_{N-1} \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(\rho E + p) \\ vC_1 \\ vC_2 \\ \cdot \\ \cdot \\ vC_{N-1} \end{pmatrix},$$

$$\mathbf{W} = \begin{pmatrix} 0 \\ \mu u_y \\ \frac{4}{3}\mu v_y \\ \mu u u_y + \frac{4}{3}\mu v v_y + kT_y - \sum_{i=1}^{N} C_i h_i \tilde{v}_i \\ -C_1 \tilde{v}_1 \\ -C_2 \tilde{v}_2 \\ \cdot \\ \cdot \\ -C_{N-1} \tilde{v}_{N-1} \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ S_1 \\ S_2 \\ \cdot \\ \cdot \\ S_{N-1} \end{pmatrix}.$$

THERMODYNAMIC AND TRANSPORT MODELS

Equation of State

$$p = p(\rho, e, C_1, C_2, ...C_{N-1})$$

$$p = R_u T \sum_{i=1}^{N} \frac{C_i}{W_i}$$

Physical Properties

- Mass diffusion is approximated by Fick's law. Binary mass diffusivity obtained from Chapman-Enskog theory.
- For the individual species: C_p, k, and μ are determined by fourth-order polynomials of temperature.
- For the gas mixture: C_p obtained by mass concentration weighting of each species. k and μ obtained using Wilke's mixing rule.

Chemistry Model of Air

- Five (5) species (O_2, N_2, O, N, NO) and eleven (11) elementary reaction steps.
- Neglecting ionization as well as thermal nonequilibrium.

SOLUTION METHOD

1. Two-stage Runge-Kutta method for time integration of the governing equations.

2. Chemical source terms treated implicitly so that the stiffness associated with the source terms will not upset numerical stability.

3. Second-order upwind differencing for convective terms, central differencing for viscous terms.

4. Upwind-based TVD scheme to eliminate oscillations and to obtain a sharp representation of discontinuities.

UPWIND DIFFERENCING

- Good Property for Capturing Discontinuities.

- Flux-Vector Splittings
  - ✓ Steger-Warming Splitting
  - ✓ Van Leer Splitting

- Flux-Difference Splittings
  - ✓ Roe Splitting
  - Osher Splitting

ROE FLUX-DIFFERENCE SPLITTING

To construct Roe flux-difference splitting, one usually defines an average state $\hat{\mathbf{U}}$ such that

$$\Delta\mathbf{F} = \hat{\mathbf{A}}\Delta\mathbf{U}, \qquad \Delta\mathbf{G} = \hat{\mathbf{B}}\Delta\mathbf{U}, \qquad \Delta(\cdot) = (\cdot)_{\mathbf{R}} - (\cdot)_{\mathbf{L}},$$

$$\hat{\mathbf{A}} = \mathbf{A}(\hat{\mathbf{U}}), \qquad \hat{\mathbf{B}} = \mathbf{B}(\hat{\mathbf{U}}), \qquad \hat{\mathbf{U}} = \hat{\mathbf{U}}(\mathbf{U_L}, \mathbf{U_R})$$

The eigenvalues of the Jacobian A are (for N=5):

$$\lambda(\mathbf{A}) = u, \quad u, \quad u-a, \quad u+a, \quad u, \quad u, \quad u, \quad u$$

A is diagonizable

$$\mathbf{A} = \mathbf{S}_{\mathbf{A}}\Lambda_{\mathbf{A}}\mathbf{S}_{\mathbf{A}}^{-1}, \qquad diag\ \Lambda_{\mathbf{A}} = \lambda(\mathbf{A}).$$

Splitting of the diagonal matrix $\Lambda_{\mathbf{A}}$ results in the splitting of $\mathbf{A}^{\pm}$:

$$\mathbf{A} = \mathbf{A}^{+} + \mathbf{A}^{-}, \qquad \mathbf{A}^{\pm} = \mathbf{S}_{\mathbf{A}}\Lambda_{\mathbf{A}}^{\pm}\mathbf{S}_{\mathbf{A}}^{-1}$$

Thus, the splitting of the flux difference $\Delta\mathbf{F}$:

$$\Delta\mathbf{F} = \Delta\mathbf{F}^{+} + \Delta\mathbf{F}^{-}, \qquad \Delta\mathbf{F}^{\pm} = \mathbf{A}^{\pm}(\hat{\mathbf{U}})\Delta\mathbf{U}.$$

Goal: Find the average state $\hat{\mathbf{U}} = \hat{\mathbf{U}}(\mathbf{U_L}, \mathbf{U_R})$.

ROE'S AVERAGE STATE

- $\Delta \mathbf{F} = \mathbf{A}(\hat{\mathbf{U}})\Delta \mathbf{U}$
- **For a calorically perfect gas:** the Roe average state is easily obtained.
- **For a real gas:** the simplicity is lost.

Choose the set of average quantities

$$(\hat{\rho}, \hat{u}, \hat{v}, \hat{e}, \hat{H}, \hat{Y}_{i,i=1,4}, \hat{p}_\rho, \hat{p}_e, \hat{p}_{\sigma_{i,i=1,4}})$$

Define the Roe-average operator μ,

$$\hat{f} = \mu(f) = \frac{f_R + d\, f_L}{1+d}, \qquad d = (\rho_L/\rho_R)^{\frac{1}{2}}, \qquad f = u, v, e, H, Y_i, \qquad \hat{\rho} = \rho_R d.$$

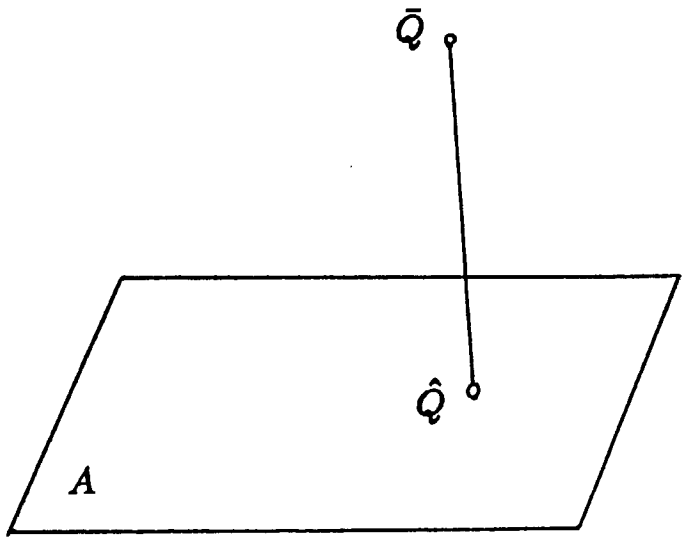
The condition left to be satisfied is:

$$\Delta p = \hat{p}_\rho \Delta \rho + \hat{p}_e \Delta e + \sum_{i=1}^{N-1} \hat{p}_{\sigma_i} \Delta C_i. \qquad (A)$$

Condition (A) contains N+1 variables for only one equation.

ROE'S AVERAGE STATE (cont'd)

$$\bar{Q} \equiv (\bar{p}_e, \bar{p}_\rho, \bar{p}_{C_i}), \qquad \bar{p}_\rho = p_\rho(\hat{\rho}, \hat{e}, \hat{C}_i), \quad etc.$$
$$\hat{Q} \equiv (\hat{p}_e, \hat{p}_\rho, \hat{p}_{C_i})$$



- $(\hat{p}_e,\ \hat{p}_\rho,\ \hat{p}_{C_i}) = (\bar{p}_e,\ \bar{p}_\rho,\ \bar{p}_{C_i})$ for a calorically perfect gas.

NUMERICAL TEST

- Constituent elements of the present flux-splitting method validated by comparison with exact solutions or experimental data in our previous work on 1-D Euler equations for reacting gases, and 2-D Navier-Stokes equations for ideal gases.

- Direct comparison of the present 2-D reacting flow N-S calculations with experimental data is hindered by the lack of suitable data for high Mach number reacting flows.

Two classes of problems are considered in the following:

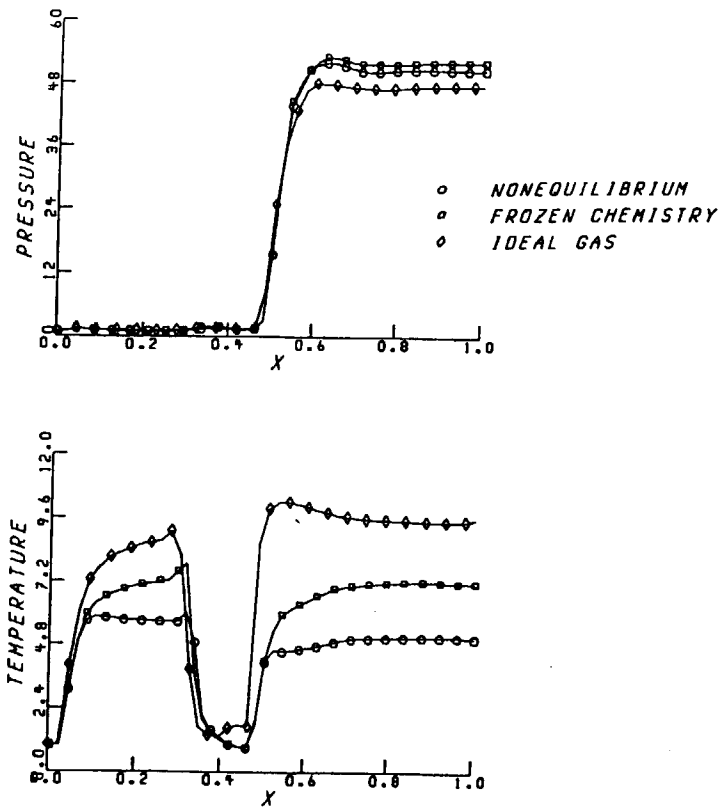
(1) shock wave/laminar boundary layer interaction problems.

(2) jet in cross flow problems.

SHOCK WAVE/BOUNDARY LAYER INTERACTION

WALL PRESSURE AND TEMPERATURE

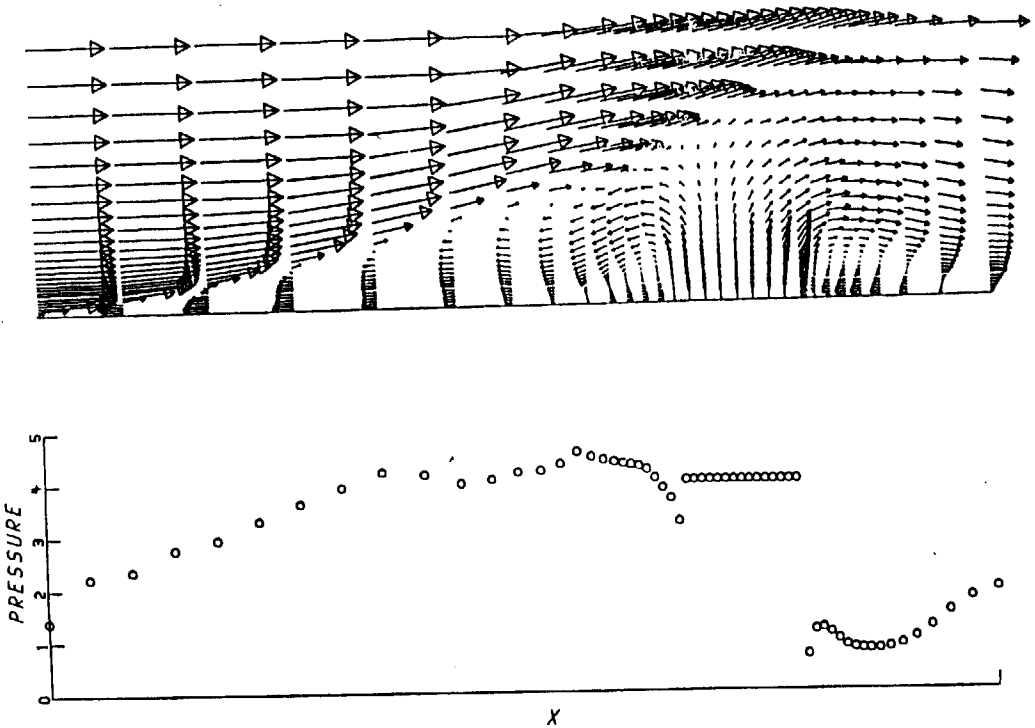
$M_\infty = 8.0, \quad \beta = 22°, \quad R_e = 1.57 \times 10^6$



JET-IN-CROSS FLOW

VELOCITY VECTORS AND WALL PRESSURE

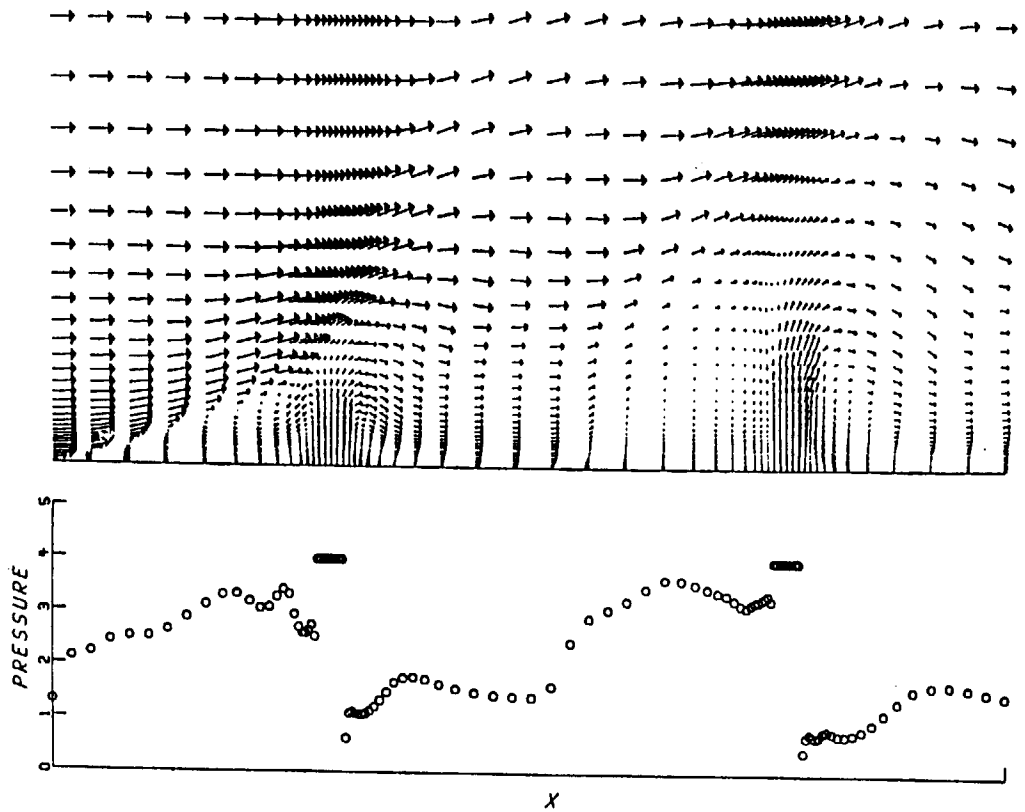
$M_\infty = 6.0, \quad R_e = 3.21 \times 10^6$



DUAL JETS-IN-CROSS FLOW

VELOCITY VECTORS AND WALL PRESSURE

$M_\infty = 6.0, \quad R_e = 3.21 \times 10^6$



SUMMARY

1. New average state of Roe's splitting for chemical reacting gases is proposed.
2. A numerical method based on Roe flux-splitting for solving the Navier-Stokes and species equations for chemical nonequilibrium gases has been developed.
3. Numerical results show the present method has the potential for calculating high Mach number flows with nonequilibrium chemistry and complex wave structure.
4. Implementation of an implicit time solver is in progress.
5. Thermal nonequilibrium is being considered in the next stage of code development.
6. Work for further code validation is needed.