INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 12, 711–726 (1991)

AN IMPLICIT CHARACTERISTIC-FLUX-AVERAGING METHOD FOR THE EULER EQUATIONS FOR REAL GASES

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SUMMARY

A formulation of an implicit characteristic-flux-averaging method for the unsteady Euler equations with real gas effects is presented. Incorporation of a real gas into a general equation of state is achieved by considering the pressure as a function of density and specific internal energy. The Riemann solver as well as the flux-split algorithm are modified by introducing the pressure derivatives with respect to density and internal energy. Expressions for calculating the values of the flow variables for a real gas at the cell faces are derived. The Jacobian matrices and the eigenvectors are defined for a general equation of state. The solution of the system of equations is obtained by using a mesh-sequencing method for acceleration of the convergence. Finally, a test case for a simple form of equation of state displays the differences from the corresponding solution for an ideal gas.

KEY WORDS Euler equations Upwind methods Real gases

1. INTRODUCTION

Current interest in hypersonic flow fields has led to the development of methods for complex chemical non-equilibrium real gas flows. Until now, some numerical methods have provided very accurate results for the flow of an ideal gas.[1,2] The reliability of these methods has been proved for two-dimensional fields[3] as well as for three-dimensional cases.[4]

The study of non-equilibrium flows requires as a first step the extension of known methods to real gas flows. The formulation of numerical methods for real gases is not yet direct. In this paper the formulation of a very efficient, implicit Riemann solver[3] for real gases is presented.

The derivation of the relations that yield the values of the flow variables on the cell faces is described. Moreover, the Jacobians of the flux vectors and the eigenvector matrices are defined for a general equation of state. The present finite volume algorithm does not consider any approximation of the interpretation of the real gas effects. The only consideration is the definition of pressure as a function of density and specific internal energy. Thus the pressure derivatives with respect to the density and the specific internal energy are incorporated in the equations.

Another flux-split algorithm has recently been developed by Glaister.[5] The incorporation of real gas effects has also been described by Colella and Glaz[6] using an approximate procedure based on a local parametrization of the equation of state. Grossman and Walters[7] have considered another approach to flux-splitting algorithms; they treat the real gas by an equivalent γ-representation, as suggested in Reference 4.

0271–2091/91/080711–16$08.00

Received January 1990
Revised May 1990

2. GOVERNING EQUATIONS AND TIME INTEGRATION

The governing equations of an inviscid compressible fluid in two dimensions are the two-dimensional Euler equations. The Euler equations can be written in conservation law form for a generalized co-ordinate system as

$$\mathbf{U}_t + \mathbf{E}_\xi + \mathbf{G}_\zeta = 0, \tag{1a}$$

where

$$\begin{aligned}
\mathbf{U} &= J(\rho, \rho u, \rho w, e)^{\mathrm{T}},\\
\mathbf{E} &= J(\rho\tilde{U}, \rho\tilde{U}u + P\xi_x, \rho w\tilde{U} + P\xi_z, (e+P)\tilde{U})^{\mathrm{T}},\\
\mathbf{G} &= J(\rho\tilde{W}, \rho u\tilde{W} + P\zeta_x, \rho w\tilde{W} + P\zeta_z, (e+P)\tilde{W})^{\mathrm{T}},\\
\tilde{U} &= u\xi_x + w\xi_z, \qquad \tilde{W} = u\zeta_x + w\zeta_z, \qquad e = \rho i + 0{\cdot}5\rho(u^2+w^2).
\end{aligned} \tag{1b}$$

Body-fitted arbitrary co-ordinates ξ, ζ are used and the Jacobian of the transformation $\xi = \xi(x, z), \zeta = \zeta(x, z)$ from Cartesian co-ordinates x, z to generalized co-ordinates is written as

$$J = x_\xi z_\zeta - z_\xi x_\zeta.$$

The quantities ρ, P, u and w represent the density, the pressure and the Cartesian velocity components respectively, while e and i are the total energy and the specific internal energy respectively. The indices $(\,)_\xi, (\,)_\zeta$ denote partial derivatives with respect to x, z. The formulation of the governing equations is completed by a general equation of state of the form

$$P = P(\rho, i).$$

The last equation for an ideal gas is written as

$$P = (\gamma - 1)\rho i,$$

where γ is the ratio of the specific heat capacities of the fluid.

To reach the steady state solution asymptotically, an implicit procedure is used which allows high CFL numbers.[2] The first-order-in-time, discretized implicit form of (1) is written as

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} + \mathbf{E}_\xi^{n+1} + \mathbf{G}_\zeta^{n+1} = 0. \tag{2}$$

A Newton method can be constructed for $\mathbf{U}^{n+1}$ by linearizing the fluxes in (2) about the known time level n:[2,4]

$$\mathbf{E}^{n+1} = \mathbf{E}^n + \mathbf{A}^n\Delta\mathbf{U}, \qquad \mathbf{G}^{n+1} = \mathbf{G}^n + \mathbf{C}^n\Delta\mathbf{U}.$$

These relations allow (2) to be written in the form

$$\frac{\Delta\mathbf{U}}{\Delta t} + (\mathbf{A}^n\Delta\mathbf{U})_\xi + (\mathbf{C}^n\Delta\mathbf{U})_\zeta = -(\mathbf{E}_\xi^n + \mathbf{G}_\zeta^n) = \mathrm{RHS}, \tag{3}$$

where

$$\mathbf{A} = \frac{\partial\mathbf{E}}{\partial\mathbf{U}}, \qquad \mathbf{C} = \frac{\partial\mathbf{G}}{\partial\mathbf{U}}$$

are the Jacobians of the flux vectors **E** and **G** respectively and

$$\Delta \mathbf{U} = \mathbf{U}^{n+1} - \mathbf{U}^{n}$$

is the time variation of the solution.

The development of the method for obtaining the solution in the case of a general equation of state consists of two parts. The first part treats the terms on the right-hand side (RHS). For this part of the solution a linear, locally one-dimensional Riemann solver (Godunov-type differencing) is employed at the cell faces of the finite volume.[2]

The characteristic-flux-averaging procedure is of third-order accuracy in space and locally monotonic.[3,8] The above method is presented in this paper for a general equation of state in order to study equilibrium gas flows, and is the first step of the extension of the algorithm to non-equilibrium real gas flows.

The second part is related to the terms on the left-hand side (LHS) and particularly with the expressions of the Jacobians **A** and **C** for the general equation of state.

3. REAL GAS FORMULATION OF THE CHARACTERISTIC FLUX-AVERAGING SCHEME

In order to reduce the complexity, we split the Euler equations into two one-dimensional equations:

$$\mathbf{U}_t + \mathbf{E}_\xi = 0, \qquad \mathbf{U}_t + \mathbf{G}_\zeta = 0.$$

The Riemann invariants are a transformation of the non-conservative Euler equations on the characteristic directions.[8] These invariants are given by

$$P - P_0 - s^2(\rho - \rho_0) = 0, \tag{4a}$$

$$(w - w_0)x - z(u - u_0) = 0, \tag{4b}$$

$$P - P_1 + \rho s[x(u - u_1) + z(w - w_1)] = 0, \tag{4c}$$

$$P - P_2 + \rho s[-x(u - u_2) - z(w - w_2)] = 0. \tag{4d}$$

The subscripts indicate the point locations $(\xi - \dot{\xi}_j \Delta t, t)$ at which P_j, ρ_j, u_j and $w_j, j = 0, 1, 2$, should be interpolated.

If we consider the cell face $i - 1/2$ between the finite volumes i and $i + 1$, we calculate from the arithmetic mean the eigenvalues and we form a mean state for the flow variables according to the formula

$$U^j_{i-1/2} = \tfrac{1}{2}[(1 + \operatorname{sign} \lambda_j) U^j_{\mathrm{l}} + (1 - \operatorname{sign} \lambda_j) U^j_{\mathrm{r}}].$$

The subscripts 'l' and 'r' denote the left and right states respectively in accordance with Reference 8. The order of accuracy of the flux difference operator is controlled by the definition of the left and right states.[8] As an example, the third-order formula is given by

$$U_{\mathrm{l}} = \tfrac{1}{6}(5U_{i-1} - U_{i-2} + 2U_i), \qquad U_{\mathrm{r}} = \tfrac{1}{6}(5U_i - U_{i+1} + 2U_{i-1}).$$

Since we make use of the homogeneous property, the invariants have to be inverted in conservative variables. Considering that the pressure can be written as a function of density and specific internal energy, $P = P(\rho, i)$, we obtain

$$\Delta P = P_\rho \Delta \rho + P_i \Delta i. \tag{5a}$$

Our goal is to formulate the equations by means of the pressure derivatives P_ρ and P_i. The transformation relations are completed by

$$\Delta u = \frac{\Delta l - u\Delta\rho}{\rho}, \tag{5b}$$

$$\Delta w = \frac{\Delta n - w\Delta\rho}{\rho}, \tag{5c}$$

where $l = \rho u$ and $n = \rho w$.

From (1b) we take

$$\Delta(\rho i) = \Delta e - \frac{2l\Delta l + 2n\Delta n}{2\rho} + \frac{l^2 + n^2}{2\rho^2}\Delta\rho. \tag{6}$$

The term $\Delta(\rho i)$ can be written as

$$\Delta(\rho i) = \rho\Delta i + i\Delta\rho.$$

From (6) we obtain

$$\rho\Delta i = \Delta e - (u\Delta l + \Delta n) + 0{\cdot}5q^2\Delta\rho - i\Delta\rho, \tag{7}$$

where

$$q^2 = u^2 + w^2.$$

Substitution of Δi from (7) in (5) yields

$$\Delta P = \Delta\rho\left(P_\rho + 0{\cdot}5q^2\frac{P_i}{\rho} - i\frac{P_i}{\rho}\right) + \frac{P_i}{\rho}[\Delta e - (u\Delta l + w\Delta n)]. \tag{8}$$

The Riemann invariants (4a)–(4d) can now be transformed by means of (5b), (5c) and (8). Analytically, the four invariants are written as

$$(\rho - \rho_0)\left(P_\rho + P_i\frac{q^2}{2\rho} - i\frac{P_i}{\rho} - s^2\right) + \frac{P_i}{\rho}[(e - e_0) - u(l - l_0) - w(n - n_0)] = 0, \tag{9a}$$

$$(\rho - \rho_0)(uz - wx) - (l - l_0)z + (n - n_0)x = 0, \tag{9b}$$

$$(\rho - \rho_1)\left(P_\rho + P_i\frac{q^2}{2}\rho - i\frac{P_i}{\rho} - s\lambda_0\right) + (l - l_1)\left(sx - u\frac{P_i}{\rho}\right) + (n - n_1)\left(sz - w\frac{P_i}{\rho}\right) + (e - e_1)\frac{P_i}{\rho} = 0, \tag{9c}$$

$$(\rho - \rho_2)\left(P_\rho + P_i\frac{q^2}{2}\rho - i\frac{P_i}{\rho} - s\lambda_0\right) + (l - l_2)\left(sx - u\frac{P_i}{\rho}\right) + (n - n_2)\left(sz - w\frac{P_i}{\rho}\right) + (e - e_2)\frac{P_i}{\rho} = 0. \tag{9d}$$

Since each of the last five expressions is zero, their weighted sums must also be zero. Multiplying each of them by the coefficients a, b, d and f and adding, we obtain

$$\rho\bar{\rho} + l\bar{l} + n\bar{n} + e\bar{e} = \rho_0\bar{\rho} + l_0\bar{l} + n_0\bar{n} + e_0\bar{e} + 2s^2(dR_1 + fR_2), \tag{9e}$$

where

$$\bar{\rho} = a(Q-s^2)+b(uz-wx)+d(Q-s\lambda_0)+f(Q+s\lambda_0), \tag{10a}$$

$$\bar{l} = d\left(sx-u\frac{P_i}{\rho}\right)-f\left(sx+u\frac{P_i}{\rho}\right)-bz-au\frac{P_i}{\rho}, \tag{10b}$$

$$\bar{n} = d\left(sz-w\frac{P_i}{\rho}\right)-f\left(sz+u\frac{P_i}{\rho}\right)-bx-aw\frac{P_i}{\rho}, \tag{10c}$$

$$\bar{e} = (a+d+f)\frac{P_i}{\rho}, \tag{10d}$$

$$R_1 = \frac{0{\cdot}5}{s^2}\left[(\rho_0-\rho_1)(s\lambda_0-Q)+(l_0-l_1)\left(u\frac{P_i}{\rho}-sx\right)+(n_0-n_1)\left(w\frac{P_i}{\rho}-sz\right)-(e_0-e_1)\frac{P_i}{\rho}\right],$$

$$R_2 = \frac{0{\cdot}5}{s^2}\left[-(\rho_0-\rho_2)(s\lambda_0+Q)+(l_0-l_2)\left(u\frac{P_i}{\rho}+sx\right)+(n_0-n_2)\left(w\frac{P_i}{\rho}+sz\right)-(e_0-e_2)\frac{P_i}{\rho}\right],$$

with

$$\lambda_0 = ux+wz, \qquad x = \frac{\xi_x}{\sqrt{(\xi_x^2+\xi_z^2)}}, \qquad z = \frac{\xi_z}{\sqrt{(\xi_x^2+\xi_z^2)}}.$$

The sound velocity s is given by

$$s^2 = P\frac{P_i}{\rho^2}+P_\rho. \tag{10e}$$

The term Q is given by

$$Q = P_\rho + P_i\frac{q^2}{2\rho}-i\frac{P_i}{\rho}. \tag{10f}$$

The system of equations (10a)–(10d) needs to be inverted for coefficients d and f. If we multiply (10b) by x and (10c) by z and add, we obtain

$$d-f = \frac{\bar{l}x+\bar{n}z+\bar{e}\lambda_0}{s}. \tag{11a}$$

Addition of (10a) and (10b) multiplied by u and (10c) multiplied by w yields

$$d+f = \frac{\bar{\rho}+\bar{l}u+\bar{n}w+\bar{e}H}{s^2}. \tag{11b}$$

The above relations have been obtained by using the known identities

$$x^2+z^2 = 1, \qquad \lambda_0 = ux+wz.$$

The total enthalpy H is given by

$$H = \frac{e+P}{\rho}. \tag{12}$$

From (11a) and (11b) we obtain the coefficients d and f:

$$d = \frac{0{\cdot}5}{s^2}[\bar{\rho} + \bar{l}(u + sx) + \bar{n}(w + sz) + \bar{e}(H + s\lambda_0)], \tag{13a}$$

$$f = \frac{0{\cdot}5}{s^2}[\bar{\rho} + \bar{l}(u - sx) + \bar{n}(w - sz) + \bar{e}(H - s\lambda_0)]. \tag{13b}$$

The above relations have also been found by Eberle[8] for the ideal gas equation of state, but for a real gas the velocity of sound is defined by (10e) and the total enthalpy by (12) or by

$$H = i + 0{\cdot}5(u^2 + w^2) + \frac{P}{\rho}. \tag{14}$$

Putting $\bar{\rho}$ equals to unity and $\bar{l}$, $\bar{u}$, and $\bar{e}$ equal to zero in (13a) and (13b) and using the scalar invariant (9e), we write out the ρ. Similarly, we find the conservative cell face flow values l, n and e from which the Euler fluxes on the RHS of (3) can be calculated. The conservative values are given by

$$\rho = \rho_0 + \bar{\rho} + r_1 + r_2, \tag{15a}$$

$$l = l_0 + r_1(u + sx) + r_2(u - sx) + xd + u\bar{\rho}, \tag{15b}$$

$$n = n_0 + r_1(w + sz) + r_2(w - sz) + zd + w\bar{\rho}, \tag{15c}$$

$$e = d\lambda_0 + (H + s\lambda_0)\rho_1 + (H - s\lambda_0)\rho_2 + \bar{e} + \bar{\rho}\left(q^2 - \rho\frac{Q}{P_i}\right) - \rho_0\frac{\rho}{P_i}Q, \tag{15d}$$

with

$$\bar{\rho} = \frac{P_i}{\rho s^2}\left(\bar{e} - e_0 - \rho_0 Q\frac{\rho}{P_i}\right), \tag{16a}$$

$$\bar{e} = ul_0 + wn_0, \tag{16b}$$

$$d = \rho_0\lambda_0 - l_0 x - n_0 z, \tag{16c}$$

$$r_1 = \frac{0{\cdot}5}{s^2}\left[\rho_1(-s\lambda_0 + Q) + l_1\left(-u\frac{P_i}{\rho} + sx\right) + n_1\left(-w\frac{P_i}{\rho} + sz\right) + e_1\frac{P_i}{\rho}\right], \tag{16d}$$

$$r_2 = \frac{0{\cdot}5}{s^2}\left[\rho_2(s\lambda_0 + Q) - l_2\left(u\frac{P_i}{\rho} + sx\right) + n_2\left(-w\frac{P_i}{\rho} + sz\right) + e_2\frac{P_i}{\rho}\right]. \tag{16e}$$

4. FORMULATION OF THE FLUX-SPLITTING ALGORITHM FOR REAL GASES

In this section the analysis of the flux-splitting procedure is presented. This formulation is needed for the calculation of the terms on the LHS. The terms $(\mathbf{A}^n\Delta\mathbf{U})_\xi$ and $(\mathbf{C}^n\Delta\mathbf{U})_\zeta$ are discretized[2,4] at the volume i, k up to second-order accuracy in space. For example, the term $(\mathbf{A}^n\Delta\mathbf{U})_\xi$ is written as

$$(\mathbf{A}^n\Delta\mathbf{U})_\xi = (\mathbf{A}^n\Delta\mathbf{U})_{i+1/2} - (\mathbf{A}^n\Delta\mathbf{U})_{i-1/2}, \tag{17a}$$

where

$$(\mathbf{A}^n\Delta\mathbf{U})_{i+1/2} = (\mathbf{T}\Lambda^+\mathbf{T}^{-1})_{i+1/2}\Delta\mathbf{U}^+_{i+1/2} + (\mathbf{T}\Lambda^-\mathbf{T}^{-1})_{i+1/2}\Delta\mathbf{U}^-_{i+1/2}, \tag{17b}$$

$$(\mathbf{A}^n\Delta\mathbf{U})_{i-1/2} = (\mathbf{T}\Lambda^+\mathbf{T}^{-1})_{i-1/2}\Delta\mathbf{U}^+_{i-1/2} + (\mathbf{T}\Lambda^-\mathbf{T}^{-1})_{i-1/2}\Delta\mathbf{U}^-_{i-1/2}, \tag{17c}$$

Λ^+ and Λ^- are the diagonal matrices of the positive and negative eigenvalues of the Jacobian $\mathbf{A}$ respectively. These matrices are defined as

$$\Lambda^+ = \max(0, \Lambda), \qquad \Lambda^- = \min(0, \Lambda).$$

The eigenvalue matrix Λ is diagonal,

$$\Lambda = \operatorname{diag}(\lambda_k^0, \lambda_k^1, \lambda_k^2, \lambda_k^3),$$

with elements

$$\lambda_k^0 = \lambda_k^1 = uk_x + wk_z, \qquad \lambda_k^2 = \lambda_k^0 + s|\nabla k|, \qquad \lambda_k^3 = \lambda_k^0 - s|\nabla k|.$$

The above elements define the eigenvalues of the matrices $\mathbf{A}$ and $\mathbf{C}$ for $k = \xi$ and $k = \zeta$ respectively.

The vectors $\Delta\mathbf{U}$ are extrapolated consistently to the RHS.[4] For the finite volume face $(i+1/2, k)$, $\Delta\mathbf{U}$ is extrapolated up to second order depending on the eigenvalues. $\mathbf{T}$ and $\mathbf{T}^{-1}$ are the matrices of the left and right eigenvectors respectively. Implementation of the method in order to include equilibrium real gas effects is achieved by derivation of the Jacobian matrices and the eigenvectors for a general equation of state. For this reason, as with the expressions on the RHS, the matrices on the LHS are defined by introducing the pressure derivatives. The Jacobian matrix $\mathbf{A}$ is defined as

$$\mathbf{A} = \frac{\partial \mathbf{E}}{\partial \mathbf{U}} = \left(\frac{\partial \mathbf{E}}{\partial \rho}, \frac{\partial \mathbf{E}}{\partial l}, \frac{\partial \mathbf{E}}{\partial n}, \frac{\partial \mathbf{E}}{\partial e} \right).$$

In accordance with the assumption that the pressure is a function of density and internal energy, the partial derivatives for the pressure are given by the relations

$$\left.\frac{\partial P}{\partial \rho}(\rho, i)\right|_{l,n,e} = \left.\frac{\partial P}{\partial \rho}(\rho, i)\right|_i + \left.\frac{\partial i}{\partial \rho}(\rho, l, n, e)\right|_{l,n,e} \left.\frac{\partial P}{\partial i}(\rho, i)\right|_\rho,$$

$$\left.\frac{\partial P}{\partial l}(\rho, i)\right|_{\rho,n,e} = \left.\frac{\partial P}{\partial i}(\rho, i)\right|_\rho \left.\frac{\partial i}{\partial l}(\rho, l, n, e)\right|_{\rho,n,e},$$

$$\left.\frac{\partial P}{\partial n}(\rho, i)\right|_{\rho,l,e} = \left.\frac{\partial P}{\partial i}(\rho, i)\right|_\rho \left.\frac{\partial i}{\partial n}(\rho, l, n, e)\right|_{\rho,l,e},$$

$$\left.\frac{\partial P}{\partial e}(\rho, i)\right|_{\rho,l,n} = \left.\frac{\partial P}{\partial i}(\rho, i)\right|_\rho \left.\frac{\partial i}{\partial e}(\rho, l, n, e)\right|_{\rho,l,n},$$

and the internal energy is defined by

$$i(\rho, l, n, e) = \frac{e}{\rho} - 0{\cdot}5\frac{l^2 + n^2}{\rho^2}.$$

The Jacobian matrices and the eigenvectors for an ideal gas can be found in Reference 9. For a real gas the same quantities are defined as follows:

$$\mathbf{A}(k = \xi), \qquad \mathbf{C}(k = \zeta) = (a_{ij}), \quad i, j = 1, 2, 3, 4,$$

$$a_{11} = 0, \qquad a_{12} = k_x, \qquad a_{13} = k_z, \qquad a_{14} = 0,$$

$$a_{21} = -u\lambda_0 + k_x Q, \qquad a_{22} = \lambda_0 + uk_x\left(1 - \frac{P_i}{\rho}\right),$$

$$a_{23} = uk_z - w\frac{P_i}{\rho}k_x, \qquad a_{24} = \frac{P_i}{\rho}k_x,$$

$$a_{31} = -w\lambda_0 + k_z Q, \qquad a_{32} = wk_x - u\frac{P_i}{\rho}k_z,$$

$$a_{33} = \lambda_0 + wk_z\left(1 - \frac{P_i}{\rho}\right), \qquad a_{34} = \frac{P_i}{\rho}k_z,$$

$$a_{41} = \lambda_0(Q - H), \qquad a_{42} = Hk_x - u\lambda_0\frac{P_i}{\rho},$$

$$a_{43} = Hk_z - w\lambda_0\frac{P_i}{\rho}, \qquad a_{44} = \lambda_0\left(1 + \frac{P_i}{\rho}\right);$$

the left-eigenvector matrix

$$\mathbf{T} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4),$$

$$\mathbf{e}_1 = (0, -\rho\tilde{k}_z, \rho\tilde{k}_x, \rho(w\tilde{k}_x - u\tilde{k}_z))^{\mathrm{T}},$$

$$\mathbf{e}_2 = (\tilde{k}_z, u\tilde{k}_z, w\tilde{k}_z, \tilde{k}_x E)^{\mathrm{T}},$$

$$\mathbf{e}_3 = \left(1, u + s\tilde{k}_x, w + s\tilde{k}_z, H + s\frac{\lambda_0}{|\nabla k|}\right)^{\mathrm{T}},$$

$$\mathbf{e}_4 = \left(1, u - s\tilde{k}_x, w - s\tilde{k}_z, H - s\frac{\lambda_0}{|\nabla k|}\right)^{\mathrm{T}};$$

and the right-eigenvector matrix

$$\mathbf{T}^{-1} = (\tilde{\mathbf{e}}_1, \tilde{\mathbf{e}}_2, \tilde{\mathbf{e}}_3, \tilde{\mathbf{e}}_4),$$

$$\tilde{\mathbf{e}}_1 = \left(\frac{1}{\rho}(u\tilde{k}_z - w\tilde{k}_x), \tilde{k}_z\left(1 - \frac{Q}{s^2}\right), \beta\left(Q - s\frac{\lambda_0}{|\nabla k|}\right), \beta\left(Q + s\frac{\lambda_0}{|\nabla k|}\right)\right)^{\mathrm{T}},$$

$$\tilde{\mathbf{e}}_2 = \left(-\frac{1}{\rho}\tilde{k}_z, u\frac{P_i}{\rho s^2}, \beta\left(s\tilde{k}_x - u\frac{P_i}{\rho}\right), -\beta\left(s\tilde{k}_x + u\frac{P_i}{\rho}\right)\right)^{\mathrm{T}},$$

$$\tilde{\mathbf{e}}_3 = \left(\frac{1}{\rho}\tilde{k}_x, w\frac{P_i}{\rho s^2}, \beta\left(s\tilde{k}_z - w\frac{P_i}{\rho}\right), -\beta\left(s\tilde{k}_z + u\frac{P_i}{\rho}\right)\right)^{\mathrm{T}},$$

$$\tilde{\mathbf{e}}_4 = \left(0, -\tilde{k}_z\frac{P_i}{\rho s^2}, \beta\frac{P_i}{\rho}, \beta\frac{P_i}{\rho}\right)^{\mathrm{T}};$$

with

$$\tilde{k}_x = \frac{k_x}{|\nabla k_x|}, \qquad \beta = \frac{0{\cdot}5}{s^2}, \qquad Q = P_\rho + P_i\frac{q^2}{2\rho} - i\frac{P_i}{\rho}.$$

All equations and matrices have been defined in accordance with the pressure derivatives with respect to density and internal energy. These can be found by an available equation of state or by curve fitting.

5. INVERSION OF THE SYSTEM OF EQUATIONS AND ACCELERATION OF THE CONVERGENCE

The solution of the system of equations (3) which includes the real gas effects is obtained by the sequence of approximations denoted by $\mathbf{q}^\nu$ such that $\lim_{\nu>1} \mathbf{q}^\nu \to \mathbf{U}^{n+1}$, where ν is the subiteration state. The equations are solved by a Newton method.[10] The Newton form is obtained by linearization of (3) around the known subiteration state ν as follows:

$$\frac{\Delta \mathbf{q}^{\nu+1}}{\Delta t} + (\mathbf{A}^\nu \Delta \mathbf{q}^{\nu+1})_\xi + (\mathbf{C}^\nu \Delta \mathbf{q}^{\nu+1})_\zeta = \frac{\mathbf{U}^n - \mathbf{q}^\nu}{\Delta t} - (\mathbf{E}_\xi^\nu + \mathbf{G}_\zeta^\nu) = \text{RHS},$$

where $\mathbf{q}^\nu$ and $\mathbf{q}^{\nu+1}$ are the solution vectors at the subiteration states ν and $\nu+1$ respectively. The solution at level $\nu+1$ is updated as

$$\mathbf{q}^{\nu+1} = \mathbf{q}^\nu + \Delta \mathbf{q}^{\nu+1}.$$

Acceleration of the convergence of the above finite volume method is obtained via a mesh-sequencing procedure.[11] The acceleration is achieved by using a coarser grid for a number of iterations during the convergence. The solution is obtained first on a sequence of coarser grids and then by interpolation up to the next finer grid. A coarse mesh can easily be formed by discarding lines of the fine mesh.

The rate of convergence for supersonic flows is usually faster than that of transonic flows. The total computational real time for supersonic and hypersonic flows is estimated at about 25%–30% of the real time if the fine grid were used for the entire calculation.

The most sensitive part of the method is the interpolation procedure. For this reason, a special treatment has been under development[12] which promises better results for the Euler and Navier–Stokes equations.

6. RESULTS

In this section the results of the flow around a 4% circular arc airfoil with freestream Mach number 4 at zero angle of attack are presented. Because of the symmetry, we study the half-plane using symmetry conditions on the upstream and downstream parts along the x-axis. The 82×31 computational grid used is shown on Figure 1. Results are given both for an ideal gas and for another simple form of the equation of state.

The ideal gas equation of state can be written in the form

$$P = (\gamma - 1)\rho i. \tag{18}$$

The ratio of the specific heat capacities depends on the gas. Typical values of γ are 1·4 for a diatomic gas and 1·2 for tetrafluoromethane. A simple extension of the ideal equation of state is the stiffened equation of state, which can be written as

$$P = c\left(\frac{\rho}{\rho_0} - 1\right) + (\gamma - 1)\rho i, \tag{19}$$

where ρ_0 is a reference density and c is a constant. The value of c depends on the non-dimensional variables. The pressure derivatives for an ideal gas are calculated by the relations

$$P_\rho = (\gamma - 1)i, \qquad P_i = (\gamma - 1)\rho.$$

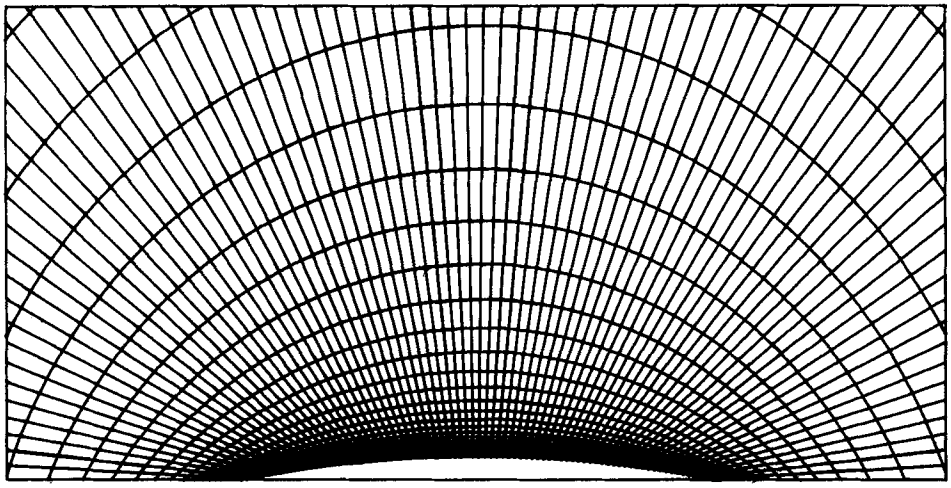

Figure 1. Computational grid

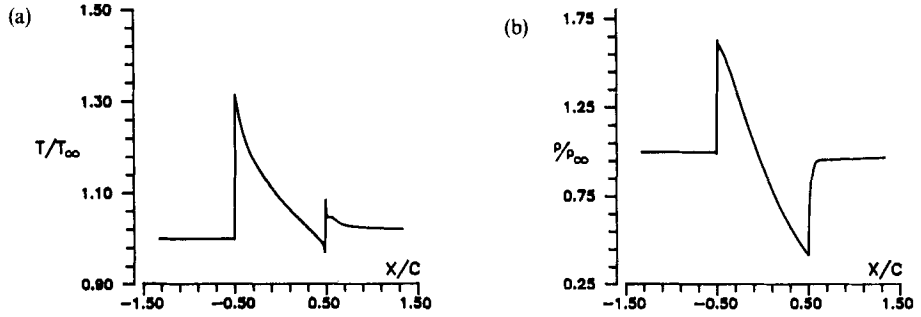

Figure 2. (a) Temperature and (b) density values along the x-axis for the stiffened equation of state (EOS) ($M = 4$, $\gamma = 1{\cdot}2$)

For a general equation of state the pressure derivatives can be calculated by an approximation formula. Glaister[5] proposed the approximations

$$P_i = \frac{1}{\Delta i}[\tfrac{1}{2}(P(\rho_R, i_R) + P(\rho_L, i_R)) - \tfrac{1}{2}(P(\rho_R, i_L) + P(\rho_L, i_L))], \tag{20a}$$

$$P_\rho = \frac{1}{\Delta \rho}[\tfrac{1}{2}(P(\rho_R, i_R) + P(\rho_R, i_L)) - \tfrac{1}{2}(P(\rho_L, i_R) + P(\rho_L, i_L))] \tag{20b}$$

for $\Delta i \neq 0$, $\Delta \rho \neq 0$ and

$$P_i = \tfrac{1}{2}(P_\rho(\rho_L, i) + P_\rho(\rho_R, i)), \tag{21a}$$

$$P_\rho = \tfrac{1}{2}(P_\rho(\rho, i_L) + P_\rho(\rho, i_R)) \tag{21b}$$

for $\Delta i = 0$, $\Delta \rho = 0$, where

$$\Delta(\cdot) = (\cdot)_R - (\cdot)_L.$$

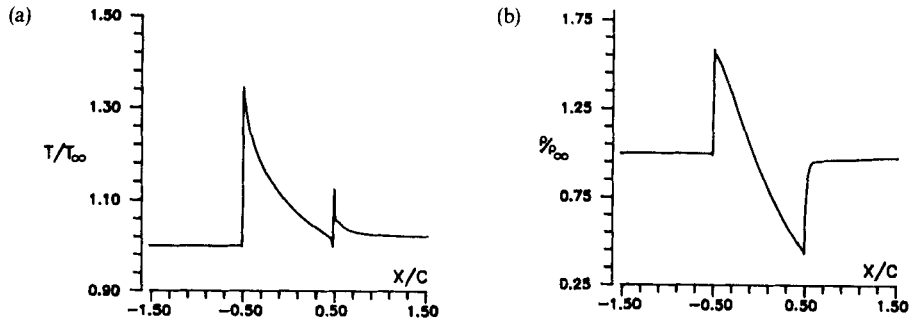

Figure 3. (a) Temperature and (b) density values along the x-axis for a perfect gas ($M = 4, \gamma = 1{\cdot}2$)

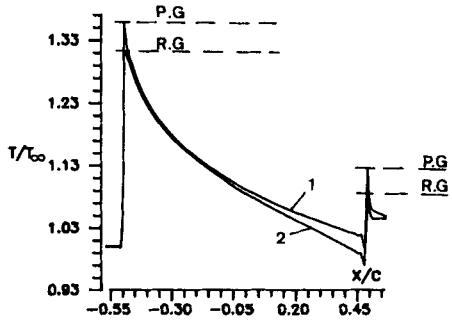

Figure 4. Differences in temperature values: 1, perfect gas (P.G); 2, stiffened EOS (R.G) ($M = 4, \gamma = 1{\cdot}2$)

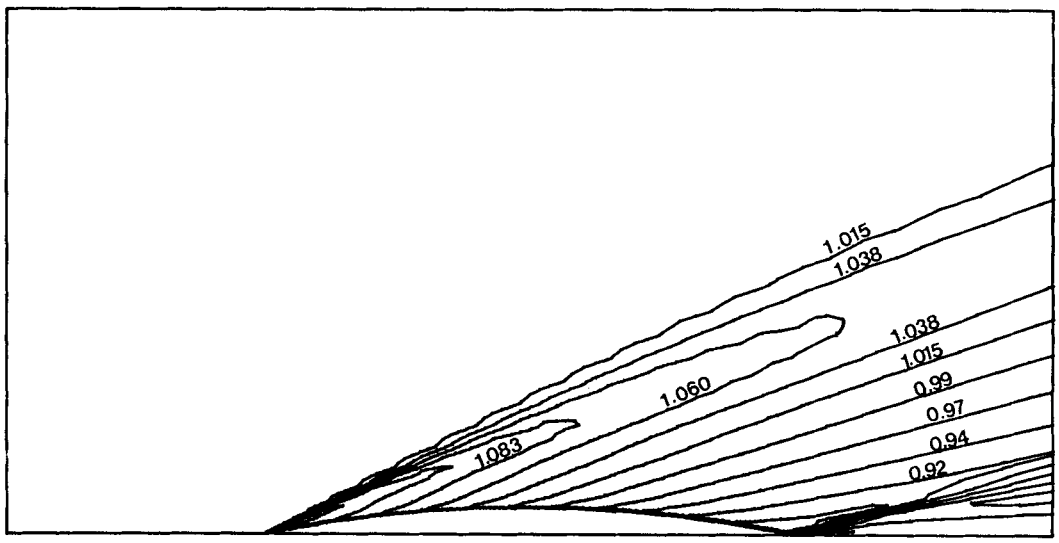

Figure 5(a). Iso-temperature lines for a perfect gas ($M = 4, \gamma = 1{\cdot}2$)

The indices R and L represent, for a cell face $i+1/2$, the volumes $i+1$ and i respectively. For $\Delta i = 0, \Delta\rho = 0$ we can also use the relations

$$P_\rho = (\tilde{\gamma}-1)i, \qquad P_i = (\tilde{\gamma}-1)\rho, \tag{22}$$

where

$$\tilde{\gamma} = \frac{P(\rho, i)}{\rho i} + 1.$$

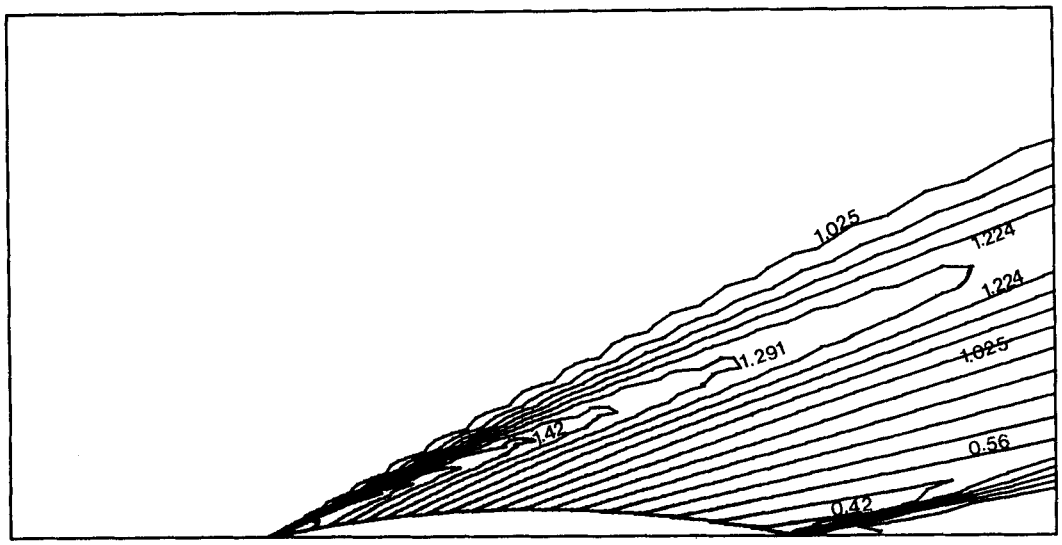

Figure 5(b). Iso-density lines for a perfect gas ($M = 4, \gamma = 1{\cdot}2$)

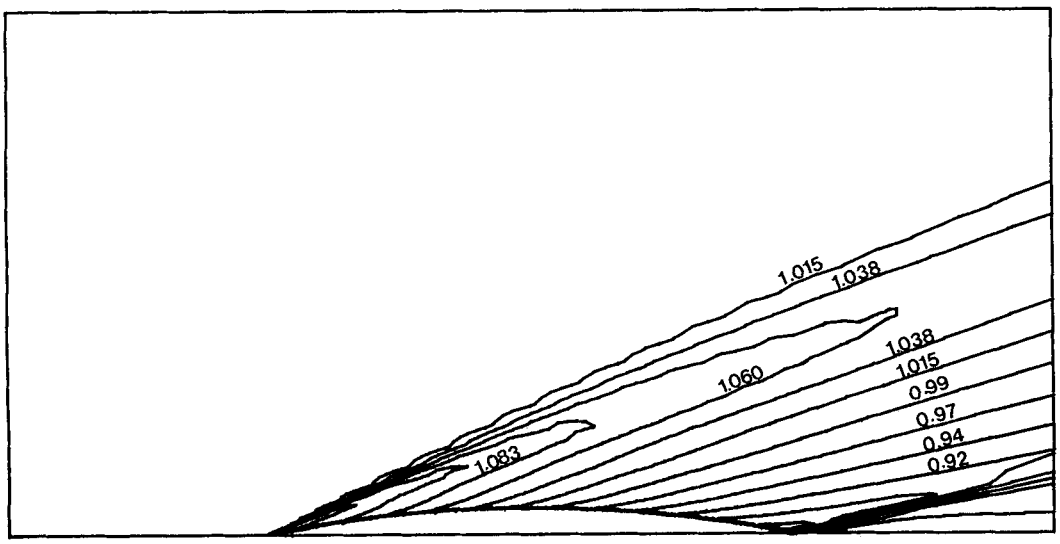

Figure 6(a). Iso-temperature lines for stiffened EOS ($M = 4, \gamma = 1{\cdot}2$)

In Figures 2(a) and 2(b) the temperature and density values respectively along the x-axis for the stiffened equation of state with $\gamma = 1{\cdot}2$ are presented. The corresponding results for an ideal gas with $\gamma = 1{\cdot}2$ are shown in Figures 3(a) and 3(b). The differences in the temperature values are shown in Figure 4. We see that the temperature jump on the leading edge and on the trailing edge is higher. The iso-temperatures and iso-density lines for the equations of state (18) and (19) have been plotted in Figures 5(a), 5(b) and 6(a), 6(b) respectively.

In Figure 7 we can see that the iso-temperature lines (R.G) for (19) have a smaller inclination with respect to the x-axis than the corresponding lines (P.G) for a perfect gas. The differences in

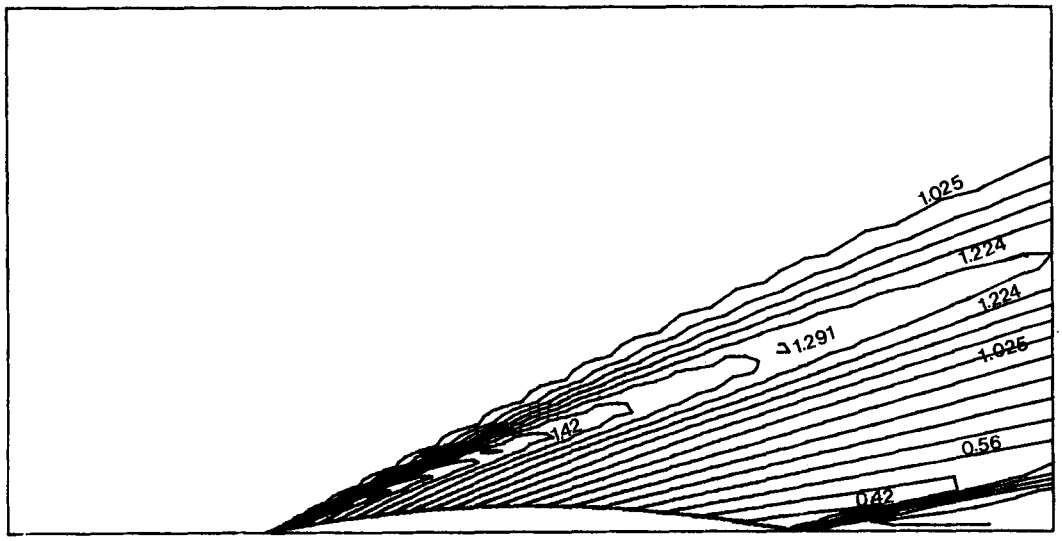

Figure 6(b). Iso-density lines for stiffened EOS ($M = 4, \gamma = 1{\cdot}2$)

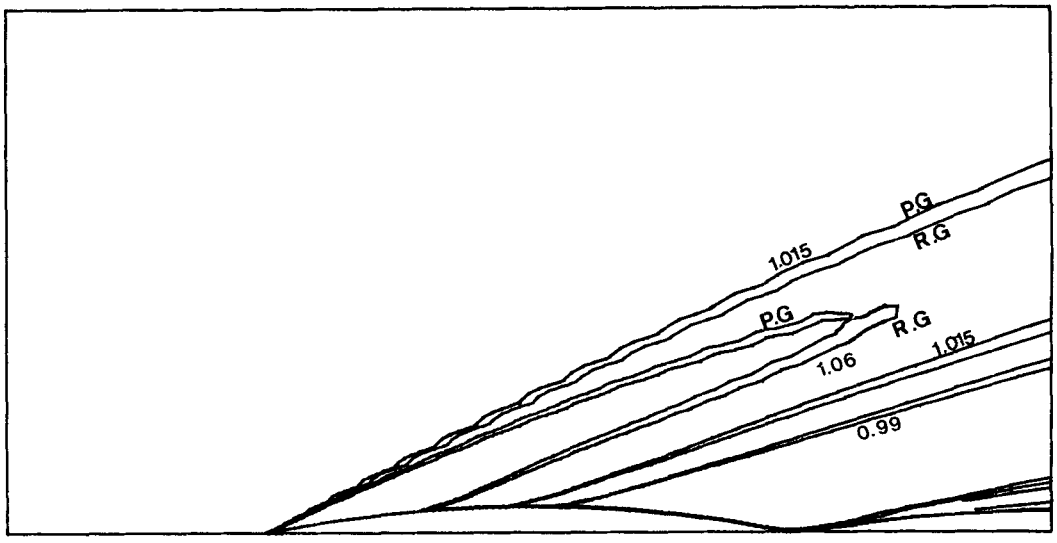

Figure 7. Comparison of iso-temperature lines between perfect gas (P.G) and stiffened EOS (R.G) ($M = 4, \gamma = 1{\cdot}2$)

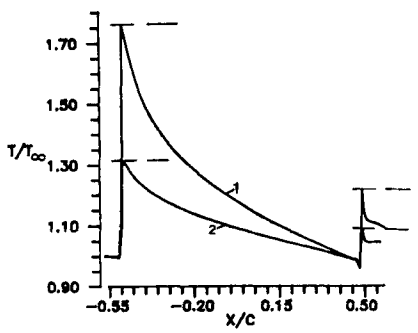

Figure 8. Comparison of temperature values: 1, perfect gas ($M = 4, \gamma = 1{\cdot}4$); 2, stiffened EOS ($M = 4, \gamma = 1{\cdot}2$)

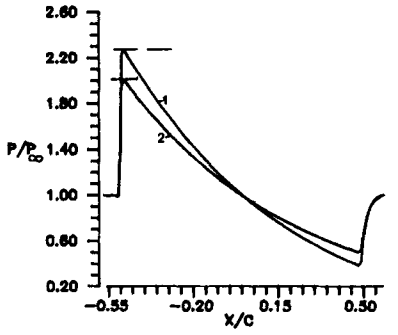

Figure 9. Comparison of pressure values: 1, perfect gas ($M = 4, \gamma = 1{\cdot}4$); 2, stiffened EOS ($M = 4, \gamma = 1{\cdot}2$)

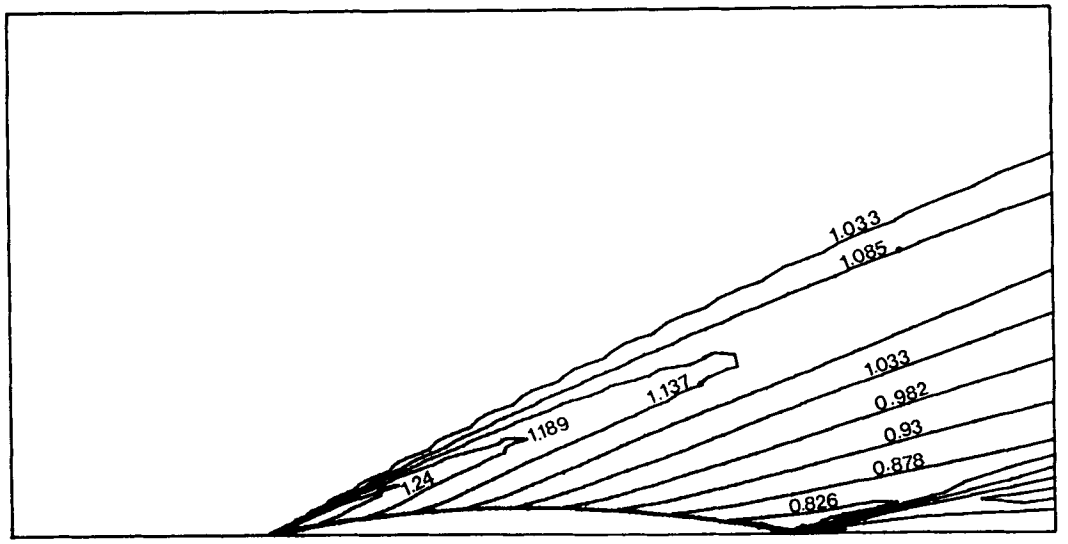

Figure 10. Iso-temperature lines for a perfect gas ($M = 4, \gamma = 1{\cdot}4$)

the temperature and pressure values between the ideal gas equation of state for $\gamma = 1{\cdot}4$ and the stiffened equation of state for $\gamma = 1{\cdot}2$ are quite significant and are shown in Figures 8 and 9 respectively. The iso-temperature lines for an ideal gas with $\gamma = 1{\cdot}4$ are presented in Figure 10. The above results have been obtained by a mesh-sequencing technique with a computational gain of about 30%.

The convergence history using three meshes versus a single grid is shown in Figure 11. The computational cost does not increase for the real gas algorithm of the present study using the simple extension of the ideal gas equation of state. The method needs only the pressure values from a curve fit. Thus the computational cost is expected not to be increased by using curve fits.

All the calculations have been performed on a DEC 3100 system. The computational time is 1 h without mesh sequences and 40 min using mesh sequences.

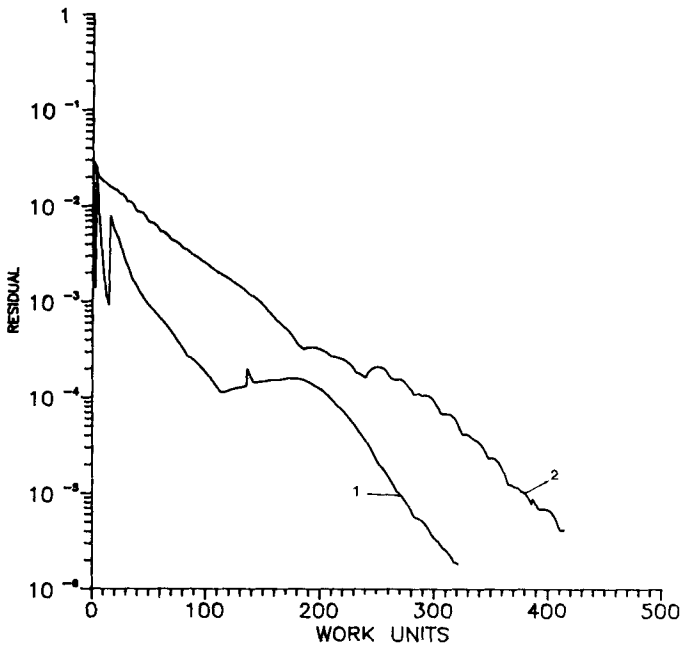

Figure 11. Convergence history: 1, mesh sequencing (three meshes); 2, single grid

7. CONCLUSIONS

In this paper the formulation of a Riemann solver with flux splitting for a general equation of state is presented. The relations for the calculation of the conservative variables on the cell faces are written including the pressure derivatives with respect to density and specific internal energy.

For the implicit part of the method the Jacobians and the eigenvector matrices are modified. Further relations are not needed for the computation of a real gas, except for the approximate calculations of the pressure derivatives from the formulae (20a, b), (21a, b) or (22). Thus the computational cost does not increase for the real gas algorithm.

A test case with a simple form of the equation of state shows the capability of the algorithm to simulate real gas flows. Using curve fits for equilibrium air, we intend to present results for high-temperature air in a future paper.

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