ON THE EFFICIENT SOLUTION OF THE EULER EQUATIONS WITH REAL GASES

P. GLAISTER

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ABSTRACT

An efficient algorithm is presented for the solution of the Euler equations of gas dynamics with a general convex equation of state. The scheme is based on solving linearised Riemann problems approximately and in more than one dimension incorporates operator splitting. In particular, only one function evaluation in each computational cell is required by using a local parameterisation of the equation of state. The scheme is applied to two standard test problems in gas dynamics for some specimen equations of state.

1. INTRODUCTION

In 1981 Roe [1] proposed an approximate linearised Riemann solver for the Euler equations of gas dynamics for an ideal gas. Following Roe, Glaister [2] developed a similar type of Riemann solver for non-ideal gases with satisfactory results. A disadvantage of Glaister's scheme is that four function evaluations are required in each computational cell to approximate the first derivatives of the equation of state. For complex equations of state, e.g. curve fits for equilibrium air [3], this can prove to be an expensive overhead. We seek here to devise a scheme that requires only one function evaluation in each cell with no deterioration in the quality of the solution. This is achieved by a local parameterisation of the equation of state, in effect a 'variable effective gamma' (VEG) scheme.

In §2 we consider the Jacobian matrix of the flux functions for the Euler equations with a general equation of state and in §3 derive an approximate Riemann solver for the solution of these equations. Finally, in §4 we display the numerical results achieved for two standard test problems in gas dynamics.

2. EQUATIONS OF FLOW

In this section we state the equations of flow considered and give the eigenvalues and eigenvectors of the Jacobian matrix of one of the corresponding flux functions.

2.1 Equations of Motion

The three dimensional Euler equations for the flow of an inviscid, compressible fluid can be written in conservation form as

$$\underset{\sim}{w}_t + \underset{\sim}{f}_x + \underset{\sim}{g}_y + \underset{\sim}{h}_z = \underset{\sim}{0} \tag{2.1}$$

where

$$\underset{\sim}{w} = (\rho, \rho u, \rho v, \rho w, e)^T \tag{2.2}$$

$$\underset{\sim}{f} = (\rho u, p+\rho u^2, \rho uv, \rho uw, u(e+p))^T \tag{2.3}$$

$$\underset{\sim}{g} = (\rho v, \rho vu, p+\rho v^2, \rho vw, v(e+p))^T \tag{2.4}$$

$$\underset{\sim}{h} = (\rho w, \rho wu, \rho wv, p+\rho w^2, w(e+p))^T \tag{2.5}$$

and

$$e = \rho i + \tfrac{1}{2}\rho(u^2 + v^2 + w^2) \quad . \tag{2.6}$$

The quantities $(\rho,u,v,w,i,p,e) = (\rho,u,v,w,i,p,e)(x,y,z,t)$ represent the density, velocity in the three coordinate directions, specific internal energy, pressure, total energy, at a general position (x,y,z) in space and at time t. In addition, we assume that there is a

thermodynamic relationship connecting p, ρ and i written as

$$p = p(\rho, i) \quad . \tag{2.7}$$

We assume further that the derivatives $p_\rho = \left.\frac{\partial p}{\partial \rho}\right|_i$ and $p_i = \left.\frac{\partial p}{\partial i}\right|_\rho$ of the equation of state (2.7) can be determined.

2.2 Jacobian

The Jacobian matrix $A = \frac{\partial \underset{\sim}{f}}{\partial \underset{\sim}{w}}$ has eigenvalues

$$\lambda_j = u \pm a, u, u, u \ , \quad j = 1, \ldots 5 \tag{2.8a-e}$$

with corresponding eigenvectors

$$\underset{\sim}{e}_{1,2} = \left(1, u \pm a, v, w, \frac{p}{\rho} + i + \tfrac{1}{2}q^2 \pm ua\right)^T \tag{2.9a-b}$$

$$\underset{\sim}{e}_3 = \left[1, u, v, w, \tfrac{1}{2}q^2 + i - \frac{\rho p_\rho}{p_i}\right] \tag{2.9c}$$

$$\underset{\sim}{e}_4 = (0, 0, 1, 0, v)^T \tag{2.9d}$$

and

$$\underset{\sim}{e}_5 = (0, 0, 0, 1, w)^T \ , \tag{2.9e}$$

where the fluid speed q and sound speed a are given by

$$q^2 = u^2 + v^2 + w^2 \tag{2.10}$$

and

$$a^2 = \frac{pp_i}{\rho^2} + p_\rho \ . \tag{2.11}$$

Similar expressions can be found for the Jacobians $\frac{\partial \underset{\sim}{g}}{\partial \underset{\sim}{w}}$ and $\frac{\partial \underset{\sim}{h}}{\partial \underset{\sim}{w}}$.

In the next section we develop an approximate Riemann solver using the results of this section.

3. APPROXIMATE RIEMANN SOLVER

In this section we develop an approximate Riemann solver for the Euler equations in three dimensions with a general convex equation of state incorporating the technique of operator splitting.

We seek to solve equations (2.1)-(2.7) approximately using operator splitting, i.e. we solve successively

$$\underset{\sim}{w}_t + \underset{\sim}{f}_x = \underset{\sim}{0} \ , \tag{3.1a}$$

$$\underset{\sim}{w}_t + \underset{\sim}{g}_y = \underset{\sim}{0} \tag{3.1b}$$

and

$$\underset{\sim}{w}_t + \underset{\sim}{h}_z = \underset{\sim}{0} \tag{3.1c}$$

along x,y and z-coordinate lines, repectively. We consider approximate solutions of equation (3.1a); then a similar analysis will give approximate solutions of equations (3.1b-c).

3.1 Parameterisation of the equation of state.

The equation of state for an ideal gas is given by

$$p = (\gamma - 1)\rho i \tag{3.2}$$

where γ is a constant and represents the ratio of specific heat capacities of the fluid. Following this, for a general equation of state $p = p(\rho,i)$ we define a new dependent variable $\gamma = \gamma(\rho,i)$ by

$$\gamma = \frac{p}{\rho i} + 1 \qquad (3.3)$$

so that the equation of state (3.7) can be rewritten as

$$p = (\gamma(\rho,i) - 1)\rho i \quad . \qquad (3.4)$$

(Many equations of state for real gases are already given in the form of equation (3.4).) Thus, $\gamma \equiv$ constant identifies an ideal gas.

From equation (3.3), the eigenvectors $\underset{\sim}{e}_{1,2}$ of equations (2.9a-b) can be written in terms of γ as

$$\underset{\sim}{e}_{1,2} = (1, u \pm a, v, w, \frac{\gamma p}{(\gamma-1)\rho} + \tfrac{1}{2}q^2 \pm ua)^T \quad . \qquad (3.5a\text{-}b)$$

In particular, for the ideal equation of state (3.2) the sound speed a is given by equation (2.11) as

$$a^2 = \frac{\gamma p}{\rho} \quad , \qquad (3.6)$$

and the fifth component of $\underset{\sim}{e}_3$ given by equation (2.9c) becomes $\tfrac{1}{2}q^2$ since $i - \frac{\rho p_\rho}{p_i} = 0$.

3.2 Wavespeeds for nearby states.

Following Godunov [4], we consider the solution at any time to consist of a series of piecewise constant states. Our aim is then to solve each of these linearised Riemann problems approximately. Consider two (constant) adjacent states $\underset{\sim}{w}_L, \underset{\sim}{w}_R$ (left and right) close to an average state $\underset{\sim}{w}$, at points L and R on an x-coordinate line. In particular, the variable γ given by equation (3.3) is piecewise constant. Now, in view of the sound speed a for ideal gases ($\gamma \equiv$ constant) given by equation (3.6) and the eigenvectors $\underset{\sim}{e}_{1,2}$ given by equations (3.5a-b), we assume that we have approximate eigenvectors

$$\underset{\sim}{r}_{1,2} = \left(1, u \pm a, v, w, \frac{a^2}{\gamma-1} + \tfrac{1}{2}(u^2+v^2+w^2) \pm ua\right)^T \qquad (3.7a\text{-}b)$$

corresponding to the average state $\underset{\sim}{w}$. (N.B. The quantity γ in equations (3.7a-b) represents an average value close to γ_L and γ_R.) In addition, because $i - \dfrac{\rho p_\rho}{p_i} = 0$ for an ideal gas, we split $\underset{\sim}{e}_3$ into two vectors as

$$\underset{\sim}{r}'_3 = \left(1, u, v, w, \tfrac{1}{2}(u^2 + v^2 + w^2)\right)^T \qquad (3.8)$$

and

$$\underset{\sim}{r}'_6 = (0,0,0,0,\beta)^T , \qquad (3.9)$$

where β represents an average value in the cell (x_L, x_R) of

$i - \rho p_{\rho/p_i}$. Finally, we approximate $\underset{\sim}{e}_{4,5}$ as

$$\underset{\sim}{r}_4 = (0,0,1,0,v)^T \tag{3.10}$$

and

$$\underset{\sim}{r}_5 = (0,0,0,1,w)^T \quad . \tag{3.11}$$

We now seek coefficients $\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5$ such that

$$\Delta\underset{\sim}{w} = \alpha_1\underset{\sim}{r}_1 + \alpha_2\underset{\sim}{r}_2 + \alpha_3\underset{\sim}{r}_3' + \alpha_4\underset{\sim}{r}_4 + \alpha_5\underset{\sim}{r}_5 + \underset{\sim}{r}_6' \tag{3.12a-f}$$

to within $O(\Delta^2)$, where $\Delta(\cdot) = (\cdot)_R - (\cdot)_L$. (N.B. The vector $\underset{\sim}{r}_6'$ is considered separately since it vanishes for an ideal gas. Also, we do not introduce another coefficient α_6 since $\underset{\sim}{r}_6'$ has only one non-zero component and is therefore not required.)

From equations (3.12a) and (3.12c-d) we obtain

$$\alpha_4 = \Delta(\rho v) - v\Delta\rho \tag{3.13}$$

$$\alpha_5 = \Delta(\rho w) - w\Delta\rho \quad , \tag{3.14}$$

but

$$\Delta(\rho U) = \rho\Delta U + U\Delta\rho \quad , \qquad U = u,v \text{ or } w \tag{3.15a-c}$$

to within $O(\Delta^2)$, so that

$$\alpha_4 = \rho\Delta v \tag{3.16}$$

and

$$\alpha_5 = \rho\Delta w \quad . \tag{3.17}$$

Also, from equations (3.12a-b) and (3.15a) we find that

$$a(\alpha_1 - \alpha_2) = \rho\Delta u \quad . \tag{3.18}$$

Using equations (3.12a) and (3.16)-(3.18) together with the relationships

$$\Delta(\rho u^2) = U^2\Delta\rho + 2\rho U\Delta U \ , \quad U = u,v \text{ or } w \tag{3.19a-c}$$

to within $O(\Delta^2)$, equation (3.12f) yields

$$\Delta(\rho i) = \frac{a^2}{\gamma-1}\Delta\rho - \frac{a^2}{\gamma-1}\alpha_3 + \beta\alpha_6 \quad . \tag{3.20}$$

However, we also know that $\rho i = \frac{p}{\gamma-1}$, therefore

$$\begin{aligned} \Delta(\rho i) = \Delta\left[\frac{p}{\gamma-1}\right] &= \frac{\Delta p}{\gamma-1} - \frac{p}{(\gamma-1)^2}\Delta\gamma \\ &= \frac{\Delta p}{\gamma-1} - \frac{\rho i}{\gamma-1}\Delta\gamma \end{aligned} \tag{3.21}$$

to within $O(\Delta^2)$, and thus equation (3.20) gives

$$\alpha_3 - \left[\Delta\rho - \frac{\Delta p}{a^2}\right] = \frac{(\gamma-1)}{a^2}\left[\beta + \frac{\rho i\Delta\gamma}{\gamma-1}\right] \quad . \tag{3.22}$$

In the ideal case $\gamma \equiv$ constant, so that $\Delta\gamma = 0$ and $i - \frac{\rho p_\rho}{p_i} = 0$, i.e. $\beta = 0$ for consistency and thus $\alpha_3 = \Delta\rho - \frac{\Delta p}{a^2}$. In the general case we would like $\alpha_3 \to \Delta\rho - \frac{\Delta p}{a^2}$ as $\Delta\gamma \to 0$, and thus we set

$$\beta = -\frac{\rho i \Delta\gamma}{\gamma-1} \tag{3.23}$$

so that

$$\alpha_3 = \Delta\rho - \frac{\Delta p}{a^2} . \tag{3.24}$$

Finally, equations (3.18) and (3.24) yield

$$\alpha_{1,2} = \frac{1}{2a^2}(\Delta p \pm \rho a \Delta u) . \tag{3.25a-b}$$

The results above imply an approximation to the eigenvector $\underset{\sim}{e}_3$ given by $\underset{\sim}{r}_3 = \underset{\sim}{r}'_3 + \underset{\sim}{r}'_6/\alpha_3$, i.e. $\underset{\sim}{r}_3 = \left[1,u,v,w,\tfrac{1}{2}(u^2+v^2+w^2) - \frac{\rho i \Delta\gamma}{(\gamma-1)\left[\Delta\rho-\frac{\Delta p}{a^2}\right]}\right]^T$, and hence an approximation to $i - \frac{\rho p_\rho}{p_i}$.

We have found $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ and α_5 such that

$$\Delta\underset{\sim}{w} = \sum_{j=1}^{5} \alpha_j \underset{\sim}{r}_j \tag{3.26}$$

to within $O(\Delta^2)$ and a routine calculation verifies that

$$\Delta \underset{\sim}{f} = \sum_{j=1}^{5} \lambda_j \alpha_j \underset{\sim}{r}_j \tag{3.27}$$

to within $O(\Delta^2)$. We are now in a position to construct the approximate Riemann solver.

3.3 Decomposition for general $\underset{\sim}{w}_L, \underset{\sim}{w}_R$

Consider the algebraic problem of finding average eigenvalues $\tilde{\lambda}_1, \tilde{\lambda}_2, \tilde{\lambda}_3, \tilde{\lambda}_4, \tilde{\lambda}_5$ and corresponding average eigenvectors $\tilde{\underset{\sim}{r}}_1, \tilde{\underset{\sim}{r}}_2, \tilde{\underset{\sim}{r}}_3, \tilde{\underset{\sim}{r}}_4, \tilde{\underset{\sim}{r}}_5$ such that relations (3.26) and (3.27) hold exactly for arbitrary states $\underset{\sim}{w}_L, \underset{\sim}{w}_R$ not necessarily close. Specifically, we seek averages $\tilde{\rho}, \tilde{u}, \tilde{v}, \tilde{w}, \tilde{a}, \tilde{\gamma}$ and $\tilde{i}$ in terms of two adjacent states $\underset{\sim}{w}_L, \underset{\sim}{w}_R$ (on an x-coordinate line) such that

$$\Delta \underset{\sim}{w} = \sum_{j=1}^{5} \tilde{\alpha}_j \tilde{\underset{\sim}{r}}_j \tag{3.28}$$

and

$$\Delta \underset{\sim}{f} = \sum_{j=1}^{5} \tilde{\lambda}_j \tilde{\alpha}_j \tilde{\underset{\sim}{r}}_j \ . \tag{3.29}$$

where

$$\Delta(\cdot) = (\cdot)_R - (\cdot)_L \ . \tag{3.30}$$

$$\underset{\sim}{w} = (\rho, \rho u, \rho v, \rho w, e)^T \ , \tag{3.31}$$

$$\underset{\sim}{f}(\underset{\sim}{w}) = (\rho u, p+\rho u^2, \rho uv, \rho uw, u(e+p))^T , \tag{3.32}$$

$$e = \rho i + \tfrac{1}{2}\rho u^2 + \tfrac{1}{2}\rho v^2 + \tfrac{1}{2}\rho w^2 , \tag{3.33}$$

$$p = p(\rho, i) , \tag{3.34}$$

$$\gamma = \frac{p}{\rho i} + 1 , \tag{3.35}$$

$$\tilde{\lambda}_{1,2,3,4,5} = \tilde{u} \pm \tilde{a}, \tilde{u}, \tilde{u}, \tilde{u} , \tag{3.36a-e}$$

$$\underset{\sim}{\tilde{r}}_1 = \left(1, \tilde{u}\pm\tilde{a}, \tilde{v}, \tilde{w}, \frac{\tilde{a}^2}{\tilde{\gamma}-1} + \tfrac{1}{2}(\tilde{u}^2+\tilde{v}^2+\tilde{w}^2) \pm \tilde{\tilde{\rho}}\tilde{u}\tilde{a}\right) , \tag{3.37a-b}$$

$$\underset{\sim}{\tilde{r}}_3 = \left[1, \tilde{u}, \tilde{v}, \tilde{w}, \tfrac{1}{2}(\tilde{u}^2+\tilde{v}^2+\tilde{w}^2) - \frac{\tilde{\tilde{\rho}}\tilde{i}\Delta\gamma}{(\tilde{\gamma}-1)(\Delta\rho - \Delta p/\tilde{a}^2)}\right] , \tag{3.37c}$$

$$\underset{\sim}{\tilde{r}}_4 = (0,0,1,0,\tilde{v})^T , \tag{3.37d}$$

$$\underset{\sim}{\tilde{r}}_5 = (0,0,0,1,\tilde{w})^T , \tag{3.38e}$$

$$\tilde{\alpha}_{1,2} = \frac{1}{2\tilde{a}^2}(\Delta p \pm \tilde{\tilde{\rho}}\tilde{a}\Delta u) , \tag{3.39a-b}$$

$$\tilde{\alpha}_3 = \Delta\rho - \frac{\Delta p}{\tilde{a}^2} , \tag{3.39c}$$

$$\tilde{\alpha}_4 = \tilde{\rho}\Delta v \tag{3.39d}$$

and

$$\tilde{\alpha}_5 = \tilde{\rho}\Delta w \ . \tag{3.39e}$$

We note that the solution to this problem is equivalent to seeking an approximation to the Jacobian A, namely $\tilde{A}$, with eigenvalues $\tilde{\lambda}_i$ and eigenvectors $\tilde{\underset{\sim}{r}}_i$, such that

$$\Delta \underset{\sim}{f} = \tilde{A}\Delta \underset{\sim}{w} \ . \tag{3.40}$$

The first step in the analysis of the above problem is to write out equations (3.28) and (3.29) explicitly, namely,

$$\Delta\rho = \tilde{\alpha}_1 + \tilde{\alpha}_2 + \tilde{\alpha}_3 \ , \tag{3.41a}$$

$$\Delta(\rho u) = \tilde{\alpha}_1(\tilde{u}+\tilde{a}) + \tilde{\alpha}_2(\tilde{u}-\tilde{a}) + \tilde{\alpha}_3\tilde{u} \ , \tag{3.41b}$$

$$\Delta(\rho v) = \tilde{\alpha}_1\tilde{v} + \tilde{\alpha}_2\tilde{v} + \tilde{\alpha}_3\tilde{v} + \tilde{\alpha}_4 \ , \tag{3.41c}$$

$$\Delta(\rho w) = \tilde{\alpha}_1\tilde{w} + \tilde{\alpha}_2\tilde{w} + \tilde{\alpha}_3\tilde{w} + \tilde{\alpha}_5 \ , \tag{3.41d}$$

$$\begin{aligned} \Delta e = \Delta\left[\rho i + \frac{\rho q^2}{2}\right] &= \tilde{\alpha}_1\left[\frac{\tilde{a}^2}{\tilde{\gamma}-1} + \tfrac{1}{2}\tilde{q}^2 + \tilde{u}\tilde{a}\right] \\ &+ \tilde{\alpha}_2\left[\frac{\tilde{a}^2}{\tilde{\gamma}-1} + \tfrac{1}{2}\tilde{q}^2 - \tilde{u}\tilde{a}\right] \\ &+ \tilde{\alpha}_3\tfrac{1}{2}\tilde{q}^2 - \frac{\tilde{\rho}\tilde{i}\Delta\gamma}{\tilde{\gamma}-1} \\ &+ \tilde{\alpha}_4\tilde{v} + \tilde{\alpha}_5\tilde{w} \ , \end{aligned} \tag{3.41e}$$

$$\Delta(\rho u) = \tilde{\alpha}_1(\tilde{u}+\tilde{a}) + \tilde{\alpha}_2(\tilde{u}-\tilde{a}) + \tilde{\alpha}_3\tilde{u} \quad , \tag{3.41f}$$

$$\Delta(p+\rho u^2) = \Delta p + \Delta(\rho u^2) = \tilde{\alpha}_1(\tilde{u}+\tilde{a})^2 + \tilde{\alpha}_2(\tilde{u}-\tilde{a})^2 + \tilde{\alpha}_3\tilde{u}^2 \quad , \tag{3.41g}$$

$$\Delta(\rho uv) = \tilde{\alpha}_1(\tilde{u}+\tilde{a})\tilde{v} + \tilde{\alpha}_2(\tilde{u}-\tilde{a})\tilde{v} + \tilde{\alpha}_3\tilde{\tilde{uv}} + \tilde{\alpha}_4\tilde{u} \quad , \tag{3.41h}$$

$$\Delta(\rho uw) = \tilde{\alpha}_1(\tilde{u}+\tilde{a})\tilde{w} + \tilde{\alpha}_2(\tilde{u}-\tilde{a})\tilde{w} + \tilde{\alpha}_3\tilde{\tilde{uw}} + \tilde{\alpha}_5\tilde{u} \quad , \tag{3.41i}$$

$$\begin{aligned}\Delta(u(e+p)) &= \Delta(up i+up) + \Delta\left[\frac{\rho uq^2}{2}\right] \\ &= \tilde{\alpha}_1(\tilde{u}+\tilde{a})\left[\frac{a^2}{\tilde{\gamma}-1} + \tfrac{1}{2}\tilde{q}^2 + \tilde{\tilde{ua}}\right] \\ &+ \tilde{\alpha}^2(\tilde{u}-\tilde{a})\left[\frac{\tilde{a}^2}{\tilde{\gamma}-1} + \tfrac{1}{2}\tilde{q}^2 - \tilde{\tilde{ua}}\right] \\ &+ \tilde{\alpha}_3\tilde{u}\tfrac{1}{2}\tilde{q}^2 - \frac{\tilde{\tilde{\tilde{up}}}\tilde{i}}{\tilde{\gamma}-1}\Delta\gamma \\ &+ \tilde{\alpha}_4\tilde{\tilde{uv}} + \tilde{\alpha}_5\tilde{\tilde{uw}} \quad ,\end{aligned} \tag{3.41j}$$

where

$$q^2 = u^2 + v^2 + w^2 \quad , \tag{3.42}$$

as before, and for convenience we have written

$$\tilde{q}^2 = \tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2 \quad . \tag{3.43}$$

Equation (3.41a) is satisfied by any average we care to define, while equation (3.41b) is the same as equation (3.41f); thus it remains to

solve equations (3.41c-j). From equations (3.41a) and (3.41f-g) we obtain a quadratic equation for $\tilde{u}$ whose only productive solution is

$$\tilde{u} = \frac{\sqrt{\rho_L}\, u_L + \sqrt{\rho_R}\, u_R}{\sqrt{\rho_L} + \sqrt{\rho_R}} . \tag{3.44}$$

In addition, from equations (3.41a), (3.41f) and (3.44) we find that

$$\tilde{\rho} = \frac{\Delta(\rho u) - \tilde{u}\Delta\rho}{\Delta u} = \sqrt{\rho_L \rho_R} . \tag{3.45}$$

Also, from equations (3.41a), (3.41c-d) and (3.45) we obtain

$$\tilde{v} = \frac{\Delta(\rho v) - \rho\Delta v}{\Delta\rho} = \frac{\sqrt{\rho_L}\, v_L + \sqrt{\rho_R}\, v_R}{\sqrt{\rho_L} + \sqrt{\rho_R}} \tag{3.46}$$

with a similar expression for $\tilde{w}$. The results given by equations (3.44)-(3.46) are identical with the ideal case given in [1].

We have now determined $\tilde{\rho}, \tilde{u}, \tilde{v}$ and $\tilde{w}$ and in view of equations (3.44)-(3.46) we can show that equations (3.41h-i) are automatically satisfied.

We are now left with equations (3.41e) and (3.41j), and noting the identity

$$\Delta\left[\frac{\rho q^2}{2}\right] - \tfrac{1}{2}\tilde{q}^2\Delta\rho - \rho(\tilde{u}\Delta u+\tilde{v}\Delta v+\tilde{w}\Delta w) = 0 , \qquad (3.47)$$

equation (3.41e) yields

$$(\tilde{\gamma}-1)\Delta(\rho i) + \tilde{\rho}\tilde{i}\Delta\gamma - \Delta p = 0 . \qquad (3.48)$$

If we define averages $\hat{\gamma}$ and $\hat{i}$ by

$$\hat{S} = \frac{\sqrt{\rho_L}\, S_L + \sqrt{\rho_R}\, S_R}{\sqrt{\rho_L} + \sqrt{\rho_R}} , \quad S = \gamma \text{ or } i , \qquad (3.49a\text{-}b)$$

we obtain the following identities

$$\Delta(\rho i) = \tilde{\rho}\Delta i + \hat{i}\Delta\rho , \qquad (3.50)$$

and

$$\begin{aligned} \Delta p &= \Delta(\rho i(\gamma-1)) \\ &= (\hat{\gamma}-1)\tilde{\rho}\Delta i + (\hat{\gamma}-1)\hat{i}\Delta\rho + \tilde{\rho}\hat{i}\Delta\gamma , \end{aligned} \qquad (3.51)$$

so that equation (3.48) yields

$$(\tilde{\gamma}-\hat{\gamma})\hat{i}\Delta\rho + (\tilde{\gamma}-\hat{\gamma})\tilde{\rho}\Delta i + \tilde{\rho}(\tilde{i}-\hat{i})\Delta\gamma = 0 . \qquad (3.52)$$

The only physical solution of equation (3.52) for all variations $\Delta\rho$, Δi and $\Delta\gamma$ is

$$\tilde{\gamma} = \hat{\gamma} \text{ and } \tilde{i} = \hat{i} , \qquad (3.53a\text{-}b)$$

given by equations (3.49a-b). It now remains to determine $\tilde{a}$.

We begin by subtracting equation (3.41e) multiplied by $\tilde{u}$ from equation (3.41j) to give

$$\frac{\tilde{a}^2\rho}{\tilde{\gamma}-1}\Delta u = \Delta(u\rho i+up) - \tilde{u}\Delta(\rho i) - \tilde{u}\Delta p$$

$$+ \Delta\left[u\frac{\rho q^2}{2}\right] - \tilde{u}\Delta\left[\frac{\rho q^2}{2}\right] - \tfrac{1}{2}\rho\tilde{q}^2\Delta u \ , \qquad (3.54)$$

which determines $\tilde{a}$. Simplifying equation (3.54) using the following identities

$$\Delta(u(\rho i+p)) - \tilde{u}\Delta(\rho i+p) = \frac{\tilde{\rho}\left[\sqrt{\rho_L}\left[i_L + \frac{p_L}{\rho_L}\right] + \sqrt{\rho_R}\left[i_R + \frac{p_R}{\rho_R}\right]\right]\Delta u}{\sqrt{\rho_L} + \sqrt{\rho_R}} \qquad (3.55)$$

and

$$\Delta\left[u\frac{\rho q^2}{2}\right] - \tilde{u}\Delta\left[\frac{\rho q^2}{2}\right] = \frac{\tilde{\rho}\left[\sqrt{\rho_L}\,\tfrac{1}{2}q_L^2 + \sqrt{\rho_R}\,\tfrac{1}{2}q_R^2\right]\Delta u}{\sqrt{\rho_L} + \sqrt{\rho_R}} \qquad (3.56)$$

we find that, after division by $\tilde{\rho}\Delta u$,

$$\tilde{a}^2 = (\tilde{\gamma}-1)(\tilde{H} - \tfrac{1}{2}\tilde{q}^2) \ , \qquad (3.57)$$

where $\tilde{H}$ is a mean enthalpy given by

$$\tilde{H} = \frac{\sqrt{\rho_L}\,H_L + \sqrt{\rho_R}\,H_R}{\sqrt{\rho_L} + \sqrt{\rho_R}} \qquad 83.58)$$

and

$$H_{L(R)} = \frac{p_{L(R)}}{\rho_{L(R)}} + i_{L(R)} + \tfrac{1}{2}q^2_{L(R)}$$

$$= \frac{\gamma_{L(R)}p_{L(R)}}{(\gamma_{L(R)}{}^{-1})\rho_{L(R)}} + \tfrac{1}{2}q^2_{L(R)} \ . \qquad (3.59)$$

(N.B. If we explicitly write out equation (3.57) we obtain

$$\tilde{a}^2 = \frac{\left[\sqrt{\rho_L}\,\frac{p_L}{\rho_L i_L} + \sqrt{\rho_R}\,\frac{p_R}{\rho_R i_R}\right]}{\sqrt{\rho_L} + \sqrt{\rho_R}}\left[\frac{\sqrt{\rho_L}\,\left[p_L/\rho_L + i_L\right] + \sqrt{\rho_R}\,\left[p_R/\rho_R + i_R\right]}{\sqrt{\rho_L} + \sqrt{\rho_R}}\right.$$

$$\left. + \frac{\sqrt{\rho_L \rho_R}\,(u_R - u_L)^2}{(\sqrt{\rho_L} + \sqrt{\rho_R})^2}\right]$$

which ensures that $\tilde{a}^2$ is positive for real data.)

By symmetry, similar results hold for the Jacobians $\frac{\partial g}{\partial w}$ and $\frac{\partial h}{\partial w}$.

Summarising, we can now apply the Riemann solver given above to the three-dimensional Euler equations with a general convex equation of state using the technique of operator splitting. We incorporate the results found here, together with the one-dimensional scalar upwind algorithm given by Roe and Baines [5], and perform a sequence of one-dimensional calculations along computational grid lines in the x,y and z-directions in turn. The algorithm along a line y = constant, z = constant can be described as follows. Suppose at time level n we have data w_L, w_R given at either end of the cell (x_L, x_R), (on a line $y = y_0, z = z_0$), then we update w to time level n+1 in an upwind manner. Thus we

$$\text{add } -\frac{\Delta t}{\Delta x}\tilde{\lambda}_j \tilde{\alpha}_j \tilde{r}_j \text{ to } w_R \text{ if } \tilde{\lambda}_j > 0$$

or

$$\text{add } -\frac{\Delta t}{\Delta x}\tilde{\lambda}_j \tilde{\alpha}_j \tilde{r}_j \text{ to } w_L \text{ if } \tilde{\lambda}_j < 0$$

where $\Delta x = x_R - x_L$, Δt is the time interval from level n to n+1 , and $\tilde{\lambda}_j, \tilde{\alpha}_j, \tilde{r}_j$ are given by

$$\tilde{\lambda}_{1,2,3,4,5} = \tilde{u} \pm \tilde{a}, \tilde{u}, \tilde{u}, \tilde{u} ,$$

$$\tilde{r}_{1,2} = (1, \tilde{u} \pm \tilde{a}, \tilde{v}, \tilde{w}, \tilde{H} \pm \tilde{u}\tilde{a})^T ,$$

$$\tilde{r}_3 = \left[1, \tilde{u}, \tilde{v}, \tilde{w}, \tfrac{1}{2}\tilde{q}^2 - \frac{\tilde{\rho}\tilde{i}\Delta\gamma}{(\tilde{\gamma}-1)\left[\Delta\rho - \frac{\Delta p}{\tilde{a}^2}\right]} \right]^T ,$$

$$\tilde{r}_4 = (0,0,1,0,\tilde{v})^T ,$$

$$\tilde{r}_5 = (0,0,0,1,\tilde{w})^T ,$$

$$\tilde{\alpha}_{1,2,3,4,5} = \frac{1}{2\tilde{a}^2}\left[\Delta p \pm \tilde{\rho}\tilde{a}\Delta u\right], \Delta\rho - \frac{\Delta p}{\tilde{a}^2}, \tilde{\rho}\Delta v, \tilde{\rho}\Delta w,$$

$$\tilde{\rho} = \sqrt{\rho_L \rho_R} , \quad \tilde{U} = \frac{\sqrt{\rho_L}\, U_L + \sqrt{\rho_R}\, U_R}{\sqrt{\rho_L} + \sqrt{\rho_R}} , \quad U = u, v, w, i, \gamma \text{ or } H$$

$$\tilde{q}^2 = \tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2 , \qquad \tilde{a}^2 = (\tilde{\gamma}-1)(\tilde{H} - \tfrac{1}{2}\tilde{q}^2) ,$$

$$\gamma_{L(R)} = \frac{p(\rho_{L(R)}, i_{L(R)})}{\rho_{L(R)} i_{L(R)}} + 1$$

and $\Delta(\cdot) = (\cdot)_R - (\cdot)_L$. Similar results apply for updating in the y and z directions.

The Riemann solver we have constructed in this section is a conservative algorithm (when incorporated with operator splitting) and has the important one-dimensional shock recognising property guaranteed by equations (3.28) and (3.29). Furthermore, the algorithm is efficient in the sense that to accommodate a non-ideal gas requires an

overhead of only a few per cent c.p.u. time; in particular, only one function evaluation of the equation of state is required in each computational cell.

In the next section we give the numerical results achieved for two standard test problems in gas dynamics using the scheme of this section.

4. NUMERICAL RESULTS

In this section we give the numerical results achieved for a one-dimensional test problem and a two-dimensional test problem using the scheme of §3.

Problem 1

This test problem is concerned with shock reflection in one-dimension of a gas governed by the Euler equations with a general equation of state. We consider a region $0 \leq x \leq 1$ divided into 50 equally spaced mesh points and the initial conditions are $(\rho,u,i,p) = (\rho_0,-u_0,i_0,p(\rho_0,i_0))$. This represents a gas of constant density and pressure moving towards the origin $x = 0$. The boundary at $x = 0$ is a rigid wall and the exact solution describes shock reflection from the wall. The equation of state chosen is that developed by R.K. Osborne at the Los Alamos Scientific Laboratory [6], and can be written in the form

$$\begin{aligned} p &= (1/(E+\phi_0))[\zeta(a_1+a_2|\zeta|) \\ &+ (b_0 + \zeta(b_1+b_2\zeta) + E(c_0+c_1\zeta))] \end{aligned}$$

where $E = \rho_0 i$, $\zeta = \frac{\rho}{\rho_0} - 1$ and the constants $\rho_0,a_1,a_2,b_0,b_1,b_2,c_1,c_2$ and ϕ_0 depend on the material in question. The particular case we choose corresponds to copper, where $\rho_0 = 8.9$, the remaining coefficients can be found in [6], and we specify $u_0 = 1$.

Three initial conditions are chosen for i_0 corresponding to shock strengths $p_+/p_0 = 100, 10$ and 2, where p_+ denotes the pressure behind the shock and $p_0 = p(\rho_0, i_0)$ denotes the pressure ahead of the shock. The results for these three cases are given in figures 1,2 and 3, together with the exact solution when the shock has moved a distance 0.3. We use the idea of flux limiters [7] to create a second order algorithm which is oscillation free, and we can modify the scheme to disperse entropy - violating solutions, (see [8]). The 'superbee' limiter is the one chosen here, (see [7]).

Problem 2

This two-dimensional test problem is concerned with Mach 3 flow in a tunnel containing a step and was originally introduced by Emery [9], but has recently been reviewed by Woodward and Colella [10]. The tunnel is 3 units long and 1 unit wide. The step is 0.2 units high and is located 0.6 units from the left hand end of the tunnel. At the left an inflow boundary condition is applied, and at the right, where the exit velocity is supersonic, all gradients are assumed to vanish. The initial conditions for the gas in the tunnel are given by $(\rho_0, u_0, v_0, p_0) = (1.4, 3, 0, 1)$ and hence i_0 from the equation of state $p_0 = p(\rho_0, i_0)$. Gas is continiually fed in at the left hand boundary with the flow variables taking the initial values given above.

The equation of state chosen is one for equilibrium air given by Srinivasan, Tannehill and Weilmuenster [3] and can be written as

$$p = (\bar{\gamma}-1)\rho i$$

where

$$\begin{aligned}\bar{\gamma} = \bar{\gamma}(\rho,i) = {} & a_1 + a_2Y + a_3Z + a_4YZ + a_5Y^2 + a_6Z^2 \\ & + a_7Y^2 + a_8YZ^2 + a_9Y^3 + a_{10}Z^3 \\ & + (a_{11} + a_{12}Y + a_{13}Z + a_{14}YZ + a_{15}Y^2 + a_{16}Z^2 + a_{17}Y^2Z \\ & + a_{18}YZ^2 + a_{19}Y^3 + a_{20}Z^3)/(1 + e^{(a_{21}+a_{22}Y+a_{23}Z+a_{24}YZ)})\end{aligned}$$

together with

$$\begin{aligned}Y &= \log_{10}(\rho/\rho_R) \\ Z &= \log_{10}(i/i_R)\end{aligned}$$

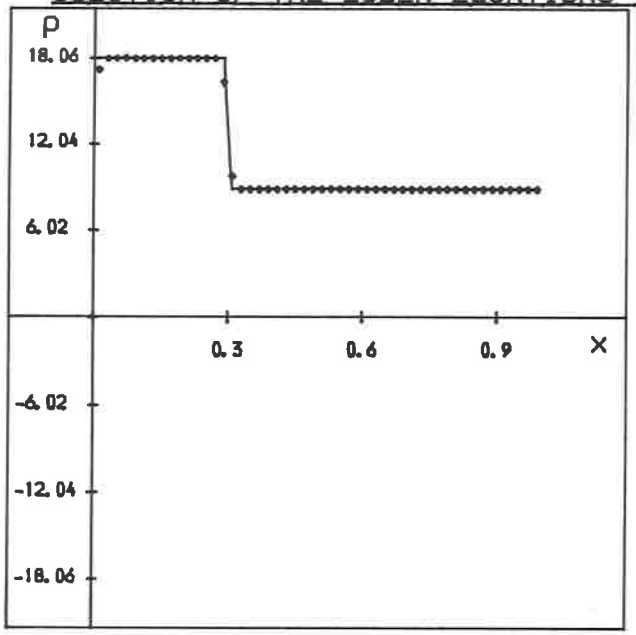
and ρ_R is a reference density and i_R is a reference internal energy. The constants a_i, $i = 1,\ldots 24$ can be found in [3]. Figures 4,5,6 and 7 display 31 equally spaced density contours at times $t = 0.5, 1.0, 1.5$ and 4.0, respectively. The figures represent formation of the bow shock, reflection at the upper wall, reflection at the lower wall, and formation of the Mach stem, respectively. A uniform 120×40 mesh was used and the second order scalar algorithm with the 'superbee' limiter, (see [7]).

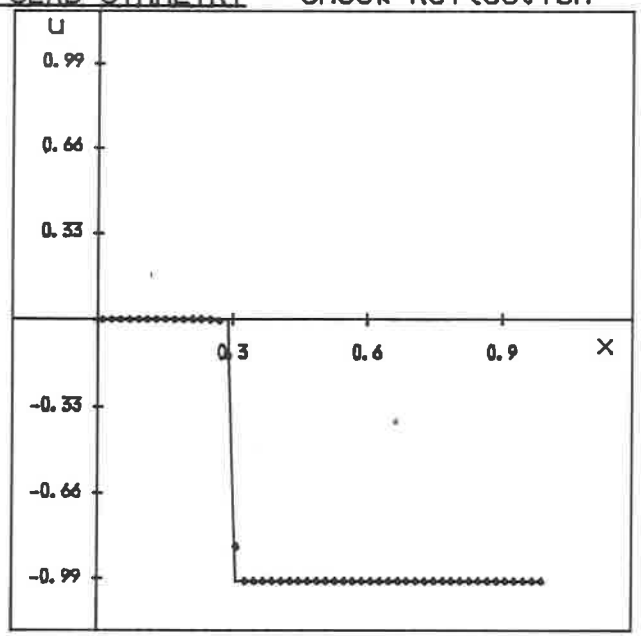
The algorithm described in §3 requires an overhead of only a few per cent over the ideal gas scheme in order to allow for non-ideal gases. Any additional expense depends on the complexity of the equation of state; however, as only one function call is required in each computational cell, this leads to an efficient algorithm.

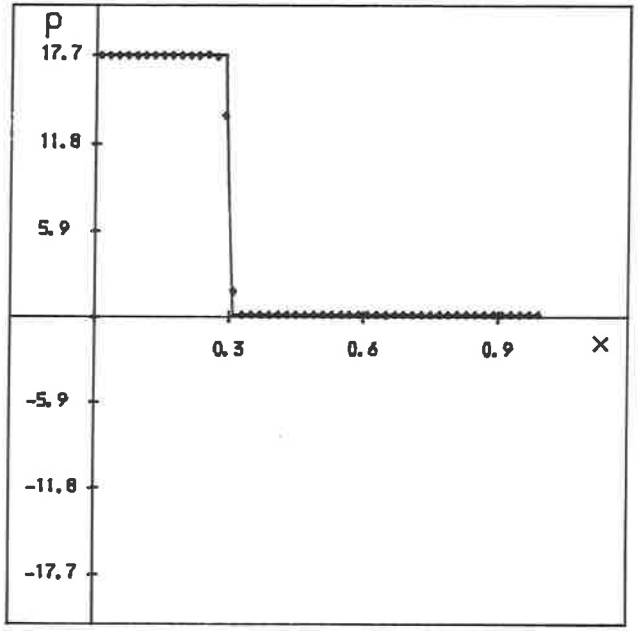
Furthermore, the satisfactory results found for Problems 1 and 2 show that no deterioration in the quality of the solution is incurred at the expense of an increase in efficiency.

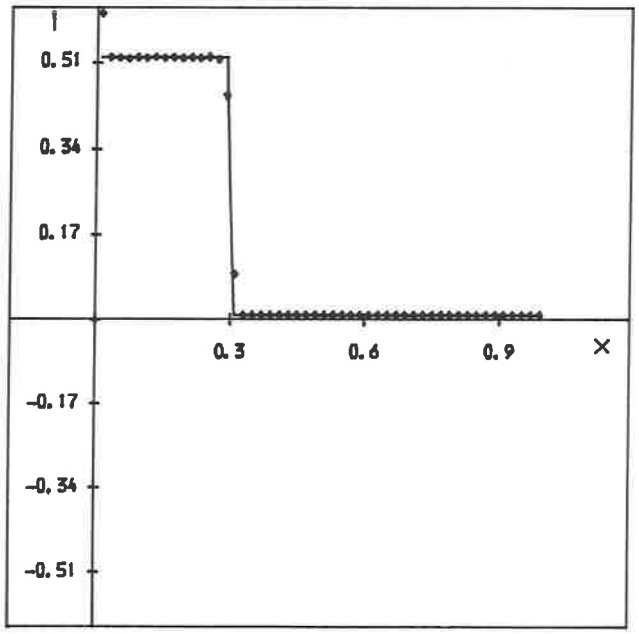
(N.B. For both problems we apply a reflection boundary condition at a rigid wall, i.e. we consider an image cell and impose equal density, pressure and tangential velocity (for two-dimensional problems), and equal and opposite normal velocity at either end of the cell.)

SOLUTION OF THE EULER EQUATIONS WITH SLAB SYMMETRY - Shock Reflection









at time t = 0.305

KEY

ρ - Density
u - Velocity
p - Pressure
I - Internal energy

—— Exact solution
◇◇◇◇◇◇ Approximate solution

PARAMETERS

General equation of state :
for Copper due to R.K. Osborne
50 Mesh points
63 Time steps
Δx = 0.02
Δt = 0.0048
Pressure ratio = 100
'Superbee' limiter used

INITIAL CONDITIONS

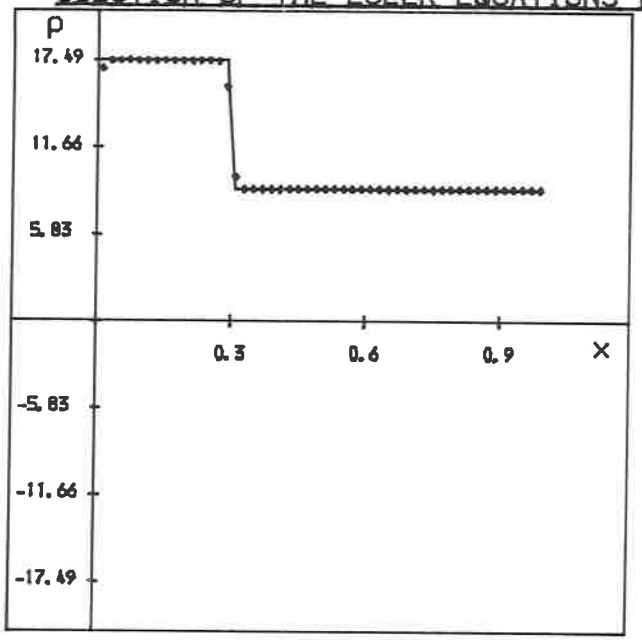
ρ =	8.900
u =	-1.000
p =	0.177
(I =	0.010)

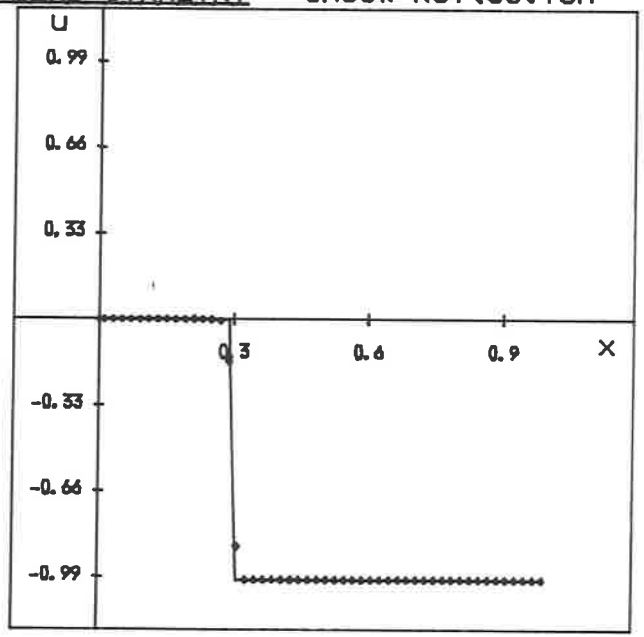
0 1

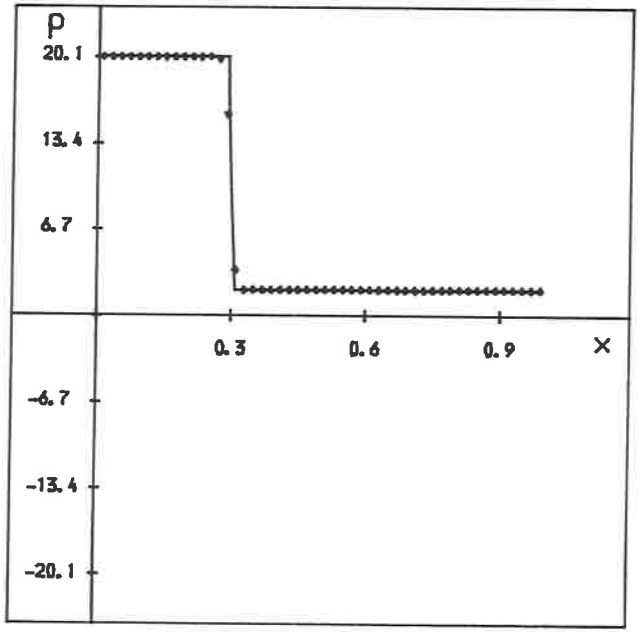
Reflected Boundary Conditions
at x = 0

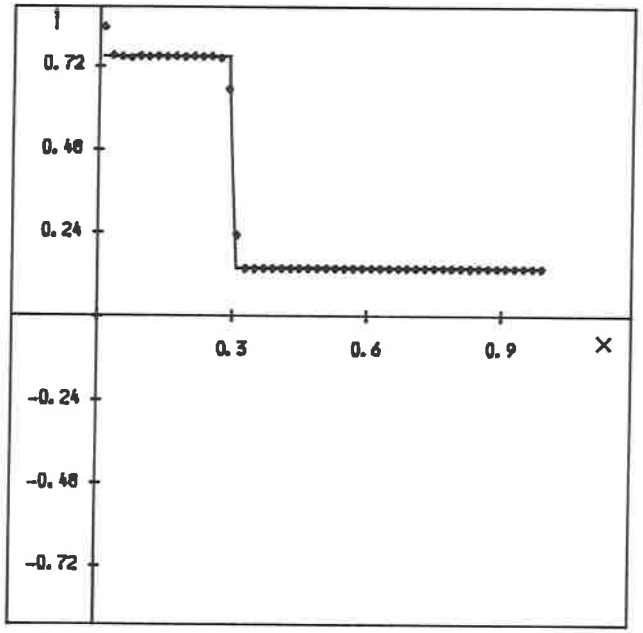
Figure 1

SOLUTION OF THE EULER EQUATIONS WITH SLAB SYMMETRY - Shock Reflection









at time t = 0.286

KEY

ρ - Density
u - Velocity
p - Pressure
I - Internal energy

—— Exact solution
◇◇◇◇◇◇ Approximate solution

PARAMETERS

General equation of state :
for Copper due to R.K. Osborne
50 Mesh points
67 Time steps
Δx = 0.02
Δt = 0.0043
Pressure ratio = 10
'Superbee' limiter used

INITIAL CONDITIONS

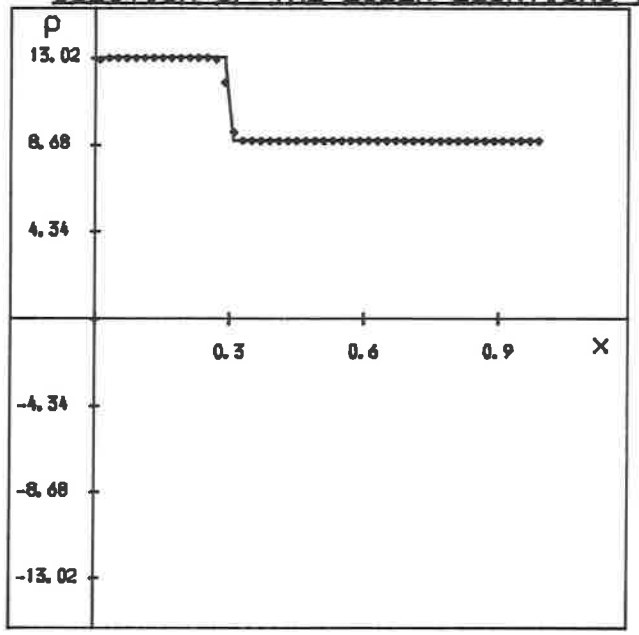
ρ =	8.900
u =	-1.000
p =	2.011
(I =	0.137)

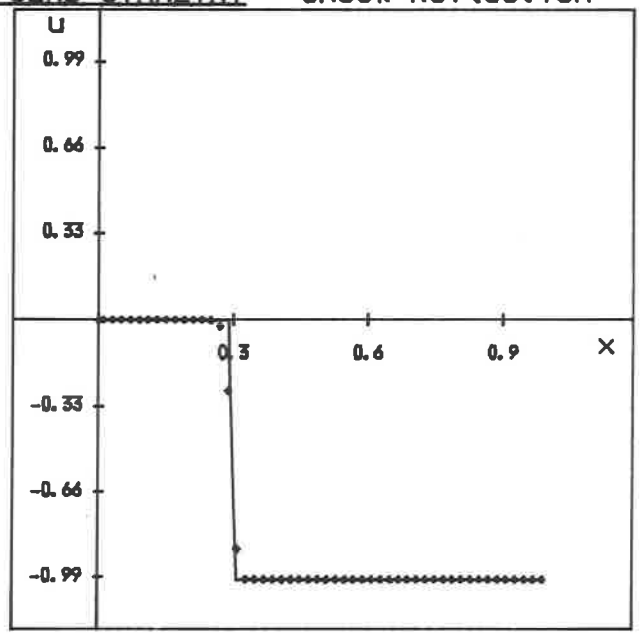
0 1

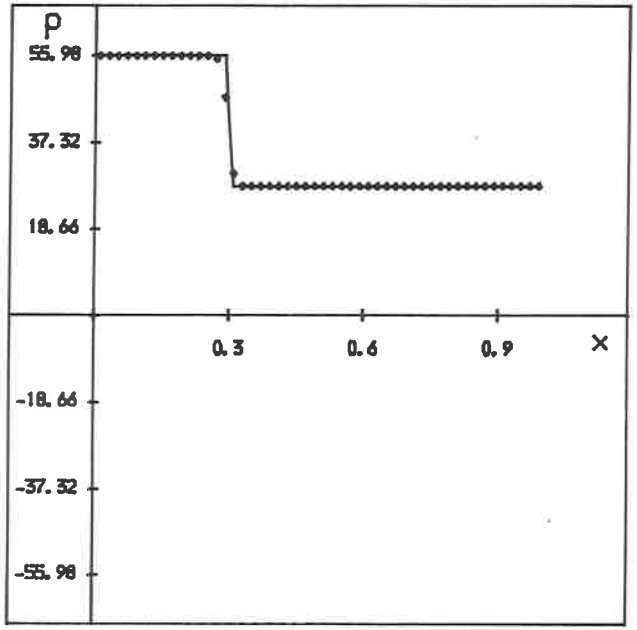
Reflected Boundary Conditions
at x = 0

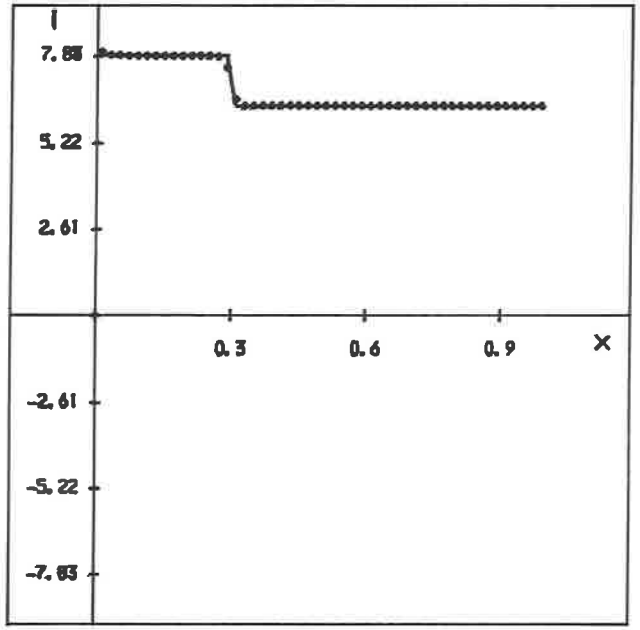
Figure 2

SOLUTION OF THE EULER EQUATIONS WITH SLAB SYMMETRY - Shock Reflection









at time t = 0.137

KEY

ρ - Density
u - Velocity
p - Pressure
I - Internal energy

—— Exact solution
◇◇◇◇◇◇ Approximate solution

PARAMETERS

General equation of state :
for Copper due to R.K. Osborne
50 Mesh points
58 Time steps
Δx = 0.02
Δt = 0.0024
Pressure ratio = 2
'Superbee' limiter used

INITIAL CONDITIONS

ρ = 8.900
u = -1.000
p = 28.000
(I = 6.348)

0 1

Reflected Boundary Conditions
at x = 0

Figure 3

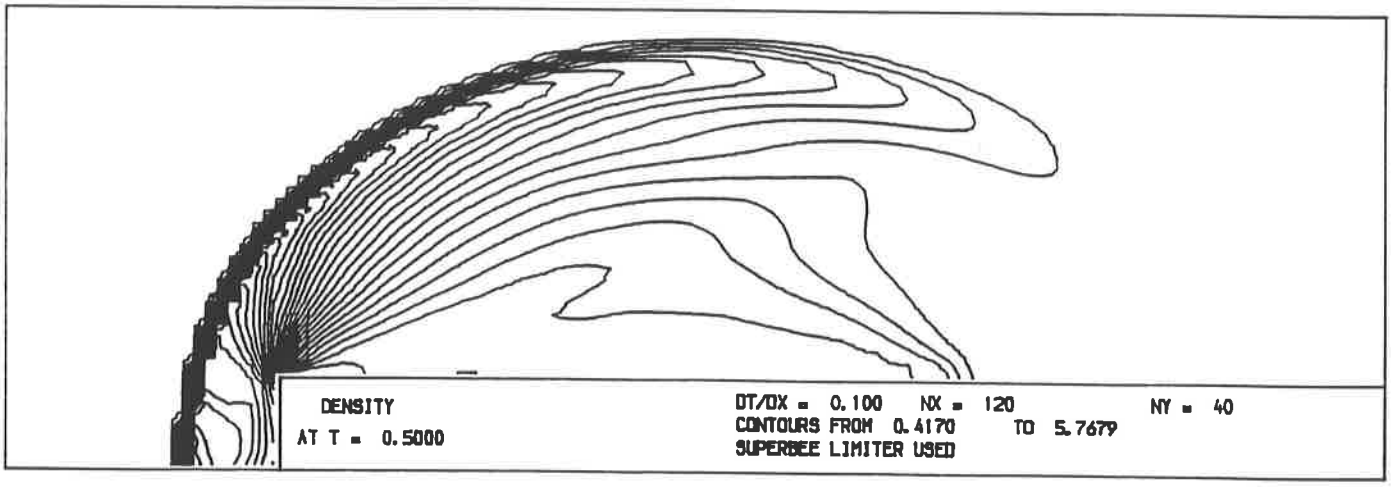


Figure 4

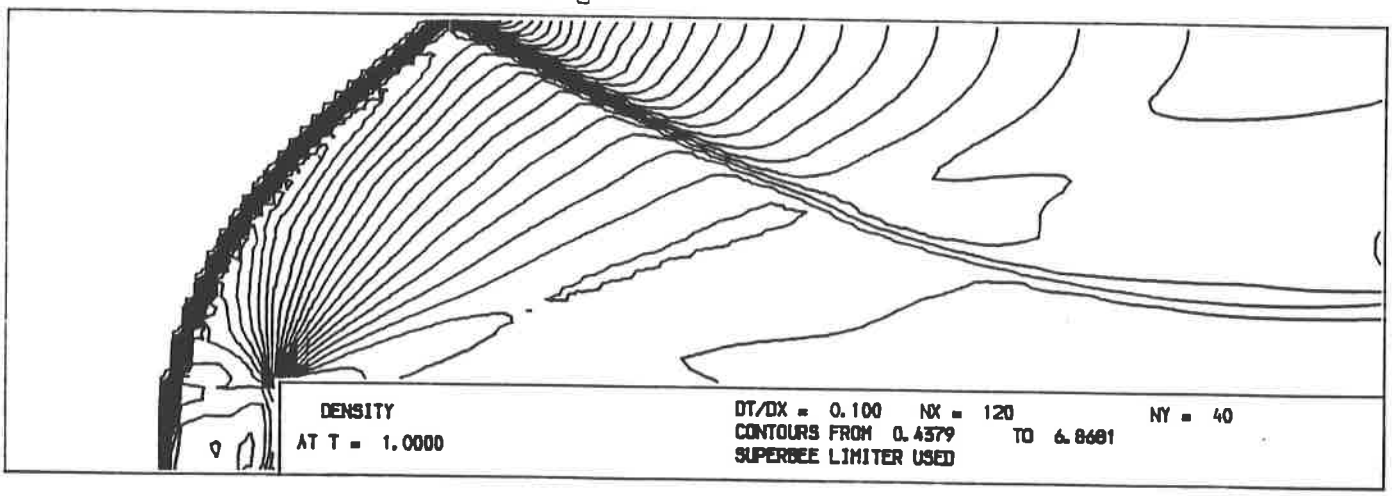


Figure 5

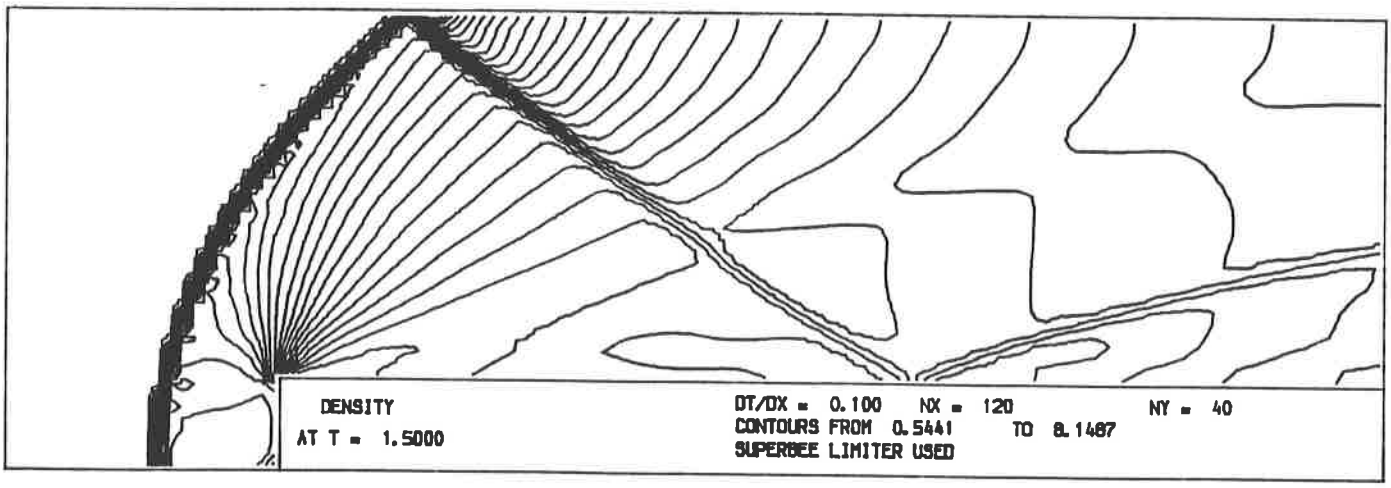


Figure 6

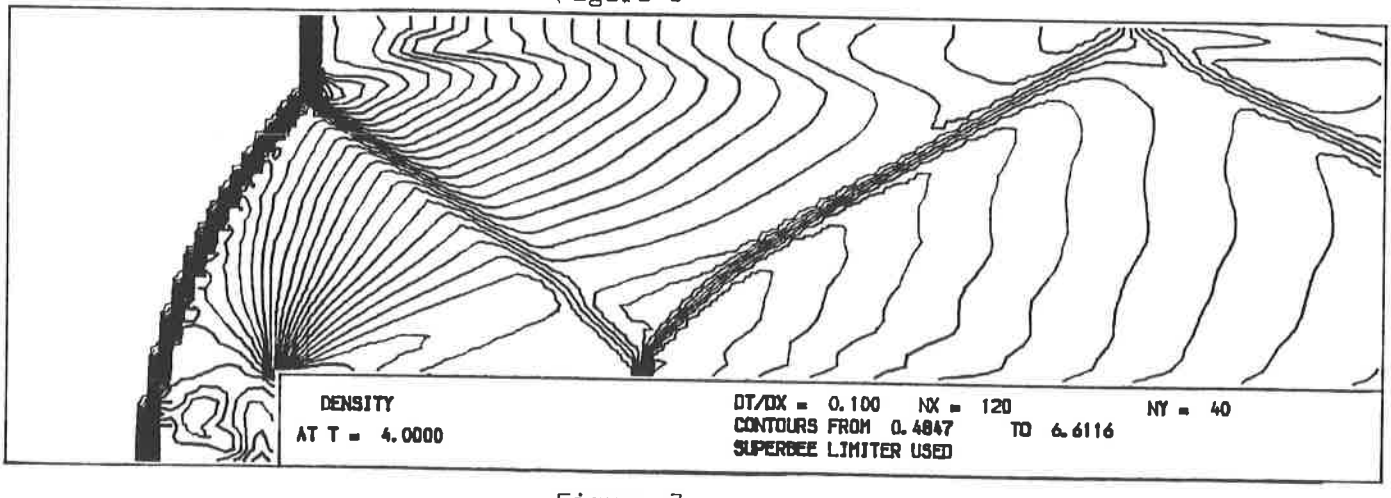


Figure 7

5. CONCLUSIONS

We have simplified the Riemann solver of Glaister [2] for the Euler equations with a general convex equation of state by local parameterisation of the equation of state. In doing so we have reduced the number of function calls to one per cell, but have retained the important shock capturing property. This results in an efficient algorithm that has produced satisfactory results for two standard test problems in gas dynamics.

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