Open-end outflow boundary approximations for the solution of the equations of unsteady one-dimensional gas flow by the Lax–Wendroff method

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Open-end outflow boundary condition approximations required in the solution of gas flow problems by the Lax–Wendroff method are presented. An upwinding method is compared with that using characteristics at the boundary, and both methods are assessed by a comparison of their solutions with the theoretical solution of a test problem. The results show that the most accurate solutions may be obtained from a hybrid version of these two methods

Keywords: *Gasflow, Lax–Wendroff method, boundary conditions*

In recent years the Lax–Wendroff method[1] has been used to compute unsteady one-dimensional gas flow in pipes. It has been shown by Warren[2] that the method has distinct advantages over unmodified characteristic methods as it can provide accurate answers to problems which involve shocks in addition to problems which involve characteristics only. The Lax–Wendroff method, however, cannot be used on the boundary of the problem and some other technique is required to approximate the conditions there. In the previous paper[2] suitable boundary condition approximations were introduced for shock tubes with closed ends; here this approach is extended to deal with shock tubes with open ends.

This paper considers an upwind boundary condition approximation in conservation form, which is appropriate for the solution of gas flow problems where shocks may be expected to occur. A test problem, consisting of a shock tube with an open end, is presented so that the upwind and characteristic methods of approximating boundary conditions can be compared with each other and with theoretical solutions.

General theory

The governing equations of one-dimensional gas flow must first be written in conservation form. For simplicity of notation it is convenient to introduce new dependent variables, the momentum, m, and the energy, e, per unit volume defined by:

$$m = \rho u, \qquad e = \rho(E + \tfrac{1}{2}u^2) \tag{1}$$

where $E = p/\rho(\gamma - 1)$. The conservation form for the equations of continuity, momentum and energy for one-dimensional flow of an ideal gas, with heat transfer and wall-friction, is now:

$$\frac{\partial V}{\partial t} + \frac{\partial G(V)}{\partial x} = B \tag{2}$$

with:

$$V = \begin{bmatrix} \rho \\ m \\ e \end{bmatrix}, \qquad G(V) = \begin{bmatrix} m \\ p + m^2/\rho \\ (e+p)m/\rho \end{bmatrix},$$

$$B = \begin{bmatrix} 0 \\ -\rho\phi \\ \rho q \end{bmatrix}$$

and the wall friction term defined by:

$$\phi = \frac{4f}{D}\frac{u}{2}|u| \tag{3}$$

The quasilinear form of these equations is:

$$\frac{\partial W}{\partial t} + A\frac{\partial W}{\partial x} = C \tag{4}$$

with:

$$W = \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}, \qquad A = \begin{bmatrix} u & \rho & 0 \\ 0 & u & 1/\rho \\ 0 & \gamma p & u \end{bmatrix},$$

$$C = \begin{bmatrix} 0 \\ -\phi \\ (\gamma - 1)\rho(q + u\phi) \end{bmatrix}$$

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Two-step Lax–Wendroff method

For a pipe subdivided by the mesh points $x_j = jh$, $j = 0, \ldots, J$, as shown in Fig 1, the Lax–Wendroff approximation to Eq (2) gives:

$$V_{j+1/2}^{n+1/2} = \frac{1}{2}(V_{j+1}^n + V_j^n) - \frac{1}{2}\frac{\Delta t}{\Delta x}(G_{j+1}^n - G_j^n) + \frac{\Delta t}{4}(B_{j+1}^n + B_j^n)$$
$$V_j^{n+1} = V_j^n - \frac{\Delta t}{\Delta x}(G_{j+1/2}^{n+1/2} - G_{j-1/2}^{n+1/2}) + \frac{\Delta t}{2}(B_{j+1/2}^{n+1/2} + B_{j-1/2}^{n+1/2}) \quad (5)$$

By applying this approximation to the grid it is possible to calculate V_j^{n+1}, for $j = 1, \ldots, J-1$. The calculation of V_0^{n+1} and V_J^{n+1} requires the consideration of the boundary conditions.

Upwind approximation at the boundary

The upwind method used at the boundary is very similar to that used for internal nodes, attributed to Lelevier by Richtmeyer and Morton[3]. In the method the time derivatives are approximated by forward differences and the space derivatives by forward or backward differences according to whether $u < 0$ or $u > 0$. As in the problems under consideration there is no possibility of the reversal of gas flow, the equations are presented only for the case $u > 0$. Applying the method to Eq (2) at node J gives:

$$\frac{\rho_J^{n+1} - \rho_J^n}{\Delta t} + \frac{m_J^n - m_{J-1}^n}{\Delta x} = 0 \quad (6)$$

$$\frac{m_J^{n+1} - m_J^n}{\Delta t} + \frac{(p + m^2/\rho)_J^n - (p + m^2/\rho)_{J-1}^n}{\Delta x} = -\rho_J^n \phi_J^n \quad (7)$$

$$\frac{e_J^{n+1} - e_J^n}{\Delta t} + \frac{((e+p)m/\rho)_J^n - ((e+p)m/\rho)_{J-1}^n}{\Delta x} = \rho_J^n q_J \quad (8)$$

The method has the special advantage that it can be used at pipe ends under outflow conditions, since the approximation is one-sided. Also, the method is conservative, which is essential for the approximation of unsteady gas flows with shocks.

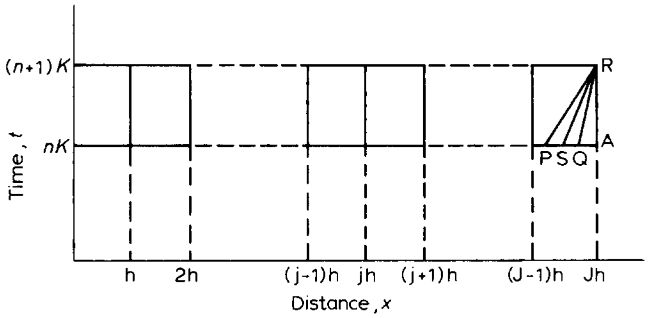


Fig 1 Computational grid for pipe of length x = Jh

In the solution of a practical problem these upwind approximations are solved simultaneously with appropriate assumptions at the boundary of the problem.

Characteristic approximation at the boundary

The characteristics and characteristic relations can be obtained from the quasilinear form.[4]

It has been shown from a consideration of the de Haller reservoir discharge problem[2] that slightly more accurate answers may be obtained by writing the characteristic equations in terms of the u, a, a_a variables used by Benson *et al*[5].

The new variables may be obtained from the relations:

$$a = \left(\gamma \frac{p}{\rho}\right)^{1/2}, \qquad a_a = \frac{a}{\left(\dfrac{p}{p_{ref}}\right)^{(\gamma-1)/2\gamma}}$$
$$p = p_{ref}\left(\frac{a}{a_a}\right)^{2\gamma/(\gamma-1)}, \quad (9)$$
$$\rho = \gamma \frac{p_{ref}}{a^2}\left(\frac{a}{a_a}\right)^{2\gamma/(\gamma-1)}$$

The characteristic relations are now:

$$da \pm \frac{\gamma-1}{2} du = \frac{\gamma-1}{2} \alpha \, dt + \frac{a}{a_a} da_a \quad (10)$$

where

$$\alpha = (\gamma-1)\frac{q}{a} \mp \phi\left(1 \mp (\gamma-1)\frac{u}{a}\right)$$

Notation

- a Speed of sound
- a_a Speed of sound after isentropic change of state to reference pressure p_{ref}
- D Pipe diameter
- E Internal energy
- f Friction factor
- p Pressure
- q Heat transfer rate per unit mass
- t Time
- u Particle velocity
- x Distance
- γ Ratio of specific heats ($\gamma = 1.4$)
- ρ Density

Subscript/superscript

$U_j^n \equiv U(jh, nk) \equiv U(x, t)$

on the $C^{(1)}$, $C^{(2)}$ characteristics, $dx/dt = u \pm a$, and:

$$da_a = \frac{1}{2}\frac{a_a}{\rho a^2}\beta\, dt \tag{11}$$

where:

$$\beta = (\gamma - 1)\rho(q + u\phi)$$

on the C characteristic, $dx/dt = u$.

These characteristic equations may be approximated by applying the method of Courant *et al*[6], or the Hartree method[7] if greater accuracy is required. The resulting equations can then be used to adapt the Lax–Wendroff method for various boundary conditions.

Using the notation of Fig 1 the Courant method leads to:

$$a_R - a_P + \frac{\gamma - 1}{2}(u_R - u_P) = \frac{\gamma - 1}{2}\alpha_A k + \frac{a_A}{(a_a)_A}[(a_a)_R - (a_a)_P] \tag{12}$$

on the $C^{(1)}$ characteristic, RP, and:

$$(a_a)_R - (a_a)_S = \frac{1}{2}\frac{(a_a)_A}{\rho_A a_A^2}\beta_A k \tag{13}$$

on the C characteristic, RS.

In the solution of a problem these characteristic approximations are solved simultaneously with the appropriate quasi-steady state conditions at the boundaries of the problem. In the computation the Courant method may be used on its own or with the Hartree method in typical predictor–corrector fashion.

Shock tube problem

The bursting of a diaphragm in a shock tube produces a complex wave pattern consisting of a shock, interface and rarefaction wave. For zero friction and heat transfer, it is possible to calculate an exact analytical solution for the incident wave before reflection occurs. The accuracy with which the Lax–Wendroff method can approximate this analytic solution has been examined by Sod[11].

Once reflection from a tube end has occurred exact analytical solutions are not available in general. However, by choosing initial values which reduce the incident wave solely to a shock, it is possible to obtain an exact analytical solution for the ensuing reflected wave. For this special case, therefore, it is possible to compare numerical with theoretical solutions.

This approach has already been used for a shock tube with a closed end[2], where it was shown that a conservative numerical approximation, obtained by incorporating reflection conditions, gave a more accurate solution than a characteristic approximation at the boundary. For the open-end problem considered here a solution obtained from a conservative approximation is compared with a solution obtained by using characteristics at the boundary.

The flow behind a shock wave may be subsonic or supersonic. Current practice assumes that for subsonic flow a reflected rarefaction wave will be initiated when the shock wave reaches the open end, but for supersonic flow the shock passes right through the open end and no reflected wave is possible[8].

The pressure ratio across a shock at which the flow behind the shock changes from subsonic to supersonic flow may be calculated by graphical methods[9]. Another possibility is to write the Rankine–Hugoniot equations in terms of a parameter $z = (p_2 - p_1)/p_1$. Following Whitham[10] the relations across a shock may be written in the form:

$$\frac{u_2 - u_1}{a_1} = \frac{z}{\gamma\left(1 + \frac{\gamma + 1}{2\gamma}z\right)^{1/2}} \tag{14}$$

$$\frac{\rho_2}{\rho_1} = \frac{1 + \frac{\gamma + 1}{2\gamma}z}{1 + \frac{\gamma - 1}{2\gamma}z} \tag{15}$$

$$\frac{a_2}{a_1} = \left[\frac{(1 + z)\left(1 + \frac{\gamma - 1}{2\gamma}z\right)}{1 + \frac{\gamma + 1}{2\gamma}z}\right]^{1/2} \tag{16}$$

where the subscripts 1 and 2 indicate conditions in front of and behind the shock respectively. The sonic condition, $u_2 = a_2$, in conjunction with Eqs (14) and (16), and $u_1 = 0$, leads to the quadratic:

$$18z^2 - 56z - 49 = 0$$

With $\gamma = 1.4$ this equation has a positive root $z = 3.823$, giving the value at which the flow behind the shock becomes sonic.

Theoretical solution

It is possible to obtain theoretical solutions to shock tube problems under the assumption of zero friction and zero heat transfer. For convenience the further assumptions at the boundary, required in obtaining these solutions, are restated here:

Theoretical quasi-steady assumption

(1) If the flow behind a shock wave is supersonic the boundary conditions are ignored.

(2) If the flow behind the shock is subsonic then the calculation is initially performed with the assumption $p = p_e$ at the boundary, where p_e is the exit pressure at the open end. If this calculation gives subsonic flow at the boundary then the calculation is terminated. If supersonic flow values are obtained at the boundary then the problem is resolved with the sonic assumption, $u_e = a_e$, replacing the constant pressure assumption at the boundary.

This theoretical quasi-steady assumption was used in obtaining solutions to the following examples where the shock tube was taken to have an open end at $x = 1.0$.

Example 1: Shock wave with supersonic flow behind

The following initial values were assumed:

$u=4.0 \quad p=29.0 \quad \rho=7.0 \quad \text{for } x<0$

$u=0.0 \quad p=1.0 \quad \rho=1.4 \quad \text{for } x>0$

With these initial values the problem has an exact solution:

$u=4.0 \quad p=29.0 \quad \rho=7.0 \quad \text{for } x/t<5.0$

$u=0.0 \quad p=1.0 \quad \rho=1.4 \quad \text{for } x/t>5.0$

for all t satisfying $0<t<0.2$.

Since the shock wave arrives at the open end at $t=0.2$, the exact solution for $t>0.2$ is:

$u=4.0 \quad p=29.0 \quad \rho=7.0$

for all x satisfying $0 \leq x \leq 1$. These solutions are illustrated in Fig 2 for various values of time.

Example 2: Shock wave with subsonic flow behind, and a reflected subsonic rarefaction wave

The following initial values were assumed:

$u=0.2988 \quad p=1.5 \quad \rho=1.867 \quad \text{for } x<0$

$u=0.0 \quad p=1.0 \quad \rho=1.4 \quad \text{for } x>0$

With these initial values the problem has an exact solution:

$u=0.2988 \quad p=1.5 \quad \rho=1.867 \quad \text{for } x/t<1.195$

$u=0.0 \quad p=1.0 \quad \rho=1.4 \quad \text{for } x/t>1.195$

for t satisfying $0<t<0.8368$.

For $t>0.8368$ the solution consists of two constant state regions separated by a rarefaction fan. In this example we have:

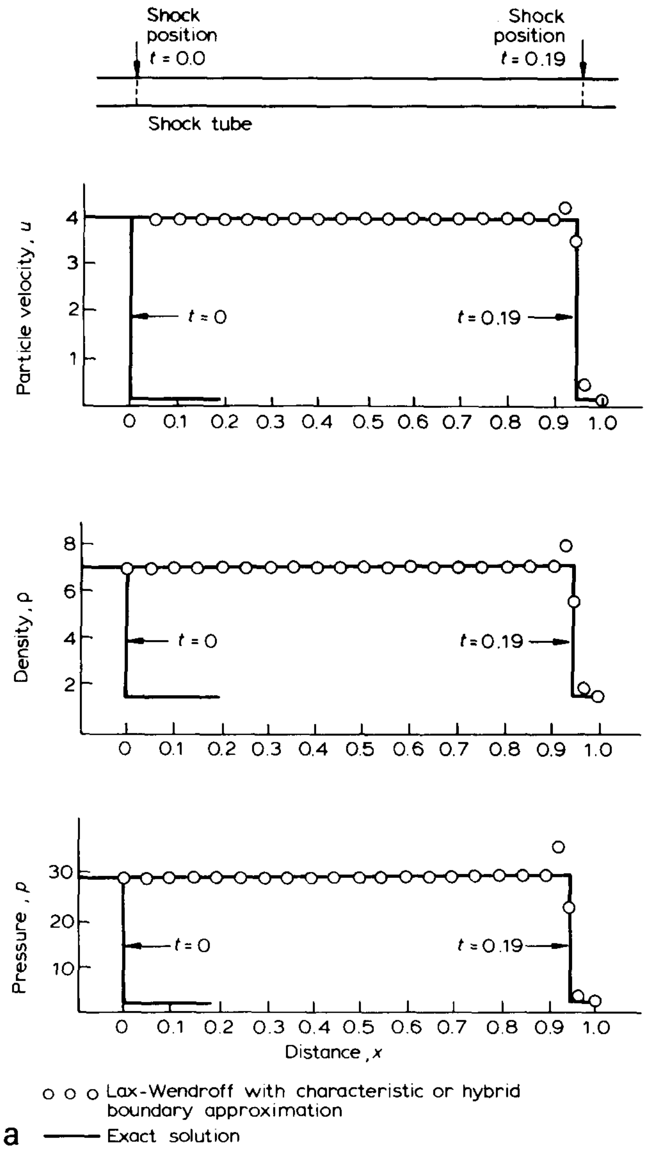
$u=0.2988 \quad p=1.5 \quad \rho=1.867$

$\text{for } 0 \leq x \leq 1.0-0.7622t'$

and:

$u=0.6 \quad p=1.0 \quad \rho=1.397$

$\text{for } 1.0-0.401t' \leq x \leq 1.0$



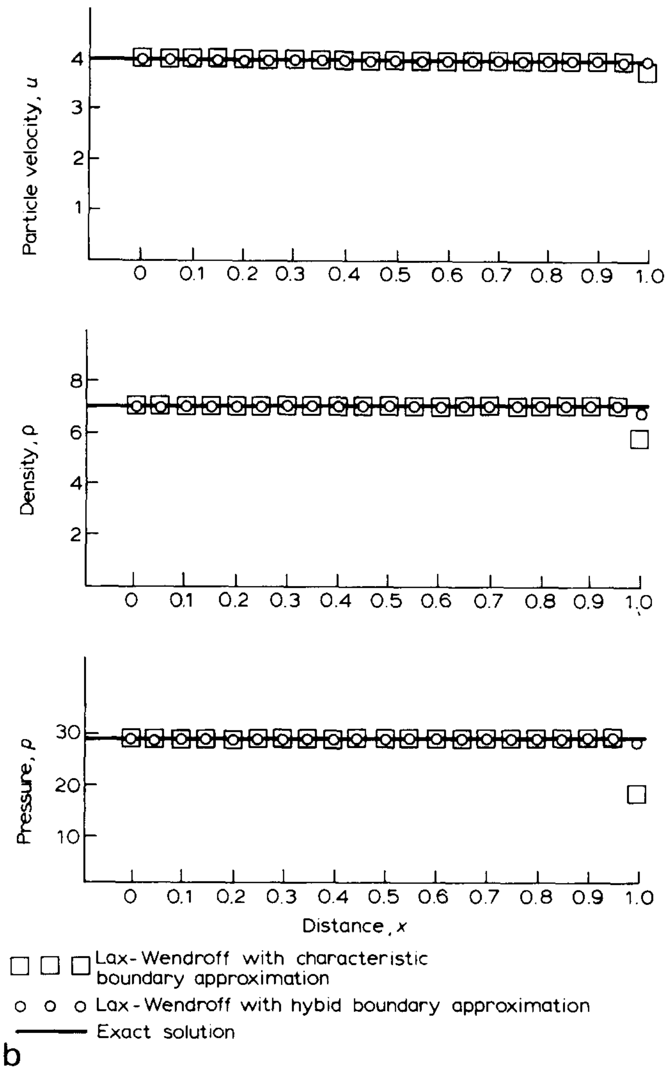


Fig 2 (a) Shock wave t = *0.0 and* t = *0.19 (b) Shock wave* t = *0.21* where the time, t', is measured from the moment when the shock arrives at the open end. The region $1.0-0.7622t' \leqslant x \leqslant 1.0-0.401t'$ constitutes the rarefaction wave region. These solutions are illustrated in Fig 3 for various values of time.

Example 3: Shock wave with subsonic flow behind, and a reflected sonic rarefaction wave

The following initial values were assumed:

$u=1.134 \quad p=4.0 \quad \rho=3.5 \quad$ for $x<0$

$u=0.0 \quad p=1.0 \quad \rho=1.4 \quad$ for $x>0$

With these initial values the problem has an exact solution:

$u=1.134 \quad p=4.0 \quad \rho=3.5 \quad$ for $x/t<1.89$

$u=0.0 \quad p=1.0 \quad \rho=1.4 \quad$ for $x/t>1.89$

for t satisfying $0<t<0.5292$.

For $t>0.5292$ the solution consists of a steady state region and a rarefaction fan. In this example we have:

$u=1.134 \quad p=4.0 \quad \rho=3.5$

for $0 \leqslant x \leqslant 1.0-0.131t'$

and a rarefaction wave in the region $1.0-0.131t' \leqslant x \leqslant 1.0$, where t' is measured from the moment when the shock arrives at the open end. The theoretical values of the flow at the open end are now:

$u=1.243 \quad p=3.538 \quad \rho=3.206$

for this example. These solutions are illustrated in Fig 4 for various values of time.

Lax–Wendroff method with upwind boundary approximation

For the numerical solution of this problem subsonic boundary conditions are required at the open end before the arrival of the shock wave, and once the shock wave has passed through the open end the possibility of subsonic, sonic or supersonic flow must be considered.

In the subsonic case, the appropriate boundary condition is:

$$p_J^{n+1} = p_e \tag{17}$$

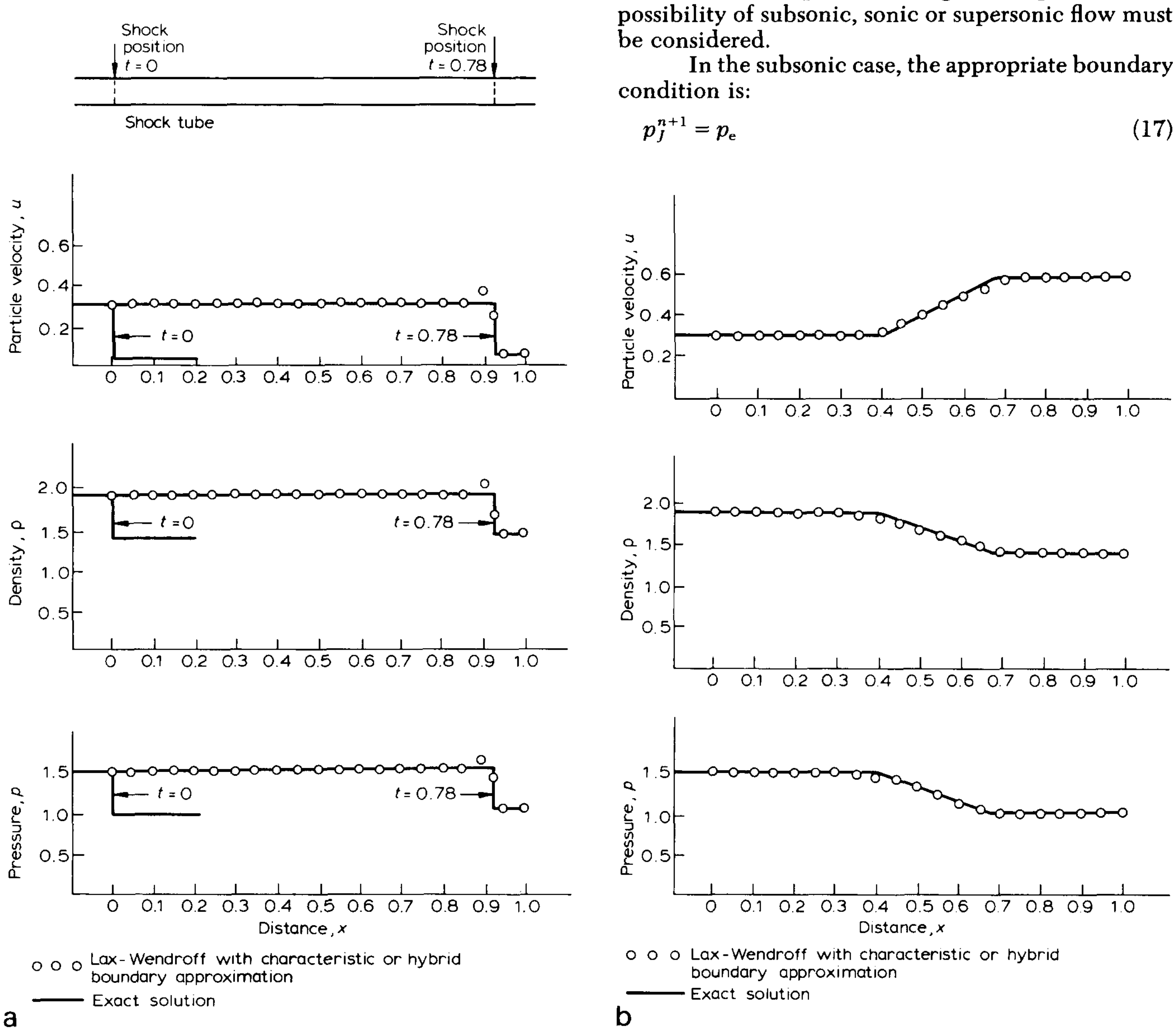


Fig 3 (a) Shock wave t = 0.0 and t = 0.78 (b) Rarefaction wave t = 1.63 where p_e is the exit pressure at the open end. The values of ρ_J^{n+1} and e_J^{n+1} can be calculated from Eqs (6) and (8), and the value of u_J^{n+1} may then be calculated from:

$$u_J^{n+1} = \left[2\left(e_J^{n+1} - \frac{p_J^{n+1}}{(\gamma-1)}\right) \Big/ \rho_J^{n+1}\right]^{1/2} \tag{18}$$

For the case of supersonic flow no imposed conditions at the boundary are required. Here the values ρ_J^{n+1}, m_J^{n+1} and e_J^{n+1} can be calculated from Eqs (6), (7) and (8), from which may be obtained:

$$u_J^{n+1} = m_J^{n+1}/\rho_J^{n+1} \tag{19}$$

and:

$$p_J^{n+1} = (\gamma-1)(e_J^{n+1} - \tfrac{1}{2}u_J^{n+1}m_J^{n+1}) \tag{20}$$

For sonic flow, once again, Eqs (6) and (8) may be used to calculate ρ_J^{n+1} and e_J^{n+1} and the sonic assumption:

$$u_J^{n+1} = \left(\gamma \frac{p_J^{n+1}}{\rho_J^{n+1}}\right)^{1/2} \tag{21}$$

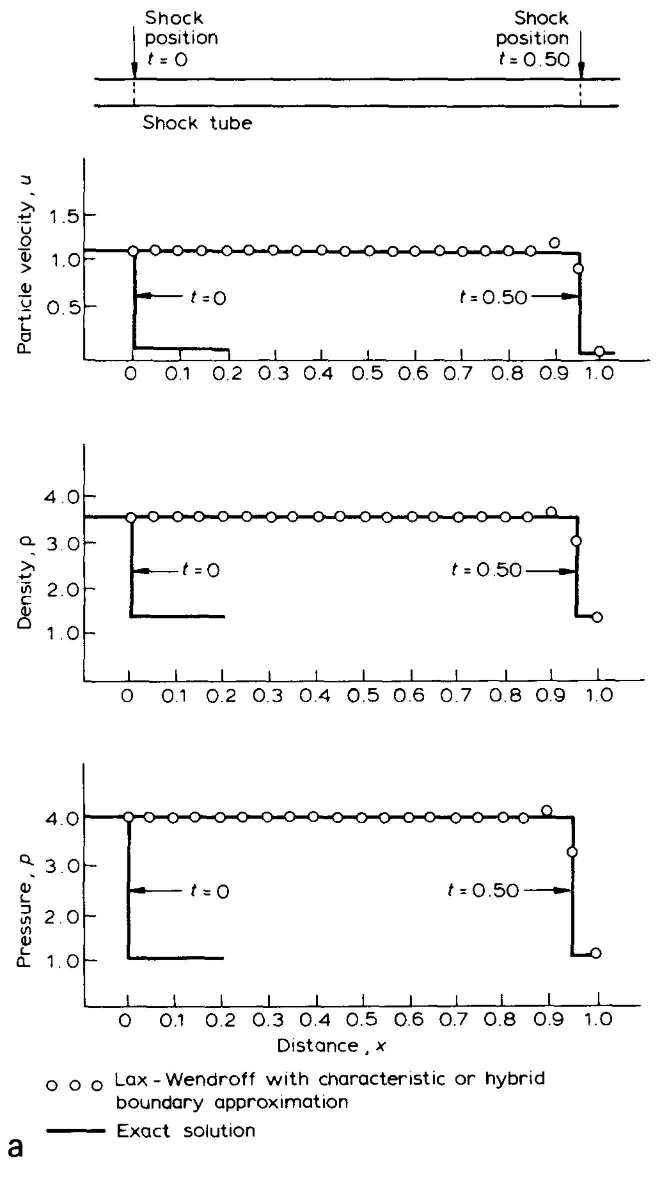
in conjunction with Eq (1) may now be used to give:

$$u_J^{n+1} = \left(\frac{\gamma(\gamma-1)}{1+\gamma(\gamma-1)/2}\frac{e_J^{n+1}}{\rho_J^{n+1}}\right)^{1/2} \tag{22}$$

Finally, the pressure, p_J^{n+1}, may be obtained from Eq (20).

Lax–Wendroff method with characteristic boundary approximation

For the solution with the characteristic approximation at the boundary a formulation of the boundary conditions in terms of the mixed variables u, a and a_a was used.



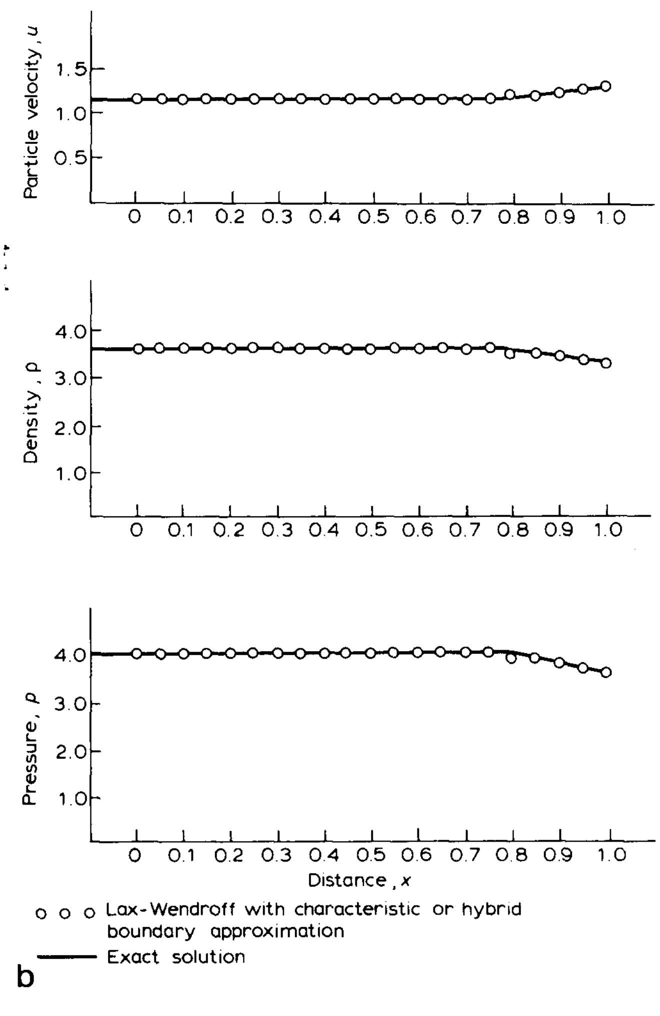


Fig 4 (a) Shock wave t = *0.0 and* t = *0.5 (b) Rarefaction wave* t = *2.06*

For subsonic flow the constant pressure condition at the pipe exit takes the form:

$$\frac{a_R}{(a_a)_R}=\left(\frac{p_e}{p_{ref}}\right)^{(\gamma-1)/2\gamma} \tag{23}$$

where p_e is the exit pressure. The required values at the boundary a_R, u_R and $(a_a)_R$ can now be obtained from Eqs (12), (13) and (23).

For supersonic flow, once again, no imposed boundary conditions are required. The three characteristic gradients are now all positive and the relations along the characteristics provide all the information that is necessary to compute the solution at the boundary. For the relation along the $C^{(2)}$ characteristic, Eq (10) with the Courant approximation gives:

$$a_R-a_Q-\frac{\gamma-1}{2}(u_R-u_Q)$$
$$=\frac{\gamma-1}{2}\alpha_A k+\frac{a_A}{(a_a)_A}[(a_a)_R-(a_a)_Q] \tag{24}$$

The three Eqs (12), (13) and (24) can now be solved for the required unknowns u_R, a_R and $(a_a)_R$.

For sonic flow, the sonic assumption $u_R=a_R$ in conjunction with Eq (12) gives:

$$a_R=\frac{2}{\gamma+1}\left[a_P+\frac{\gamma-1}{2}u_P+\frac{\gamma-1}{2}\alpha_A k\right.$$
$$\left.+\frac{a_A}{(a_a)_A}((a_a)_R-(a_a)_P)\right] \tag{25}$$

where the entropy measure variable, $(a_a)_R$, can be calculated from Eq (13). With the sound speed, a_R, now known it is possible to calculate p_R and ρ_R from the isentropic relationships.

Computational quasi-steady assumption

The theoretical quasi-steady assumption cannot be programmed directly on a computer, and the manner of its implementation is now discussed.

The first problem is to distinguish supersonic from subsonic flow behind a shock. This was achieved by evaluating average flow values from the nodes adjacent to the open end. In the implementation this average was computed from values at the five points adjacent to the end node.

In the case of supersonic flow adjacent to the open end there are now two possibilities. In the first case there may be subsonic flow at the open end, because the shock has not arrived, and in this case the subsonic flow equations are used at the open end. The other possibility is that there is supersonic flow at the open end, in which case the supersonic flow equations are used.

In the case of subsonic flow adjacent to the open end there are two possibilities once again. Either there may be subsonic flow at the open end, in which case the subsonic equations are used, or there is supersonic flow at the open end, in which case the sonic equations, limiting the flow, are used.

This computational quasi-steady assumption was used in all of the numerical calculations and would appear to have a quite general applicability.

Computational notes

Solutions to the examples were calculated using the Lax–Wendroff method with the upwind and characteristic approximations at the boundary for various mesh lengths, Δx, with the time increment, Δt, obtained from $\max(|u|+a)\Delta t/\Delta x=0.9$ in order to satisfy the Courant–Friedrichs–Lewy stability criterion[3].

The computations led to the following general observations:

- Both the upwind and characteristic boundary approximation methods showed deficiencies when used on their own.
- The upwind method provided slightly greater accuracy than the characteristic method for shocks with supersonic flow behind the shock.
- The characteristic method provided greater accuracy than the upwind method in the calculation of the rarefaction wave arising from a shock with subsonic flow behind the shock.

The theoretical reason for these observations is, of course, that a characteristic method is not suitable for flow calculations in which large shocks occur. For shocks with subsonic flow behind the shock, these errors have much less significance and are outweighed by the accuracy with which the rarefaction wave may be calculated. The rarefaction wave can be calculated accurately because the method of Courant *et al*, with mixed variables, provides an exact solution for homentropic flows[2]. Further, the upwind method is not suitable for the calculation of a rarefaction wave, because one of the conservation equations has to be abandoned in accommodating the required boundary condition.

Lax–Wendroff method with hybrid boundary approximation

The most accurate solutions to the examples were obtained from a hybrid version of the previous two methods, incorporating their best features. This hybrid version may be summarised:

(1) Values of the flow variables at the open end are calculated using the subsonic equations of the characteristic method. If the resultant flow is subsonic or sonic the calculation is terminated.

(2) If the flow is supersonic at the open end the average values of the flow at the five nodes adjacent to the open end are calculated.

(3) If in (2) a region of subsonic flow adjacent to the boundary is established then the sonic equations of the characteristic method are used to calculate the flow values at the open end.

(4) If in (2) a region of supersonic flow adjacent to the boundary is established then the supersonic equations of the upwind method are used to calculate the flow values at the open end.

In Figs 2, 3 and 4 the results of computations with this hybrid method at the boundary are compared with results obtained from using the characteristic method at the boundary. In both sets of calculations a mesh length of $\Delta x=0.025$ was used.

Conclusion

This paper has proposed boundary condition approximations that may be used in the solution of gas flow problems by the Lax–Wendroff method. Their application has been examined by considering the solution of a shock tube problem with an open end. Through the choice of suitable parameters it has been shown that this problem may be used as a benchmark for the comparison of numerical methods of solution. The test problem has been used to compare the accuracy of an upwind approximation with that of a characteristic approximation at the boundary. The results have shown that the upwind method provides slightly greater accuracy for supersonic flow, and the characteristic method provides greater accuracy for subsonic flow, behind a shock. The most accurate results have been obtained by using a hybrid version of these two methods.

In conclusion it would appear that the Lax–Wendroff method, in conjunction with this hybrid method, has the potential for solving many problems where shocks cross pipe boundaries. An example of practical interest arises in an autoclave system when a shock impinges on a plate at the end of a pipe, and this problem is currently under investigation.

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