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Low Mach Number Instability of an Explicit Numerical Scheme

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ABSTRACT

In this paper we describe a low Mach number instability which occurs in a scheme we have advocated for the solution of gas dynamics and multiphase flow problems. We illustrate the instability and explain its origin using a simplified Von Neumann stability analysis. Finally, we present a simple modification to the scheme which completely eliminates the instability.

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Nomenclature

A	area factor
C	Courant number
C_v	specific heat at constant volume
c_s	speed of sound
e	internal energy
M	Mach number
$\dot{m}$	mass flow rate
p	pressure
T	temperature
t	time
v	velocity
x	space coordinate

Greek Symbols

ρ	density
δ	non-dimensional wave-number (defined in eq. (8))
γ	ratio of specific heats
λ	eigenvalue of the stability matrix
Δt	time-step
Δx	space-step

Subscripts

exit	condition at the exit
inlet	condition at the inlet
tot	stagnation value
0	reference value

1 Introduction

A very fundamental problem in numerical simulations of complex physical phenomena is the proper distinction and recognition of purely numerical instability effects from physically caused instabilities inherent in the system studied. It is entirely possible for a numerical scheme to be stable and accurate for a range of physical conditions and yet become unstable and totally unsuitable for problems lying outside that range. Unless the user is aware of this, it is easy to mistake the manifestations of a numerical instability for a genuine physical one. The purpose of this paper is to report an interesting numerical instability associated with the explicit, first-order scheme we have advocated earlier as a suitable practical and robust method for solving gas dynamics [1], and multiphase fluid dynamics [2]. Somewhat unusually, the instability manifests itself at low flow Mach numbers and exhibits a threshold.

We first describe a simple flow situation in one-dimensional gas dynamics which is typical of how the instability arises. With numerical examples we show that it is indeed a low Mach number instability with a threshold. We then present a simplified Von Neumann stability analysis of the scheme which qualitatively explains all the features shown by the numerics. We also describe and illustrate two distinct methods of totally eliminating the instability in those situations where it might be expected to arise. Finally, we show by concrete examples how the same instability occurs when the scheme is used to calculate the nonhyperbolic multiphase equations and how it is suppressed in that context. The present results clarify and put in context our earlier, correct, results obtained with the scheme in question. Users of this scheme should be aware of the stability limits discussed here and methods of enhancing the scheme to suppress instability in those cases when it can be expected to arise.

2 A typical example

We consider one dimensional, transient, compressible inviscid flow of a perfect gas in a nozzle. The governing equations are [3],

$$\frac{\partial \rho}{\partial t} + \frac{1}{A}\frac{\partial}{\partial x}(\rho v A) = 0 \tag{1}$$

$$\frac{\partial \rho v}{\partial t} + \frac{1}{A}\frac{\partial}{\partial x}(\rho v^2 A) = -\frac{\partial p}{\partial x} \tag{2}$$

$$\frac{\partial}{\partial t}\left(\rho(e + v^2/2)\right) + \frac{1}{A}\frac{\partial}{\partial x}\left(\rho v A(e + v^2/2 + p/\rho)\right) = 0 \tag{3}$$

$$p = (\gamma - 1)C_v \rho T \tag{4}$$

$$e = C_v T. \tag{5}$$

In the above equations, γ, C_v are constants characteristic of the gas, whilst $A(x)$ is a user specified area function describing the geometry of the nozzle. The initial-boundary value problem for the above system (including sources) has been discussed by us elsewhere [4]. For the present purposes, the following remarks suffice:-

1. The solution domain is $0 < x < L$. The "inlet plane" is at $x = 0$, whilst $x = L$ is the location of the exit plane, as shown in Figure 1.

2. At the inlet, we specify p_{tot} and ρ_{tot}.

3. At the exit, p_{exit}/p_{tot} is prescribed.

4. Initial data are given for ρ, v and p at $t = 0$.

The details of the solution procedure and the determination of the inlet mass flow rate $\dot{m}_{inlet}$ follow the methods described in earlier publications and do not concern us [1,4,5]. The above problem is well-posed for both subsonic and transonic (i.e. choked flow) and is expected to lead to the well-known steady nozzle flow with or without a standing shock. If the flow is wholly subsonic, it must be isentropic provided the initial entropy distribution is uniform. In the case of choked flow, the entropy must increase in the final steady-state monotonically from the inlet to the exit planes.

We remark that in our scheme, equation (1) is conservatively upwind-differenced spatially and is explicit in time and preserves the positivity of ρ (and conserves the total mass in a closed domain) provided that the condition $|v_{max}\Delta t| < \Delta x$ is satisfied. Equation (2) is also conservatively differenced and explicit first-order in Δt. However, the velocities at $t + \Delta t$ are obtained from equation (2) *after* the new densities are available by a solution of equation (1). In the original scheme, equation (2) was solved using the pressures at time t. The finite-difference forms of equation (2) is used to advance the velocity field. The ρv at the old time are used in the convective term to transport $v(x, t + \Delta t)$. Thus, a tri-diagonal matrix solution is required to obtain $v(x, t + \Delta t)$. The treatment of equation (3) is straightforward, since the new v's are available.

For numerical stability, this scheme requires the more stringent condition,

$$(c_s + |v|)_{max} < \frac{\Delta x}{\Delta t},$$

where c_s is the local sound speed. As we shall shortly show, this condition is necessary but not always sufficient for numerical stability. As our first example, we consider the nozzle flow of a perfect gas in the geometry illustrated in Figure 1. The grid sizes and other parameters have been chosen for convenience rather than great quantitative accuracy. We note that, $L = 230\text{mm}, \Delta x = 1.92\text{mm}$ and $\Delta t = 0.5\mu\text{s}$, except in one case. The sound speed for the chosen conditions is of the order of 1000m/s. This implies a Courant number, $C = c_s\Delta t/\Delta x, = 0.4$. The results obtained in three distinct cases will be considered. In all the cases, the following parameters and conditions were the same: p_{tot}, ρ_{tot} at inlet; uniform pressure, density and velocity at $t = 0$; the exit pressure ratio was held constant in time; the calculations were carried out with the same conservative, explicit, upwind difference scheme for a time of $t = 20\text{ms}$ (i.e. for 4×10^4 time-steps). A detailed description of all the parameters and conditions used is given elsewhere [4]. The three cases correspond to the exit pressure ratios (p_{exit}/p_{tot}) and inlet and exit Mach numbers (M_{inlet}, M_{exit}), shown in Table 1. It should be noted that the exit pressure ratio is specified as a boundary condition in all three cases whilst the code calculates M_{inlet} and M_{exit} as a function of time. In all cases, M_{exit} reaches a steady value after about 10ms. It is the steady values that are given in the table.

Figure 2 shows the Mach number M as a function of distance x, when all the fields have reached their steady-state. Figure 2a corresponds to case a in Table 1. It shows

Case	p_{exit}/p_{tot}	M_{inlet}	M_{exit}
a	0.75	0.37	0.52
b	0.88	0.30	0.39
c	0.91	(not converged)	0.33

Table 1: The effect of exit pressure ratio on the inlet and exit Mach numbers.

that the flow goes sonic at the throat and accelerates sharply until a maximum Mach number of about 1.2 is reached just aft of the throat section. As the flow area increases further, a standing shock forms and the flow returns to subsonic conditions. Figure 3 shows the entropy, which is always monotone increasing as a function of x. It also shows that the flow is isentropic (or nearly so) both behind and in front of the standing shock. The small rise at the front part of the throat is due to numerical dissipation and the fact that the one-dimensional flow model is strictly invalid at "corners" in the area profile. This example demonstrates that the explicit, conservative scheme described by us in earlier references can and does lead to stable, qualitatively consistent and quantitatively accurate solutions [1,4] (provided $\Delta x/L$ is small enough) under the conditions of case a. Figure 2b shows $M(x)$ at $t = 20$ms for case b. In this case, the flow is seen to be entirely subsonic and very nearly isentropic (see figure 3) as expected. M_{inlet} is now somewhat lower than case a at 0.3. It is clear from these two examples that the scheme is well able to handle mixed (i.e. supersonic-subsonic-transonic) flow regimes as well as completely subsonic flows with no hint of numerical instability.

The real surprise then is represented by case c which only differs from the other two in having a slightly higher exit pressure ratio of 0.91. The expected value of the inlet Mach number in steady, fully subsonic, isentropic nozzle flow conditions is 0.27. However, Figure 2c demonstrates that a violent numerical instability exists in the region between the inlet plane and the beginning of the constant area throat section. This figure leads to several interesting observations:

1. a very modest change in the inlet Mach numbers from 0.3 to 0.27 is sufficient for the instability which is entirely numerical in origin;

2. case c corresponds to a saturated (i.e. the field values are not unbounded in time) instability;

3. the instability is confined to a sharply defined "zone".

Thus, Figure 2c shows that the correct steady solution for the given conditions is indeed calculated by the code for $x > 0.065$m. Indeed there is no hint of any difficulty with the solution in the exit zone where M falls to 0.33.

3 Analysis of the instability and its resolution

The numerical instability illustrated above for our scheme is remarkable in that for given values of the local Courant number $C(x)$, it occurs below a threshold value of the local flow Mach number $M(x)$. Fortunately, a very simple and direct explanation of this behaviour can be given. The practical approach to the elimination of the instability itself is quite straightforward and will be demonstrated. As cases a and b illustrate, such a resolution may not always be called for but it is sufficiently "easy" as to be worth implementing in general.

To understand the nature of this numerical instability, let us consider an extreme case. Thus, let us set $A(x) = A_0$ (i.e. a uniform channel), and $M_{inlet} = 0$ (i.e. no flow) in equations (1)–(5). If we consider an initial value problem for the system with a small initial disturbance about a uniform thermodynamic equilibrium state with spatially periodic conditions at $x = 0$ and L, we have the familiar problem of linearized acoustics. Making the isentropic assumption, it is easily shown (and long recognised in the literature [6]) that the scheme described earlier is *unconditionally unstable* for arbitrary finite values of $C = \frac{c_s \Delta t}{\Delta x}$. For the scheme to converge, we require $\Delta t \sim O((\Delta x)^2)$. It is plain that if M were not exactly zero but sufficiently small, the instability must persist since the numerical dissipational stability produced by upwind differenced terms in the continuity and momentum equations cannot outweigh the basic "acoustic" instability of the explicit (forward time, staggered space) scheme. However, case b suggests very strongly that if M satisfies a condition like $M > C$, the scheme is indeed stable. This can be explicitly demonstrated by a simple Von Neumann stability analysis in the case when the channel is uniform and the unperturbed flow is uniform, subsonic and isentropic.

Thus, assume $\rho(x,t) = \rho_0 + \tilde{\rho}(x,t), v(x,t) = v_0 + \tilde{v}(x,t)$, with $\tilde{\rho}/\rho_0 << 1$ and $v_0 > 0$. It is convenient to set

$$\rho(n\Delta t, m\Delta x) = \rho_0 + \tilde{\rho}_n \exp\{ikm\Delta x\} \tag{6}$$

and

$$v(n\Delta t, (m + \frac{1}{2})\Delta t) = v_0 + \tilde{v}_n \exp\{ik(m + \frac{1}{2})\Delta x\} \tag{7}$$

where k is a wave number, m, n are integers and $1 \le m \le N$, where $N\Delta x = L$. We introduce the non-dimensional parameters,

$$\delta = k\Delta x; \qquad M = \frac{v_0}{c_s} = \frac{v_0}{\sqrt{\gamma p_0/\rho_0}}; \quad C = \frac{c_s \Delta t}{\Delta x}. \tag{8}$$

Putting $\tilde{\rho}^*_{n+1} = \tilde{\rho}_{n+1}/\rho_0$, $\tilde{v}^*_{n+1} = \tilde{v}_{n+1}/c_s$, , we obtain, from the continuity and the momentum equations (assuming an isentropic equation of state) the linearized finite-difference equations

$$\tilde{\rho}^*_{n+1} = \tilde{\rho}^*_n(1 - MC(1 - e^{-i\delta})) - 2Ci\sin(\delta/2)\tilde{v}^*_n \tag{9}$$

and

$$\begin{aligned} \tilde{v}^*_{n+1} &= \tilde{v}^*_n \left[1 - MC(1 - e^{-i\delta})\right] \\ &+ \tilde{\rho}^*_n \left[M^2C(e^{i\delta/2} - e^{-3i\delta/2}) - 2iC\sin(\delta/2)\right]. \end{aligned} \tag{10}$$

Let $A(\delta) \equiv 1 - e^{-i\delta}, B(\delta) \equiv e^{i\delta/2} - e^{-3i\delta/2}$ and $D(\delta) \equiv 2i\sin(\delta/2)$. The eigenvalues λ of the Von Neumann matrix are given by the secular equation,

$$(1 - MCA - \lambda)^2 + C^2 D(M^2 B - D) = 0. \tag{11}$$

Consider first the simple "no flow" situation when $M = 0$, in which case

$$\lambda = 1 \pm CD. \tag{12}$$

Plainly, the scheme is unconditionally unstable for $C \neq 0$, $\delta \neq 0$.

Although equation (11) is the complete dispersion relation, we are only interested in circumstances when $C \leq 1$. Furthermore, we shall actually assume that M is small enough for the condition $M^2 << M$ to hold. If then follows (neglecting $O(M^2)$ terms), that,

$$\lambda = 1 - MC + \cos\delta MC \pm 2iC\sin(\delta/2) - iMC\sin\delta. \tag{13}$$

It is easy to show that $|\lambda| < 1$ if and only if

$$C < M(1 \pm 2C\cos\delta/2). \tag{14}$$

For arbitrary δ, $1 \pm 2C\cos(\delta/2) > 0$ if $C < 1/2$. The inequality (14) implies the following stability condition (i.e. condition *sufficient* for stability):

$$M > C \qquad (\text{for} \quad C < 1/2). \tag{15}$$

Since, for consistency, we require M^2 negligible compared with M, the condition $C < 1/2$ is not really restrictive. In terms of basic flow variables the stability condition (15) may also be written as

$$v_0 \frac{\Delta x}{\Delta t} > c_s^2. \tag{16}$$

In this form, the meaning of this condition can be readily understood. $c_s^2 \Delta t$ is the basic "anti-diffusion" present in this explicit numerical scheme, driving the instability. When a flow v_0 is present, the upwind-differencing leads (in leading order of $\frac{v_0}{c_s}$) to a "numerical diffusion" stabilizing the scheme, represented by the diffusivity $v_0\Delta x$. When the net stabilizing diffusivity, $v_0\Delta x - c_s^2\Delta t$ is non-negative, the scheme is stable. Our simulations show that this result is approximately valid locally even though the simplified Von Neumann analysis presented above is not. The result also appears to be valid when area changes occur. Our examples show that an explicit numerical scheme discarded as unsuitable in the literature owing to its manifest instability can actually be used (unchanged) to obtain perfectly valid, stable results under other conditions with substantial flows present.

Returning to case c, the next question we ask is, can we show that equation (16) is indeed sufficient? Figure 4 shows the result of running case c with the *only* change being $\Delta t = 0.25\mu s$ (i.e. $C \leq 0.2$). Clearly there is now no hint of instability anywhere and the solution coincides with that shown in figure 2c where the latter is converged. The instability can indeed be suppressed by satisfying the condition (16) without altering the scheme. We next present a very modest enhancement of the scheme which removes the need for condition (16). Returning to the "no flow" case ($M \equiv 0$), we retain the stability equation for the finite-differenced continuity equation in its usual explicit form:

$$\tilde{\rho}^*_{n+1} = \tilde{\rho}^*_n - 2Ci\sin(\delta/2)\tilde{v}^*_n. \tag{17}$$

However, in the momentum equation, instead of using the pressure at time-level n, we use an isentropic estimate $p^{est}(m\Delta x, (n+1)\Delta t)$, obtained using $\rho(m\Delta x, (n+1)\Delta t)$ thus:

$$p^{est}(m\Delta x, (n+1)\Delta t) = p(m\Delta x, n\Delta t)\left\{\frac{\rho(m\Delta x, (n+1)\Delta t)}{\rho(m\Delta x, n\Delta t)}\right\}^{\gamma}. \tag{18}$$

Note that equation (18) is actually exact if the flow is locally isentropic. In the limit as $\Delta t \to 0$, $p^{est} \to p(m\Delta x, (n+1)\Delta t)$ except at shocks or detonation fronts. Thus, equation (18) is expected to preserve *numerical* consistency in the usual sense and is, in general, an excellent estimate of the pressure at the new time-level. Using the appropriate linearized form of equation (18) in the momentum equation, we obtain, as a replacement for equation (10),

$$\tilde{v}^*_{n+1} = \tilde{v}^*_n - 2Ci\sin(\delta/2)\tilde{\rho}^*_{n+1} \tag{19}$$

in the limit as $M \to 0$. Although equation (19) is formally implicit, $\tilde{\rho}^*_{n+1}$ can be eliminated using equation (17) and the set of equations is effectively explicit. The eigenvalues of the Von Neumann matrix are given by

$$\lambda^2 + \lambda(4C^2\sin^2(\delta/2) - 2) + 1 = 0. \tag{20}$$

Thus a necessary and sufficient condition for the roots to be of unit modulus is

$$(4C^2\sin^2(\delta/2) - 2)^2 < 4,$$
$$\text{i.e.} \qquad C < 1. \tag{21}$$

Thus, provided the usual Courant condition (required anyway for accuracy) is satisfied, the scheme using equation (18) is stable for arbitrary Mach numbers (in particular for $M = 0$), and yet is effectively explicit.

The above prediction was verified by repeating the calculation of case c with $\Delta t = 0.5\mu s$, (giving $C \approx 0.4$) but using p^{est} in the momentum equations. This time the code produced a completely converged result indistinguishable from that given in Figure 4, which is the same solution obtained with the original scheme but using a smaller time-step. It is therefore clearly more practical to use the "enhanced" explicit scheme which costs no more than the original scheme for given accuracy and yet does not suffer from the extra condition (given in equation (16)), which is more stringent in subsonic flow than the condition $C < 1$.

It may be tempting to conclude that the results are rather specific. To show that this not the case, we conclude with an example drawn from our multiphase calculations. The example is taken from our simulations of multiphase detonations in melt/water mixtures. The model is fully described elsewhere [2]. We must emphasise that there is nothing wrong with our earlier calculations since these were obtained using a small enough time-step for the instability to be suppressed. Figure 5a shows the result of a simulation with a time-step of $0.5\mu s$ and a maximum Courant number of 0.18. The instability is evident in the regions of low flow velocity.

The method of removing the instability described above needed to be modified for this case, since the equation of state is more complicated in this situation [2]. In fact the equation of state is such that it is easier to derive an estimate for the advanced time pressure assuming that the internal energy remains constant rather than the entropy, as suggested in equation (18). Figures 5b shows that with this practice the instability is again completely suppressed.

In the multiphase flow case there is no simple Von Neumann analysis and yet the comparison shows that the instability exists and can be removed in a similar manner to that used in the gas dynamics case. It is very remarkable that this particular instability does not apparently care whether the underlying system of equations is hyperbolic or not. The fact that it can be suppressed in both cases by exactly the same prescription shows that multiphase equations are not necessarily more "ill-posed" or pathological as regards their macroscopic behaviour than the hyperbolic equation systems of gas dynamics, provided the flow simulation is qualitatively consistent and faithful [7].

Finally, we should note that the instability can always be removed by using the new pressure field in the momentum equations, therefore making them fully implicit, and iterating the solution. We found this practice to be the optimal one in our multiphase flow simulations, since it allowed us to take much larger time-steps. However, the modified explicit scheme was found to be preferable in our gas dynamics work, since the computational time-step was limited by other constraints (a large heat source) [4].

4 Conclusions

We have demonstrated a novel low Mach number instability arising in a class of explicit, positive faithful schemes arising in gas and multiphase fluid dynamics. A simple modification of the scheme which preserves its explicit character and is consistent with the governing partial differential equations is shown to be effective in removing the Mach number-Courant number threshold condition characterising the instability. Simplified Von Neumann stability analyses are presented together with a complementary set of numerical examples to illustrate and clarify the nature of the instability and its practical resolution.

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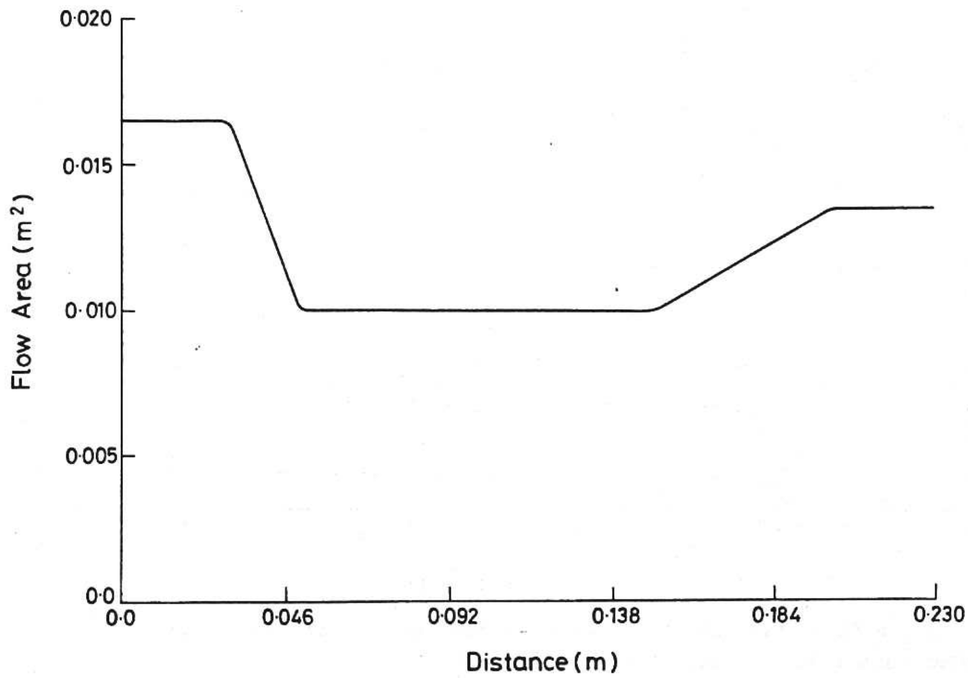


Fig. 1 The geometry used in the duct flow example.

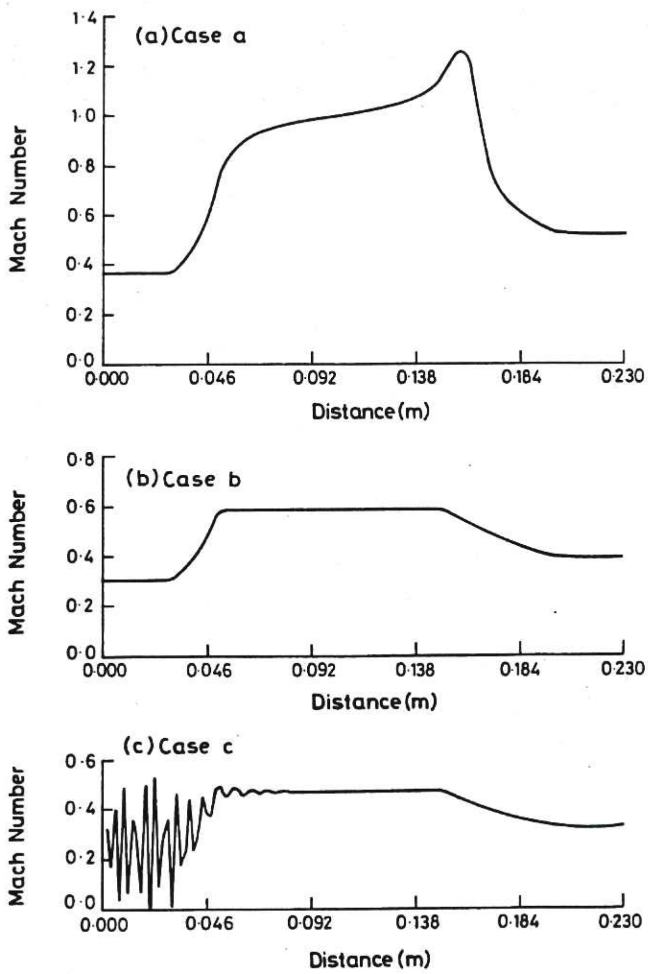


Fig. 2 The Mach number profiles for the three different cases. The Mach number at inlet decreases in successive cases.

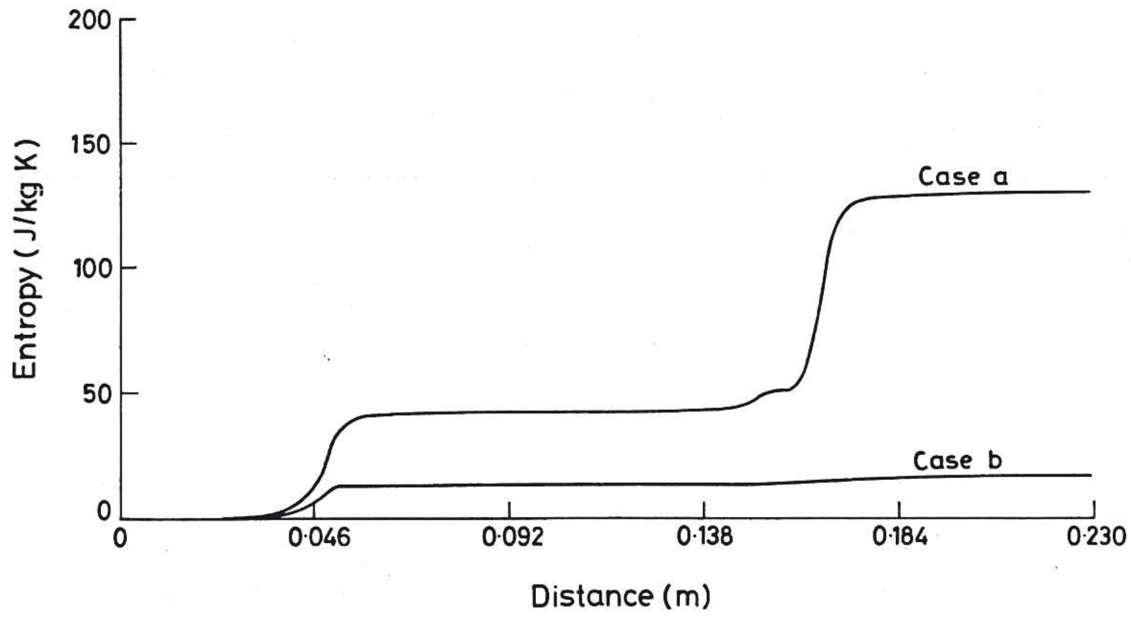


Fig. 3 The entropy profile for the two converged duct flow calculations. (The entropy values shown are increases above the inlet value.)

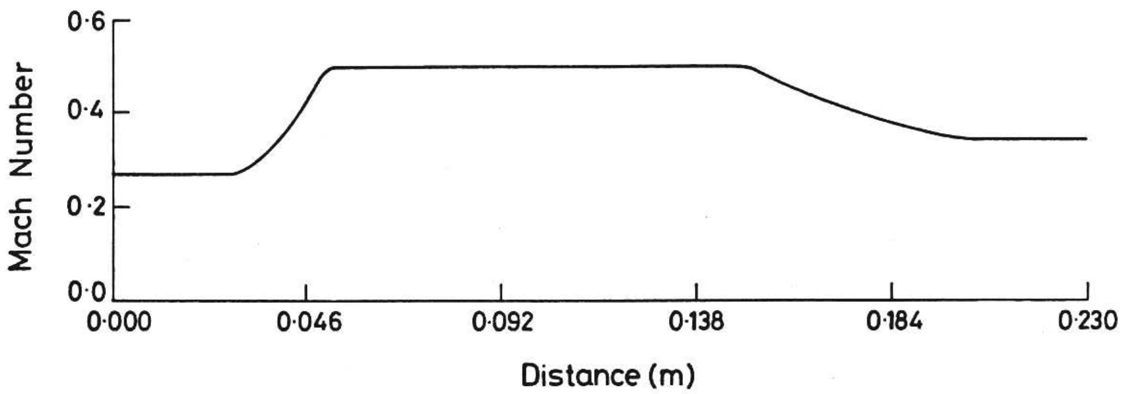
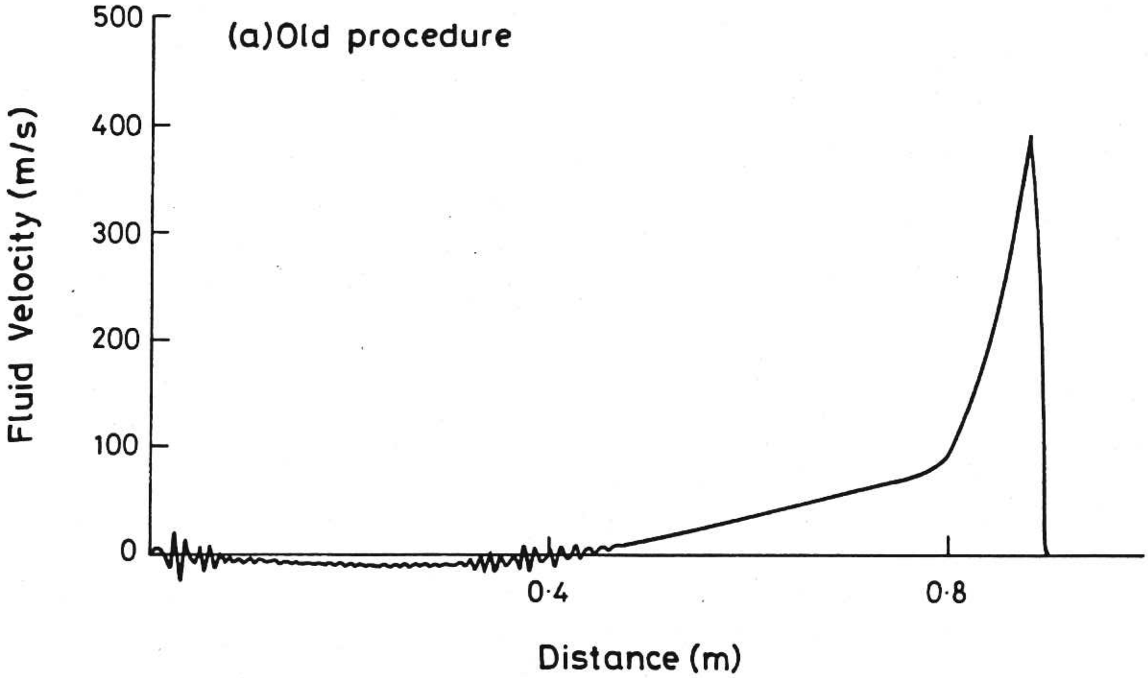


Fig. 4 The Mach number profile for case c of figure 2, obtained using a smaller time-step or the modified scheme.



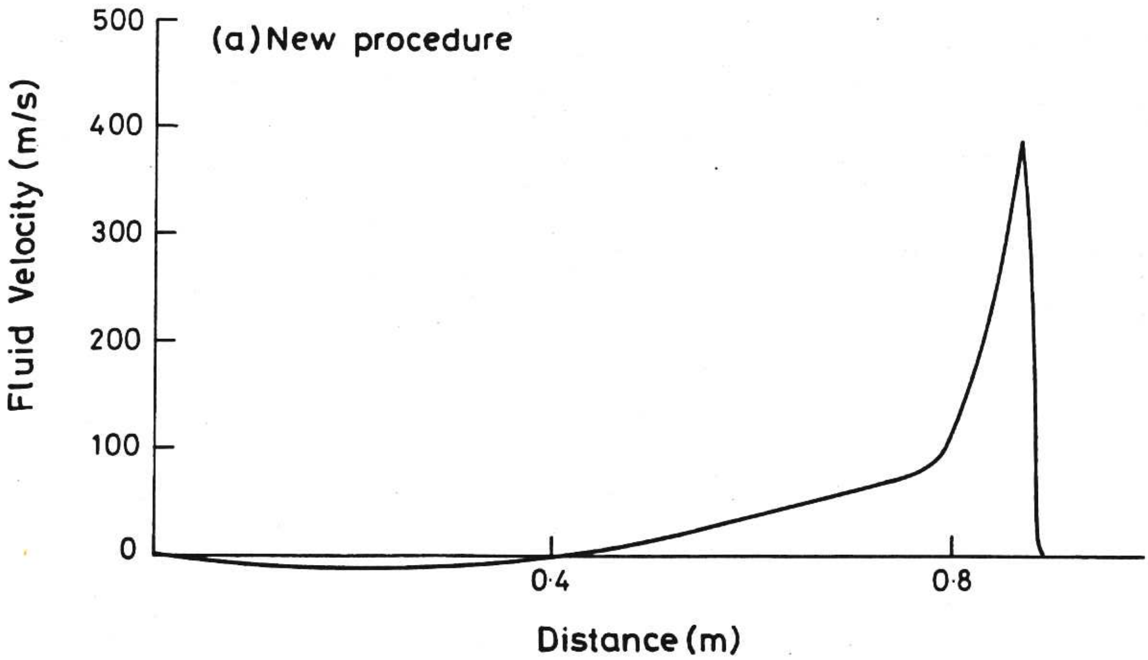


Fig. 5 An example of the same instability in a multiphase flow system. The figures show the results of simulations with and without the modified scheme.