Journal of Computational Mathematics, Vol.9, No.4, 1991, 337–347.

A MODIFIED MACCORMACK'S SCHEME*

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Abstract

In this paper a modified MacCormack's scheme is presented. The scheme is based on flux vector splitting. The test computations show that the proposed modified scheme produces much better numerical results than original MacCormack's scheme.

§1. Introduction

A numerical flux function plays a very important role in solving hyperbolic equations of conservation laws by finite difference methods. The first order accurate numerical flux scheme may be most dependable in providing solutions which are free of computational noise, but it possesses sufficiently large dissipative trunction error so that discontinuities are smeared out on grids.

The higher order numerical flux schemes[5,7] possess the peculiar property that nonphysical oscillations in the solution can be generated in the vicinity of steep gradient regions[12]. This computational noise may degrate or destroy the accuracy of solution. Undesirable physical features of the simulated flow such as negative masses or energy densities may develop in solving gasdynamic equations.

As a consequence, the development of higher order monotonic or TVD numerical schemes has continued. Some examples of these schemes are in [1,2,10]. In these schemes nonlinear filtering techniques are used for higher order numerical algorithms. In general, constraints are imposed on the gradients of the dependent variable [9] or on the gradients of the flux functions [4] in these algorithms. This technique effectively removes computation noise from steep gradient solutions.

A modified MocCormack's scheme is presented in this paper. The algorithm is based on flux vector splitting [8] for systems and the flux limeter may be treated in a relatively simple and convenient way. The test calculations show that the numerical results are of higher resolution.

§2. Description of The Algorithm

In this section we will briefly describe the general algorithm. A modified MacCormack's scheme is described in the next section.

* Received August 13 1988.

To illustrate the basic notion we consider the numerical algorithm for a one-dimensional system of conservation laws

$$\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} = 0, \tag{1}$$

where W and the flux function $F(W)$ are m-component column vectors.

Now computing x-spatial is divided into cells of equal width, Δx. We take W at the center of the jth cell. At time $n\Delta t$, these variables, W_j^n, are known on the cells. The objective is to compute the dependent variables one time step later, W_j^{n+1}. The algorithm is accomplished as follows

Step 1. The predictor solution is calculated at $(n+1)\Delta t$ using a first order accurate scheme for computing the spatial derivative in (1)

$$\widetilde{W}_j = W_j^n - \lambda\left(F^{nf}_{j+\frac{1}{2}} - F^{nf}_{j-\frac{1}{2}}\right), \tag{2}$$

where $\lambda = \dfrac{\Delta t}{\Delta x}$ and $F^{nf}_{j+\frac{1}{2}}$ is a first order numerical flux at the boundary between the jth and $(j+1)$th cells. An example of a first order scheme is the upwind method [3]. This step should not introduce ripples into the solution.

Step 2. An anti-diffusion flux is calculated

$$F^a_{j+\frac{1}{2}} = F^{nh}_{j+\frac{1}{2}} - F^{nf}_{j+\frac{1}{2}}, \tag{3}$$

where $F^{nh}_{j+\frac{1}{2}}$ is a higher order approximation to the spatial derivative in (1). The solutions computed by the higher order flux, $F^{nh}_{j+\frac{1}{2}}$, contain ripples.

Step 3. The predictor solution which is monotonic, $\tilde{W}$, and the higher order flux are used in conjunction with a nonlinear filter to obtain the resulting solutions at time $(n+1)\Delta t$

$$W_j^{n+1} = \tilde{W}_j - \lambda(F^{ac}_{j+\frac{1}{2}} - F^{ac}_{j-\frac{1}{2}}). \tag{4}$$

The objective is to control the flux, $F^{ac}_{j+\frac{1}{2}}$, in and out of cells so as to decrease the diffusion introduced by the first order scheme. Here $F^{ac}_{j+\frac{1}{2}}$ is adjusted as follows

$$F^{ac}_{j+\frac{1}{2}} = \begin{cases} S_{j+\frac{1}{2}} \min(\alpha|F^a_{j+\frac{3}{2}}|, |F^a_{j+\frac{1}{2}}|, \alpha|F^a_{j-\frac{1}{2}}|), \text{ when} \\ \qquad S_{j+\frac{1}{2}} = \mathrm{Sign}(F^a_{j+\frac{1}{2}}) = \mathrm{Sign}(F^a_{j+\frac{3}{2}}) = \mathrm{Sign}(F^a_{j-\frac{1}{2}}); \\ 0, \qquad \text{otherwise}, \end{cases} \tag{5}$$

where α is a constant between 1 and 2. From (4) and (2) we can see that the scheme is of higher order if $F^{ac}_{j+\frac{1}{2}} = F^a_{j+\frac{1}{2}}$, and it is the first order scheme (2) when parameter $\alpha = 0$.

Using the algorithm described above we have constructed some schemes already. One of them is a modified MacCormack's scheme in the next section.

§3. Modified MacCormack's scheme

As well known, MacCormack's second order scheme[7] for the one- dimensional system of conservation laws (1) is

$$\tilde{W}_j = W_j^n - \lambda(F_j^n - F_{j-1}^n), \tag{6.1}$$

$$W_j^{n+1} = \frac{1}{2}(W_j^n + \tilde{W}_j) - \frac{\lambda}{2}(\tilde{F}_{j+1} - \tilde{F}_j), \tag{6.2}$$

where $\tilde{F}_j = F(\tilde{W}_j)$. The predictor (6.1) is an upwind scheme. Its necessary local stability condition is that all the eigenvalues of the Jacobian matrix $A = \dfrac{\partial F(W)}{\partial W}$ are positive.

The corrector (6.2) can be rewritten as

$$W_j^{n+1} = \tilde{W}_j - \frac{\lambda}{2}(\tilde{F}_{j+1} - F_j^n - \tilde{F}_j^n + F_{j-1}^n), \tag{7}$$

and then the anti-diffusion flux can be written as

$$F_{j+\frac{1}{2}}^a = \tilde{F}_{j+1} - F_j^n. \tag{8}$$

Therefore we obtain a modified version of MacCormack's scheme

$$\tilde{W}_j = W_j^n - \lambda(F_j^n - F_{j-1}^n), \tag{9.1}$$

$$W_j^{n+1} = \tilde{W}_j - \frac{\lambda}{2}(F_{j+\frac{1}{2}}^{ac} - F_{j-\frac{1}{2}}^{ac}), \tag{9.2}$$

$$F_{j+\frac{1}{2}}^a = \tilde{F}_{j+1} - F_j^n, \tag{9.3}$$

$$F_{j+\frac{1}{2}}^{ac} = \text{ the same as right of (5) }, \tag{9.4}$$

when all eigenvalues of the Jacobian matrix A are positive. In the case that all eigenvalues of A are negative, the modified MacCormack's scheme can be written as

$$\tilde{W}_j = W_j^n - \lambda(F_{j+1}^n - F_j^n), \tag{10.1}$$

$$W_j^{n+1} = \tilde{W}_j - \frac{\lambda}{2}(F_{j+\frac{1}{2}}^{ac} - F_{j-\frac{1}{2}}^{ac}), \tag{10.2}$$

$$F_{j+\frac{1}{2}}^a = \tilde{F}_j - F_{j+1}^n, \tag{10.3}$$

$$F_{j+\frac{1}{2}}^{ac} = \text{ the same as right of (5).} \tag{10.4}$$

By virtue of (9) and (10), the flux vector splitting scheme by Steger and Warming [8] can be used so that a split version of modified MacCormack's scheme can be written when the eigenvalues are of mixed signs. The split version is

$$\tilde{W}_j = W_j^n - \lambda[(F^+)_j^n - (F^+)_{j-1}^n + (F^-)_{j+1}^n - (F^-)_j^n], \tag{11.1}$$

$$W_j^{n+1} = \tilde{W}_j - \frac{\lambda}{2}(F_{j+\frac{1}{2}}^{ac} - F_{j-\frac{1}{2}}^{ac}), \tag{11.2}$$

$$F_{j+\frac{1}{2}}^a = \tilde{F}_{j+1}^+ - (F^+)_j^n + \tilde{F}_j^- - (F^-)_{j+1}^n, \tag{11.3}$$

$$F_{j+\frac{1}{2}}^{ac} = \text{ the same as right of (5).} \tag{11.4}$$

In the scheme (11) F^+ and F^- are subvectors so that F is split into two parts

$$F = F^+ + F^-, \tag{12}$$

when the nonlinear flux vector $F(W)$ is homogeneous function of degree one in W. F^+ corresponds to subvectors associated with the positive eigenvalues of A and F^-, the negative eigenvalues. The detailed derivation of this splitting $F = F^+ + F^-$ can be found in [8].

According to linear stability theory, the necessary stability condition of the scheme (11) is

$$\max_k |a_k \lambda| \le 1, \tag{13}$$

where $a_k (k = 1, 2, \cdots, m)$ are the eigenvalues of the Jacobian matrix A.

§4. Algorithms for Two Spatial Dimensions

Splitting the spatial operators, we can extend the method described above to the two-dimensional system of conservation laws

$$\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + \frac{\partial G(W)}{\partial y} = 0. \tag{14}$$

By that we mean that we solve the following equations alternately:

$$\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} = 0, \tag{15.1}$$

$$\frac{\partial W}{\partial t} + \frac{\partial G(W)}{\partial y} = 0. \tag{15.2}$$

Let $W_{j,k}^n$ be the numerical solution at $x = j\Delta x$, $y = k\Delta y$, $t = n\Delta t$, with Δx the mesh size in the x-direction and Δy the mesh size in the y-diriction. Also let $\bar{F}_{j+\frac{1}{2},k}^n$ and $\bar{G}_{j,k+\frac{1}{2}}^*$ be the numerical fluxes in x- and y-direction, respectively. The modified MacCormack's scheme can be implemented in two spatial dimension by the method of fractional steps as follows:

$$\tilde{W}_{j,k}^n = W_{j,k}^n - \frac{\Delta t}{\Delta x}[(F^+)_{j,k}^n - (F^+)_{j-1,k}^n + (F^-)_{j+1,k}^n - (F^-)_{j,k}^n],$$

$$W_{j,k}^* = \tilde{W}_{j,k}^n - \frac{\Delta t}{2\Delta x}(\bar{F}_{j+\frac{1}{2},k} - \bar{F}_{j-\frac{1}{2},k}) = L_x W_{j,k}^n; \tag{1.6.1}$$

$$\tilde{W}_{j,k}^* = W_{j,k}^* - \frac{\Delta t}{\Delta y}[(G^+)_{j,k}^* - (G^+)_{j,k-1}^* + (G^-)_{j,k+1}^* - (G^-)_{j,k}^*],$$

$$W_{j,k}^{n+1} = \tilde{W}_{j,k}^* - \frac{\Delta t}{2\Delta y}(\bar{G}_{j,k+\frac{1}{2}} - \bar{G}_{j,k-\frac{1}{2}}) = L_y W_{j,k}^*. \tag{1.6.2}$$

That is

$$W_{j,k}^{n+1} = L_y L_x W_{j,k}^n. \tag{17}$$

The fluxes $\bar{F}_{j+\frac{1}{2},k}$ and $\bar{G}_{j,k+\frac{1}{2}}$ are written as follows

$$\bar{F}_{j+\frac{1}{2},k} = S_{j+\frac{1}{2},k}\max[0,\min(S_{j+\frac{1}{2},k}\alpha\Delta F^n_{j+\frac{3}{2},k}, |\Delta F^n_{j+\frac{1}{2},k}|, S_{j+\frac{1}{2},k}\alpha\Delta F^n_{j-\frac{1}{2},k})],$$

$$\Delta F^n_{j+\frac{1}{2},k} = (\tilde{F}^+)^n_{j+1} + (\tilde{F}^-)^n_{j,k} - (F^+)^n_{j,k} - (F^-)^n_{j+1,k},$$

$$S_{j+\frac{1}{2},k} = \mathrm{Sign}(\Delta F^n_{j+\frac{1}{2},k}), \quad \tilde{F}^n = F(\tilde{W}^n);$$

$$\bar{G}_{j,k+\frac{1}{2}} = (S_{j,k+\frac{1}{2}}\max[0,\min(S_{j,k+\frac{1}{2}}\alpha\Delta G_{j,k+\frac{3}{2}}, |\Delta G_{j,k+\frac{1}{2}}|, S_{j,k+\frac{1}{2}}\alpha\Delta G^n_{j,k-\frac{1}{2}})],$$

$$\Delta G^*_{j,k+\frac{1}{2}} = (\tilde{G}^+)^*_{j,k+1} + (\tilde{G}^-)^*_{j,k} - (G^+)^*_{j,k} - (G^-)^*_{j,k+1},$$

$$S_{j,k+\frac{1}{2}} = \mathrm{Sign}(\Delta G_{j,k+\frac{1}{2}}), \quad \tilde{G}^* = G(\tilde{W}^*).$$

In order to retain the original time accuracy of the method, we use the following fractional step operators

$$W^{n+1}_{j,k} = L_x L_y L_y L_x W^n_{j,k}. \tag{18}$$

§5. Numerical Experiments for approximation to Euler equations of gasdynamics

In this section results are presented for the numerical solution of the Euler equations of gasdynamics. In one-dimension the Euler equations of gasdynamics can be written in the conservation law form (1), where

$$W = \begin{pmatrix} \rho \\ m \\ E \end{pmatrix}, \quad F(W) = \begin{pmatrix} m \\ \dfrac{m^2}{\rho} + p \\ (E+p)\dfrac{m}{\rho} \end{pmatrix}, \tag{19}$$

$$p = (\gamma - 1)(E - \frac{m^2}{2\rho}). \tag{20}$$

here ρ, $m = \rho u$, p and E are the density, momentum, pressure and total energy, respectively. u is velocity and γ is the ratio of specific heats.

The Jacobian matrix $A = \dfrac{\partial F(W)}{\partial W}$ is easily computed as

$$A = \begin{pmatrix} 0 & 1 & 0 \\ \dfrac{(\gamma-3)u^2}{2} & (3-\gamma)u & \gamma - 1 \\ (\gamma-1)u^3 - \dfrac{\gamma E u}{\rho} & \dfrac{\gamma E}{\rho} - \dfrac{3(\gamma-1)u^2}{2} & \gamma u \end{pmatrix}. \tag{21}$$

The eigenvalues of A are

$$a_1 = u, \quad a_2 = u + c, \quad a_3 = u - c, \tag{22}$$

here $c^2 = \dfrac{\gamma p}{\rho}$ is the local sound speed.

We can readily verify that the nonlinear flux vector $F(W)$ in (19) is homogeneous function of degree one in W. subvectors F^+ and F^- required in the scheme can be found in [8].

$$F^{\pm}=\frac{\rho}{2\gamma}\begin{pmatrix} 2(\gamma-1)a_1^{\pm}+a_2^{\pm}+a_3^{\pm} \\ 2(\gamma-1)ua_1^{\pm}+a_2^{\pm}(u+c)+a_3^{\pm}(u-c) \\ (\gamma-1)a_1^{\pm}u^2+\frac{a_2^{\pm}}{2}(u+c)^2+\frac{a_3^{\pm}}{2}(u-c)^2+X \end{pmatrix}, \tag{23}$$

where

$$X=\frac{(3-\gamma)(a_2^{\pm}+a_3^{\pm})c^2}{2(\gamma-1)}, \tag{24}$$

and

$$a_k^{\pm}=\frac{a_k^{\pm}\pm|a_k^{\pm}|}{2}\pm\varepsilon,\quad k=1,2,3, \tag{25}$$

where $\varepsilon\geq 0$ is a parameter.

Some examples are given here to illustrate the performance of the proposed modified MacCormack's scheme. In numerical tests for one dimension the results are compared to the exact solution. The numerical values are shown by circles. The exact solution is shown by a solid line. In these examples the parameter $\alpha=2$ is chosen.

(I) In one dimension the test example is the shock tube problem whose solution belongs to the Riemann problem. The initial conditions are given as follows:

$$W_L=\begin{pmatrix}5\\0\\0.6\end{pmatrix},0\leq x\leq 35;\quad W_R=\begin{pmatrix}1\\0\\0.12\end{pmatrix},\quad 35\leq x\leq 70;\quad \gamma=\frac{5}{3}.$$

The solution for $t\geq 0$ consists of a shock wave travelling to the right followed by a contact discontinuity and a rarefaction wave. The density and energy are discontinuous across the contact, while the velocity and pressure are not. Comparison to the exact solution is made at time $t=60$ in Fig. 1. The calculation was performed under $\Delta t=0.75$ and 140 cells.

In Fig. 1a-b we show the results obtained by the scheme (11) with $\varepsilon=0.05$, and by the scheme of flux vector splitting [8], respectively.

In Fig. 2 we apply the scheme (11) to a different set of data for the Riemann problem:

$$W_L=\begin{pmatrix}0.445\\0.311\\8.298\end{pmatrix},0\leq x\leq 8;\quad W_R=\begin{pmatrix}0.5\\0\\1.4275\end{pmatrix},\quad 8\leq x\leq 14,$$

and $\gamma=1.4$. The example is taken from [2]. The calculation was performed with 100 time steps under $\Delta t=0.02$ and 140 cells.

In two dimension the Euler equations of gasdynamics can be written in (14), where

$$W=\begin{pmatrix}\rho\\m\\n\\E\end{pmatrix},\quad F(W)=\begin{pmatrix}m\\ \frac{m^2}{\rho}\\ \frac{mn}{\rho}\\ \frac{(E+p)m}{\rho}\end{pmatrix},\quad G(W)=\begin{pmatrix}n\\ \frac{mn}{\rho}\\ \frac{n^2}{\rho}\\ \frac{(E+p)n}{\rho}\end{pmatrix}. \tag{26}$$

with $m = \rho u$, $n = \rho v$ and $p = (\gamma - 1)\Big(E - \frac{(m^2+n^2)}{2\rho}\Big)$. The primitive variable of (26) are density, velocity components u and v, and pressure p. The engenvalues of $A = \frac{\partial F(W)}{\partial W}$ and $B = \frac{\partial G(W)}{\partial W}$ are

$$f_1 = f_2 = u, \quad f_3 = f_1 + c, \quad f_4 = f_1 - c,$$

and

$$g_1 = g_2 = v, \quad g_3 = g_1 + c, \quad g_4 = g_1 - c.$$

The subvectors $F^{\pm}$ or $G^{\pm}$ can be written in the following form:

$$H^{\pm} = \frac{\rho}{2\gamma}\begin{pmatrix} 2(\gamma-1)a_1^{\pm} + a_3^{\pm} + a_4^{\pm} \\ 2(\gamma-1)ua_1^{\pm} + (u+ck_f)a_3^{\pm} + (u-ck_f)a_4^{\pm} \\ 2(\gamma-1)va_1^{\pm} + (v+ck_g)a_3^{\pm} + (u-ck_g)a_4^{\pm} \\ (\gamma-1)(u^2+v^2)a_1^{\pm} + Z_1 + Z_2 + X \end{pmatrix}, \tag{27}$$

where

$$Z_1 = 0.5a_3^{\pm}[(u+ck_f)^2 + (v+ck_g)^2], \quad Z_2 = 0.5a_4^{\pm}[(u-ck_f)^2 + (v-ck_g)^2]$$

and

$$X = \frac{(3-\gamma)(a_3^{\pm} + a_4^{\pm})c^2}{2(\gamma-1)}.$$

The flux subvectors $F^{\pm}$ are obtained from (27) if $k_f = 1$, $k_g = 0$ and $a^{\pm} = 0.5(f_k \pm |f_k|)$ (k=1,2,3) are inserted in (27). Likewise, $G^{\pm}$ are obtained from (27) if $k_f = 0$, $k_g = 1$ and $a^{\pm} = 0.5(g_k \pm |g_k|)$ $(k = 1, 2, 3)$ are inserted in (27).

(II) The first test problem for two dimension is a steady state flow of air ($\gamma = 1.4$) through a duct containing a step. Initially the flow is everywhere to the right at Mach 3, with $\gamma = 1.4$, $p = c = 1$. The duct width is 1, its length is 3, and the step of height 0.2 is located a distance of 0.6 from the entrance. This problem has been used by Harten[2], van Leer[10], Woodward and Colella[11], Li Yin-fan[6] and others. The results in Fig. 3 were obtained with a uniform Cartesian cell with $\Delta x = \Delta y = 0.05$. At the exit an outflow boundary condition is applied. The complicated system of shock reflections, rarefaction waves and contact discontinuities are presented at $t = 4$.

The second two dimensional test problem is an unsteady problem whose geometry and initial data are shown in Fig. 4a. The shock wave is located on a step which is a distance of 3.75 from the left boundary and its height is 0.75. At the right boundary inflow is applied. All the results were obtained with a uniform Cartesian cell with $\Delta x = \Delta y = 0.05$. The density contours at $t = 0.52$, 1 and 1.52 are shown in Fig. 4b ,c and d. The shock regular reflection and Mach rarefactions are presented.

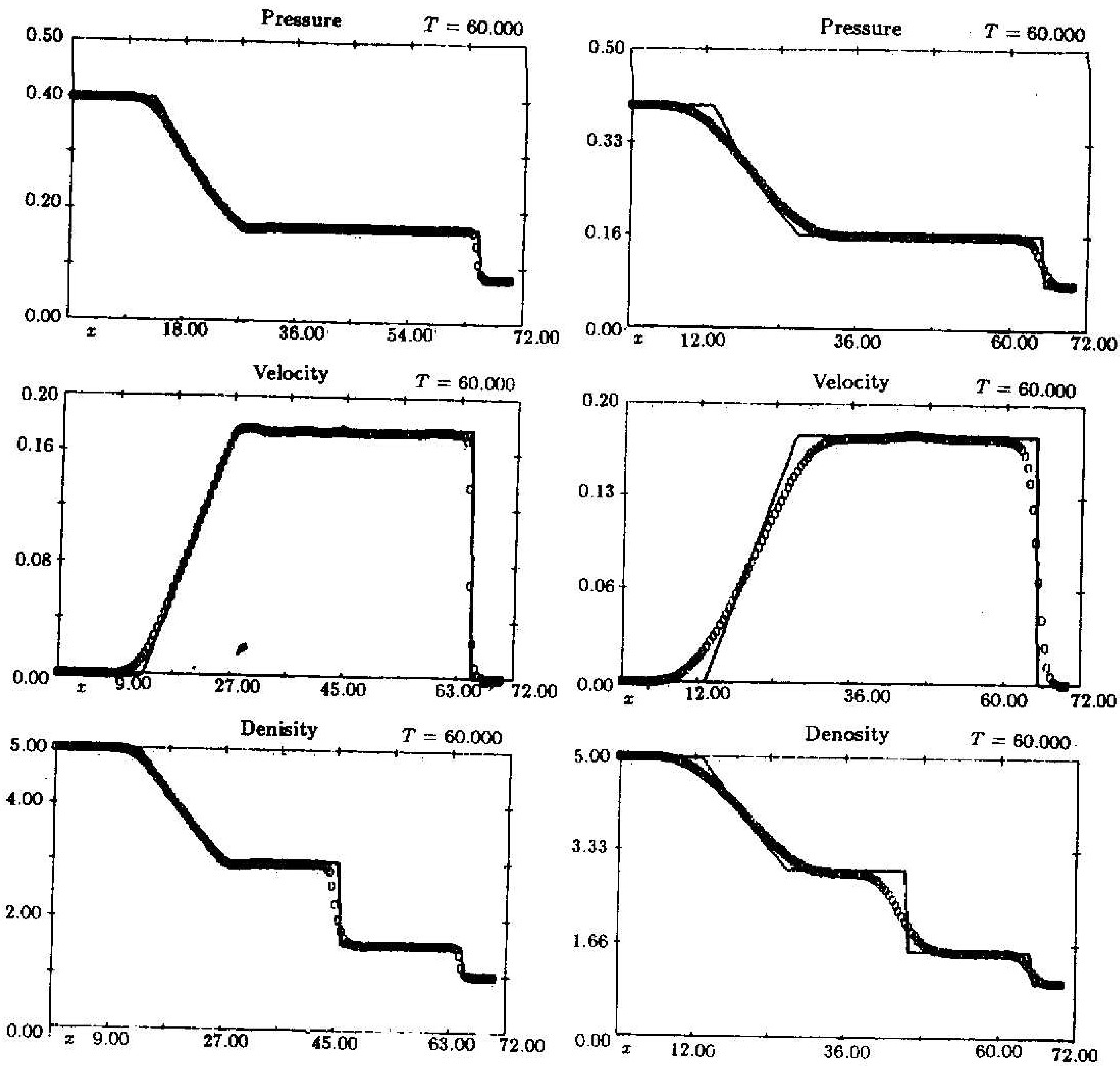
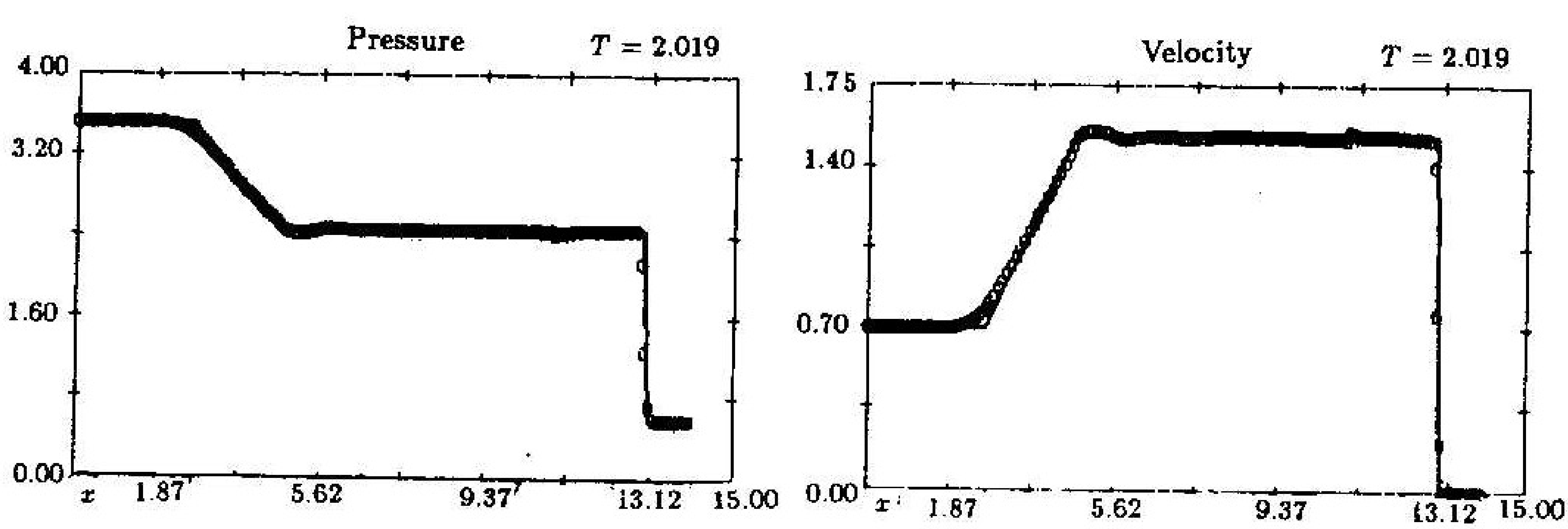


Fig. 1. Numerical results at $T = 60$ for the first shock tube problem
a) with $\varepsilon = 0.05$ in (25),
b) using flux vector splitting scheme [8]



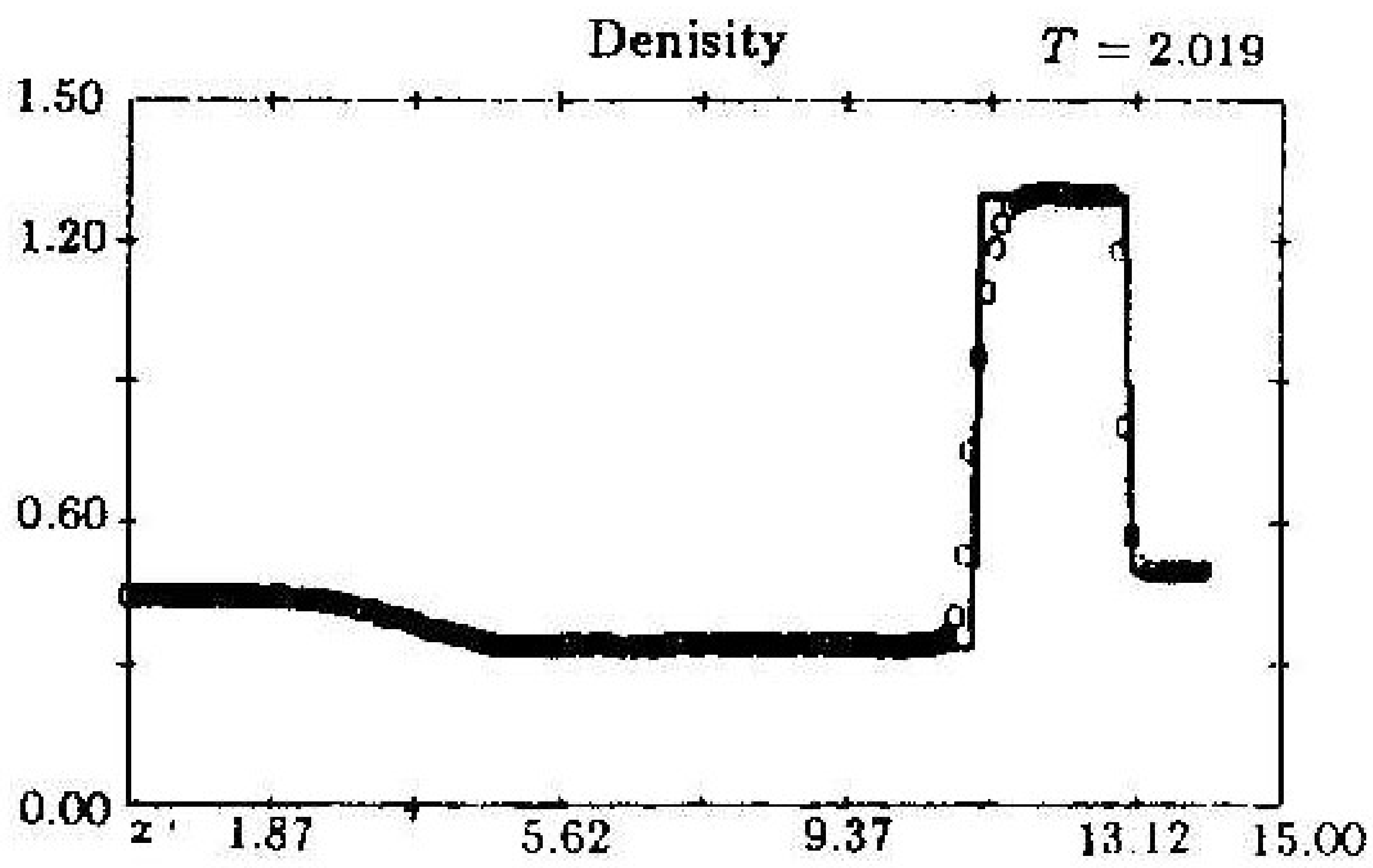


Fig. 2. Numerical results with $\varepsilon = 0.05$ at $T = 2$ for the second shock tube problem

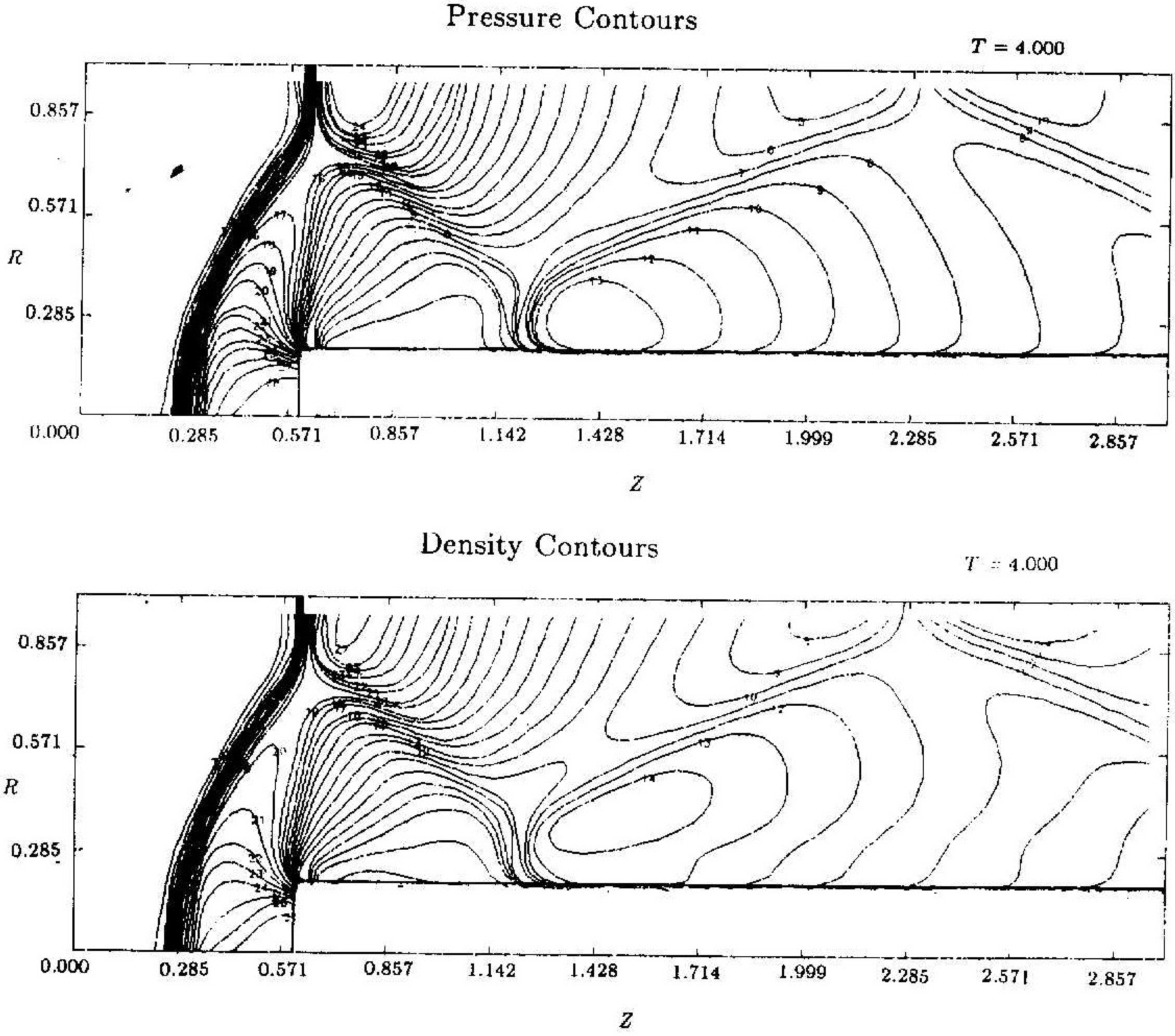


Fig. 3. Pressure (3a) and density (3b) contours for Mach 3 steady flow with a Step at $T = 4$

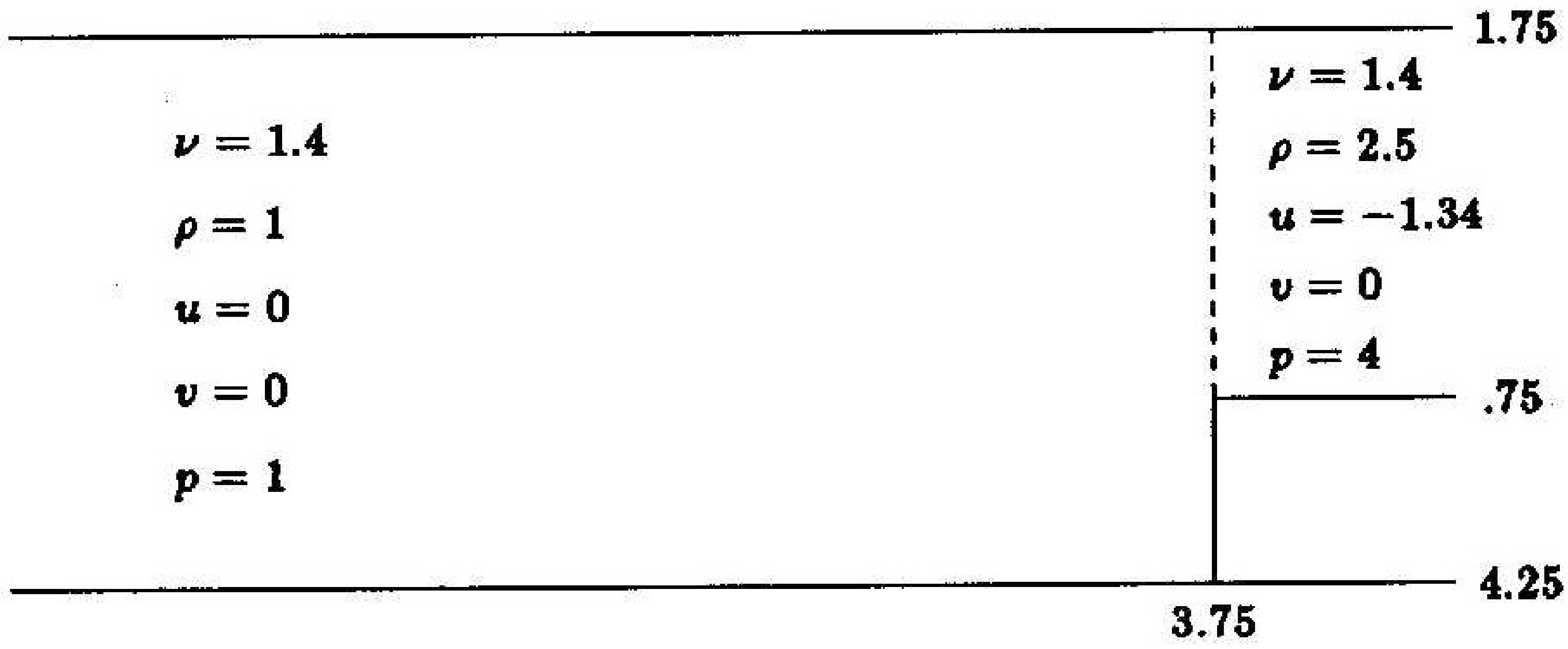
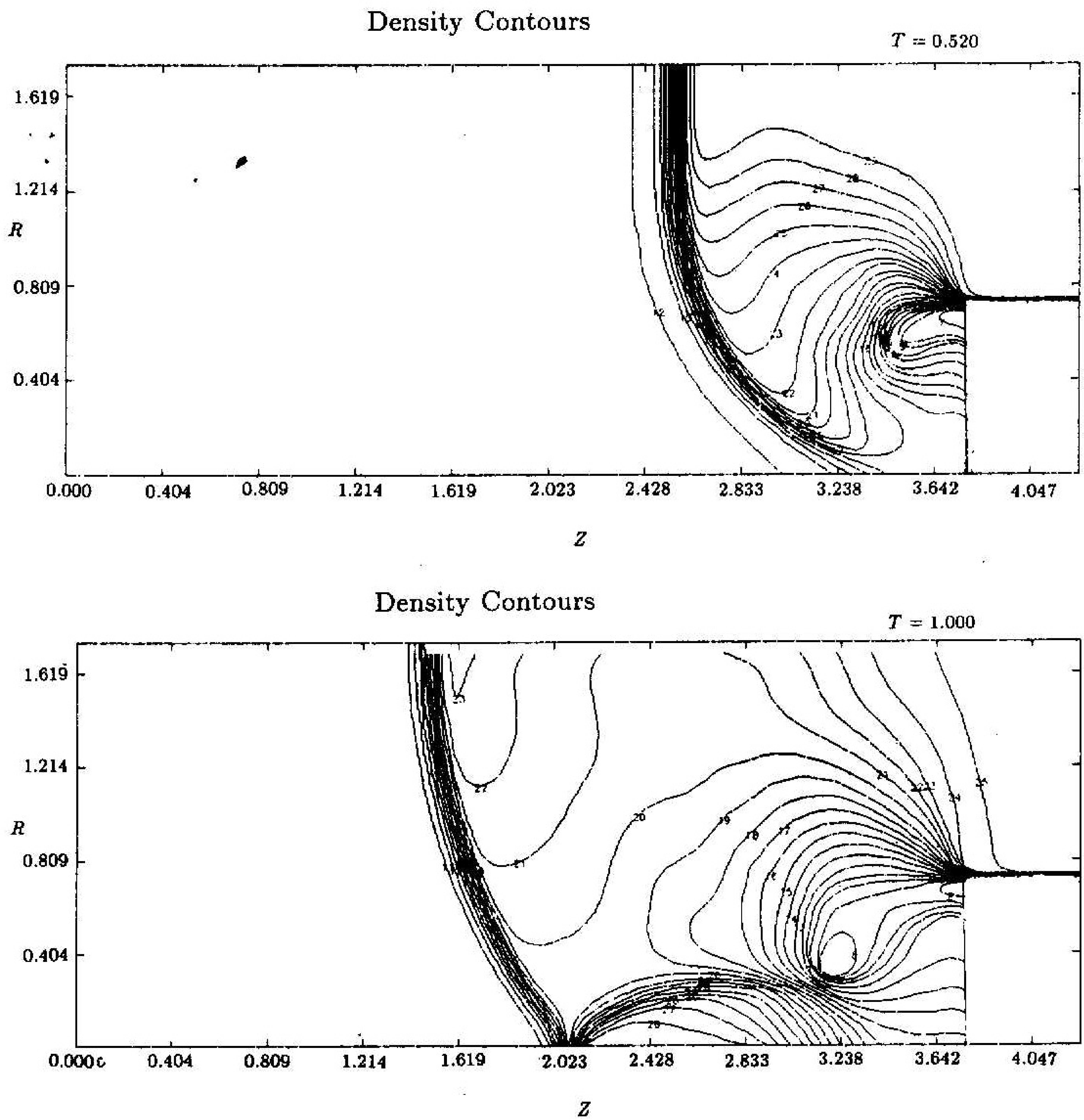


Fig.4. a) Geometry and initial value for unsteady flow



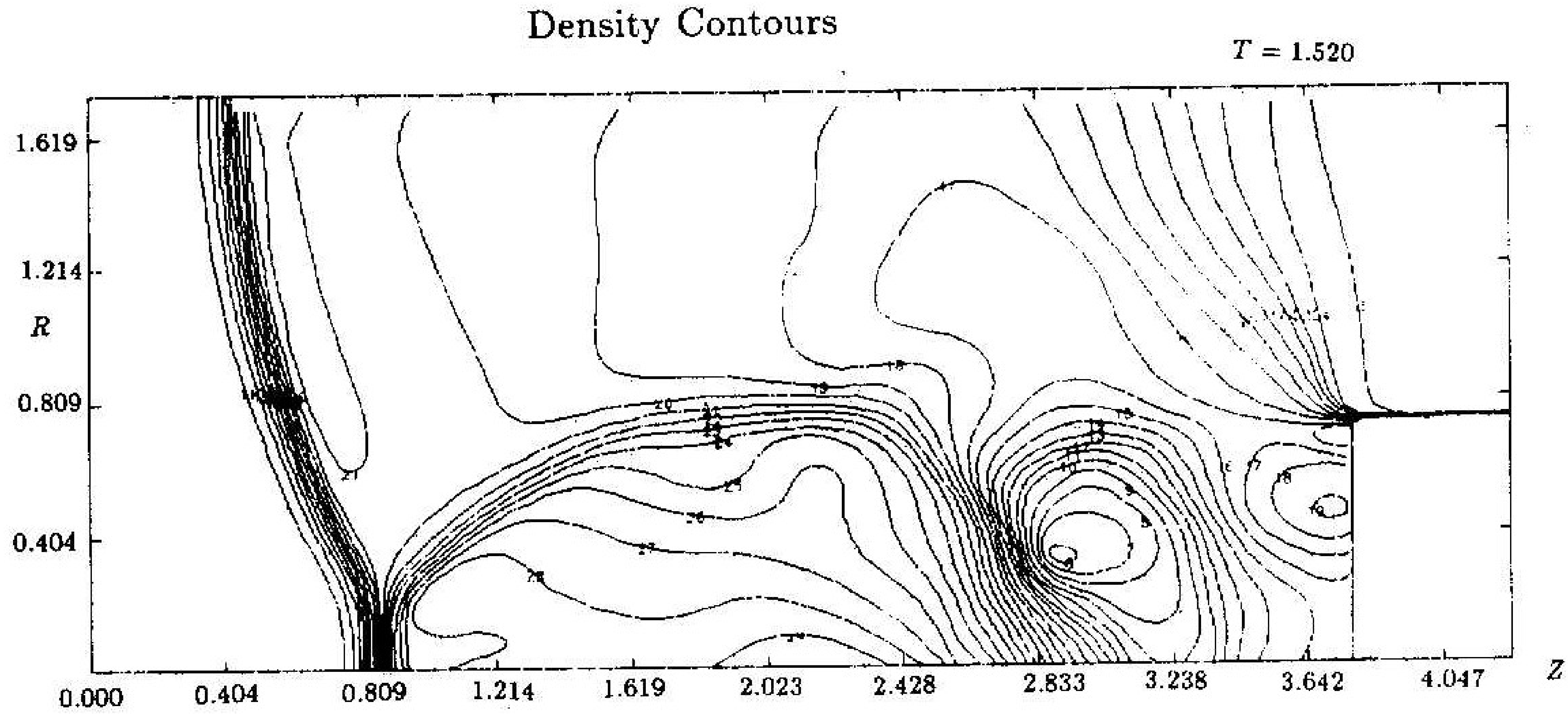


Fig.4. b), c) and d); density contours at $T = 0.5$, 1 and 1.5

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