Appropriate boundary conditions for the solution of the equations of unsteady one-dimensional gas flow by the Lax–Wendroff method

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This paper presents a new characteristic approximation to the boundary conditions, required in the solution of gas flow problems by the Lax–Wendroff method. The accuracy of this and other currently used methods is assessed by a comparison with the exact solutions of two test problems

Key words: *gas flow, 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. The method, however, cannot be used on the boundaries of the problem where some other technique is required to approximate the conditions. This paper compares the available choices for the boundary condition approximation by considering the solution of two test problems, the reservoir discharge problem and the shock tube reflection problem.

One method of approximating the boundary conditions is to use characteristics as in MacLaren *et al*[2]. This paper constructs a new characteristic formulation in terms of the primitive variables and compares it with solutions obtained from the mixed-variable method originally used by Benson *et al*[3]. Another method, suggested by Lax[4], is to use reflected boundary conditions and these are considered in the shock reflection problem. The accuracy of these various methods of solution is assessed by a comparison with the exact solutions of the proposed test problems.

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Governing equations

Following MacLaren *et al*[2], the equations of continuity, momentum, and energy for one-dimensional flow of an ideal gas, with heat transfer and wall friction, may be written in the conservation form:

$$\frac{\partial V}{\partial t}+\frac{\partial G(V)}{\partial x}=B \tag{1}$$

with

$$V=\begin{bmatrix}\rho\\ \rho u\\ \frac{1}{2}\rho u^2+p/(\gamma-1)\end{bmatrix}$$

$$G(V)=\begin{bmatrix}\rho u\\ \rho u^2+p\\ \frac{1}{2}\rho u^3+\gamma/(\gamma-1)\,up\end{bmatrix}\qquad B=\begin{bmatrix}0\\ -\rho\phi\\ \rho q\end{bmatrix}$$

and the wall friction term defined by:

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

The normal form of these equations is:

$$\frac{\partial W}{\partial t}+A\frac{\partial W}{\partial x}=C \tag{3}$$

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

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

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with

$$W=\begin{bmatrix}\rho\\ u\\ p\end{bmatrix}\qquad A=\begin{bmatrix}u & \rho & 0\\ 0 & u & 1/\rho\\ 0 & a^2\rho & u\end{bmatrix}$$

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

These equations are written in terms of particle velocity, pressure and density and it would be convenient to formulate a method of solution in terms of these primitive variables.

Two-step Lax–Wendroff method

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

$$\begin{aligned} V_{j+1/2}^{n+1/2} &= \tfrac{1}{2}(V_{j+1}^n + V_j^n) - \frac{1}{2}\frac{\Delta t}{\Delta x}(G_{j+1}^n - G_j^n) \\ &\quad + \frac{\Delta t}{4}(B_{j+1}^n + B_j^n) \\ V_j^{n+1} &= V_j^n - \frac{\Delta t}{\Delta x}(G_{j+1/2}^{n+1/2} - G_{j-1/2}^{n+1/2}) \\ &\quad + \frac{\Delta t}{2}(B_{j+1/2}^{n+1/2} + B_{j-1/2}^{n+1/2}) \end{aligned} \tag{4}$$

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.

Characteristics and characteristic relations

The characteristics and characteristic relations can be obtained from the normal form[5]. The characteristic relations on the $C^{(1)}$, $C^{(2)}$ characteristics, where $dx/dt = u \pm a$, can be written in the form:

$$\frac{1}{\rho a}\,dp \pm du = \alpha\, dt \tag{5}$$

where

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

The characteristic relation on the C characteristic, where $dx/dt = u$, may be written in the form:

$$dp - a^2\, d\rho = \beta\, dt \tag{6}$$

where

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

The advantage of using approximations based on these forms is that no change of variable is necessary when used with the Lax–Wendroff method.

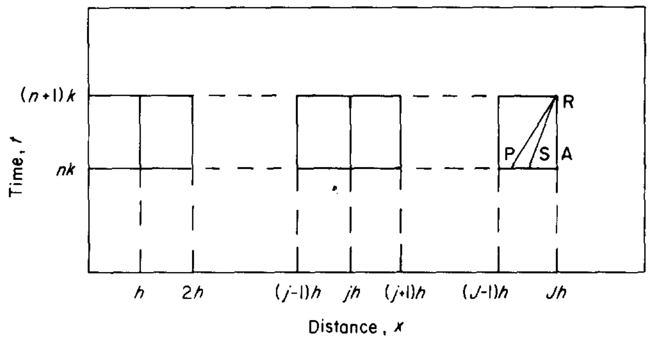

Fig 1 Computational grid for pipe of length x = Jh

The characteristics may also be written in terms of the u, a, a_a variables used by Benson *et al*[3]. The change to the new variables may be obtained from the relations:

$$\begin{aligned} a &= \left(\gamma\frac{p}{\rho}\right)^{1/2} & a_a &= \frac{a}{(p/p_{ref})^{(\gamma-1)/(2\gamma)}} \\ p &= p_{ref}\left(\frac{a}{a_a}\right)^{2\gamma/(\gamma-1)} & \rho &= \gamma\frac{p_{ref}}{a^2}\left(\frac{a}{a_a}\right)^{2\gamma/(\gamma-1)} \end{aligned} \tag{7}$$

The characteristic relations are now:

$$da \pm \frac{(\gamma-1)}{2}\,du = \frac{\gamma-1}{2}\alpha\, dt + \frac{a}{a_a}\,da_a \tag{8}$$

on the $C^{(1)}$, $C^{(2)}$ characteristics and:

$$da_a = \frac{1}{2}\frac{a_a}{\rho a^2}\beta\, dt \tag{9}$$

on the C characteristic. For homentropic flow, this formulation has the advantage that the equations are readily integrable.

Approximation of the characteristic equations

The characteristic equations of the previous section 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.

In terms of the u, p, ρ variables, and the notation of Fig 1, the Courant method leads to:

$$\begin{aligned} &x_R - x_P = (u_A + a_A)k \\ &\frac{1}{\rho_A a_A}(p_R - p_P) + u_R - u_P = \alpha_A k \end{aligned} \tag{10}$$

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

$$\begin{aligned} &x_R - x_S = u_A k \\ &p_R - p_S - a_A^2(\rho_R - \rho_S) = \beta_A k \end{aligned} \tag{11}$$

on the C characteristic.

The Hartree approximation was also used giving:

$$\begin{aligned} &x_R - x_P = \tfrac{1}{2}(u_R + a_R + u_P + a_P)k \\ &\frac{1}{2}\left(\frac{1}{\rho_R a_R} + \frac{1}{\rho_P a_P}\right)(p_R - p_P) + u_R - u_P = \tfrac{1}{2}(\alpha_R + \alpha_P)k \end{aligned} \tag{12}$$

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

$$\begin{aligned} x_R - x_S &= \tfrac{1}{2}(u_R + u_S)k \\ p_R - p_S - \tfrac{1}{2}(a_R^2 + a_S^2)(\rho_R - \rho_S) &= \tfrac{1}{2}(\beta_R + \beta_S)k \end{aligned} \quad (13)$$

on the C characteristic.

In terms of the u, a, a_a variables the Courant method leads to:

$$a_R - a_P + \frac{\gamma-1}{2}(u_R - u_P) = \frac{\gamma-1}{2}\alpha_A k + \frac{a_A}{(a_a)_A}[(a_a)_R - (a_a)_P] \quad (14)$$

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

$$(a_a)_R - (a_a)_S = \frac{1}{2}\frac{(a_a)_A}{\rho_A a_A^2}\beta_A k \quad (15)$$

on the C characteristic, RS. Approximations may be derived similarly along the $C^{(2)}$ characteristic.

In the solution of a problem these characteristic approximations are solved simultaneously with the appropriate quasi-steady 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.

Reservoir discharge problem

A test problem of practical importance is the reservoir discharge problem of de Haller[8]. The quasi-steady state conditions at the pipe ends are readily available[5]. Two types of boundary condition are required depending upon whether the flow is subsonic or sonic at the boundary.

The calculation is now considered of the unknowns at the open end at which there is outflow. In terms of the u, p, ρ variables, for subsonic flow, the appropriate boundary condition is:

$$p_R = p_e \quad (16)$$

where p_e is the exit pressure, and for sonic flow the relation:

$$u_R = \left(\gamma \frac{p_R}{\rho_R}\right)^{1/2} \quad (17)$$

must hold. For subsonic flow Eqs (10), (11), and (16) are linear and, hence, may easily be solved for u_R, p_R, and ρ_R. For sonic flow Eqs (10), (11), and (17) may be reduced to the solution of a non-linear equation in the variable p_R.

In terms of the u, a, a_a variables the corresponding boundary conditions are:

$$\frac{a_R}{(a_a)_R} = \left(\frac{p_e}{p_{ref}}\right)^{\gamma-1/2\gamma} \quad (18)$$

and

$$u_R = a_R \quad (19)$$

In this case, for both sonic and subsonic flow, a set of linear equations in u_R, a_R and $(a_a)_R$ is obtained.

The equations at the reservoir end may be obtained from quasi-steady-state considerations in a similar manner.

Exact solution

By making an assumption of homentropic flow, the exact theoretical solution is known for the initial and final flow values. The initial flow at the outlet, and along the pipe before the rarefaction wave is reflected from the reservoir end, can be calculated using Riemann invariants. For sonic flow at the outlet the solution is:

$$u = a = \frac{2}{\gamma+1}a_0 \quad (20)$$

where a_0 is the initial value of the sound speed for the gas in the pipe. Once the wave interaction has ceased a further theoretical check is available from the steady-state values down the pipe. For sonic flow at the outlet the solution is:

$$u = a = \left(\frac{2}{\gamma+1}\right)^{1/2} a_{stag} \quad (21)$$

where a_{stag} is the sound speed of the gas in the reservoir.

Computational notes

Lax–Wendroff calculations, with both the primitive and the mixed-variable methods of boundary approximation, have given values which indicate that convergence to the theoretical solution, where available, could be obtained by using a sufficiently fine mesh interval. Computations with the different boundary variables and the same mesh interval showed that a similar accuracy could be obtained by both methods apart from some initial values at the outflow end where the change of variable produced slightly more accurate results.

The relative accuracy of the computations with the primitive and mixed variable methods may be illustrated, and also compared with theoretical solutions, by assuming that the flow is homentropic. The discharge from a reservoir and pipe of unit length with initial values $p = 1.0$, $\rho = 1.4$, $u = 0.0$, into an exhaust region at a pressure $p = 0.0$, was considered. The Lax–Wendroff method with a mesh-length $\Delta x = 0.1$ was applied to this problem and the time increment, Δt, was obtained from max $(|u| + a)\,\Delta t/\Delta x = 0.9$ to satisfy the Courant–Friedrichs–Lewy stability criterion[9]. The upper limit for this criterion is 1.0 and the choice of 0.9 allows a reasonable margin of safety for the calculation. The numerical solutions to this problem at the exit and reservoir ends of the pipe are shown in Fig 2. As can be seen, close agreement has been obtained between the two methods except for some initial values. The numerical results at the pipe exit also show good agreement with the initial theoretical values, $p = 0.2791$, $\rho = 0.5626$, $u = 0.8333$, and the final theoretical values, $p = 0.5283$, $\rho = 0.8875$ and $u = 0.9129$.

Error analysis

It is of interest to examine the causes of the initial errors at the pipe exit, for the special case of homentropic flow. In the following, it is assumed that there is sonic flow at the pipe exit. A similar analysis may be made for the case of subsonic flow at the exit.

In the Courant approximation with the u, a, a_a variables, Eqs (14) and (15) are solved along with the condition for sonic flow, Eq (19).

Eqs (14), (15) and (19) represent three equations which may be solved for the three unknowns a_R, u_R, and $(a_a)_R$. As $\alpha \equiv \beta \equiv 0$ for the problem under consideration, the value of the entropy measure variable at the open end, $(a_a)_R$, equals the initial value, and the solution of Eqs (14), (15) and (19) is:

$$(a_a)_R = (a_a)_S \tag{22}$$

and

$$u_R = a_R = \frac{2}{\gamma+1}\left[a_P + \frac{(\gamma-1)}{2}u_P\right] \tag{23}$$

The accuracy of this solution may be assessed by integrating the characteristic Eqs (8) and (9) exactly to give:

$$a + \frac{\gamma-1}{2}u = \text{constant} \tag{24}$$

on the RP characteristic and

$$a_a = \text{constant} \tag{25}$$

on the RS characteristic. Eq (24) is, of course, just the Riemann Invariant which holds under the conditions of homentropic flow, Eq (25). The solution of Eqs (24) and (25) at the point R is identical to the solution given in Eqs (22) and (23), showing that in this case the Courant method of solution is exact for homentropic flow.

In the approximation with the u, p, ρ variables, the Courant method uses Eqs (10) and (11). The accuracy of this approximation may be determined from attempting to integrate Eqs (5) and (6). An explicit integration of these equations is obstructed by the variation of $(\rho a)^{-1}$ in Eq (5) along the RP characteristic and a^2 in Eq (6) along the RS characteristic. The Courant approximation takes these coefficients as constant with values at the point A of Fig 1. An integration now gives the Courant method in terms of the u, p, ρ variables as in Eqs (10) and (11). Providing that the variables are continuous in the neighbourhood of the Point A, the error in this assumption may be made arbitrarily small by decreasing the mesh size and bringing the values at R and P as close as is necessary to the values at A. However, for the problem under consideration, both for subsonic and sonic flow, the instantaneous opening of the valve at A introduces a discontinuity into the solution at A and, hence, there will always be an error in using the Courant method with the u, p, ρ variables in the form shown in Eqs (10) and (11). It is for this reason that slightly more accurate results were obtained by the change of variable in the previous section for the initial flow values. In the subsequent flow this initial discontinuity is immediately smoothed out and, as Fig 2 shows, close agreement between the two methods of approximating the boundary conditions can be obtained.

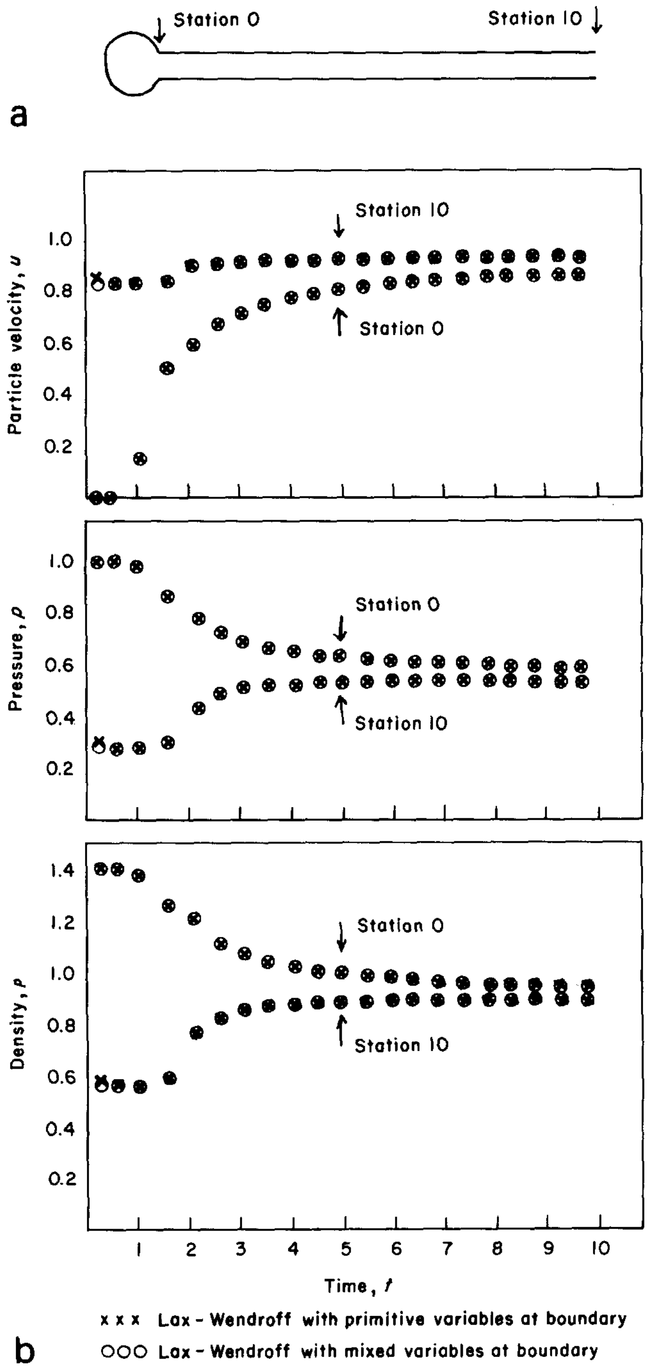

Fig 2 (a) Reservoir and discharge pipe (b) Computed values at pipe exit and reservoir end

Shock tube problem

The Lax–Wendroff method may also be used to produce accurate answers for one-dimensional problems in the presence of shocks. With this facility it has an advantage over unmodified characteristic methods of solution which produce errors in the presence of shocks[5].

The one-dimensional equations of gas flow may be solved by characteristic methods provided that the solutions are continuous. However, discontinuous solutions may also occur, eg in shock tube problems. It is also possible that, after a finite time, solutions may develop shocks arising from the steepening of a compression wave. For accurate solutions to these problems characteristic methods must be modified to account for these internal discontinuities.

In contrast with characteristic methods, the solution by the Lax–Wendroff method requires no modification in the presence of shocks. However, as is discussed in the following sections, the calculations show that particular care must be taken with the boundary approximations, when using the Lax–Wendroff method, if accurate solutions are required.

The shock tube problem is a test problem of the greatest importance as theoretical solutions to this problem are available and can be used as a benchmark for comparisons with numerical solutions. The Lax–Wendroff method was applied to Eq (1) with the assumption that friction and heat transfer terms were negligible so that the numerical solution could be compared with an exact theoretical solution.

The shock tube was assumed to be closed at the end $x = 1.0$ and the Riemann problem was considered with the initial values:

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

for $x < 0$, and (26)

$$u = 0.0 \qquad p = 1.0 \qquad \rho = 1.4$$

for $x > 0$.

With these initial values the problem has an exact solution:

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

for $x/t < 5.0$ and (27)

$$u = 0.0 \qquad p = 1.0 \qquad \rho = 1.4$$

for $x/t > 5.0$.

Incident shock wave

The Lax–Wendroff method with a mesh length $\Delta x = 0.025$ was applied to this problem and the time increment, Δt, was obtained from max $[(|u| + a)\,\Delta t]/\Delta x = 0.9$ to satisfy the Courant–Friedrichs–Lewy stability criterion. The exact and Lax–Wendroff solutions to this problem are shown in Fig 3 at time $t = 0.16$.

Fig 3 shows that the Lax–Wendroff method provides a good solution except at the shock itself where the shock discontinuity has been replaced by a shock band (x_1, x_0) within which there is a rapid variation in the variables. The best resolution of a shock wave by a numerical method is over one mesh length and, as can be seen in the Figure, the Lax–Wendroff method fails to achieve this ideal representation. In the shock band the 'clean' shock is 'smeared' by an approximation based over a few mesh intervals but the bandwidth is, nevertheless, many magnitudes greater than that of a physically real shock. Across the shock band the Rankine–Hugoniot equations:

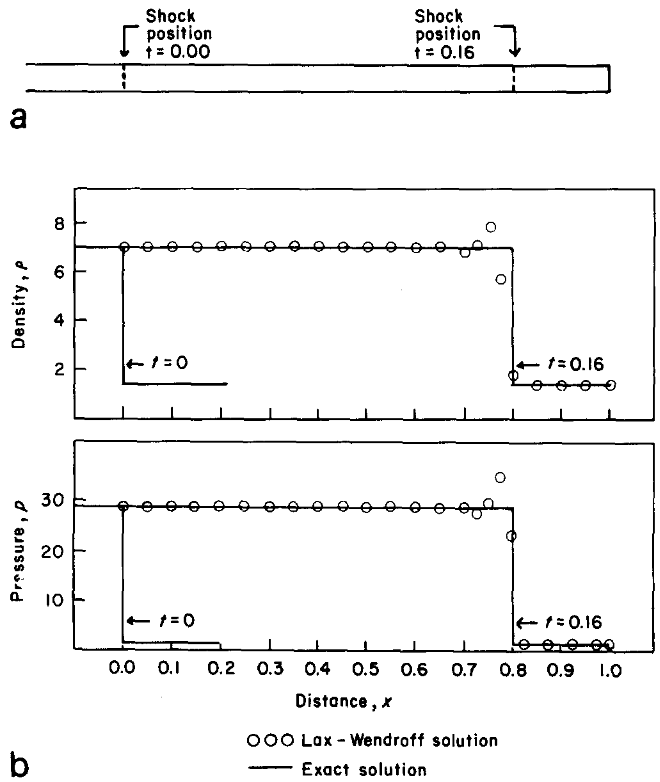

Fig 3 (a) Shock tube (b) Incident shock wave

$$U(\rho_1 - \rho_0) = \rho_1 u_1 - \rho_0 u_0$$
$$U(\rho_1 u_1 - \rho_0 u_0) = \rho_1 u_1^2 + p_1 - \rho_0 u_0^2 - p_0 \qquad (28)$$
$$U(E_1 - E_0) = u_1(E_1 + p_1) - u_0(E_0 + p_0)$$

hold, where $E = \frac{1}{2}\rho u^2 + \rho e$, and U is the shock speed. Richtmeyer and Morton[10] have verified that solutions obtained by the Lax–Wendroff method approximate both the Rankine–Hugoniot conditions and the shock speed to a high accuracy. This high accuracy is to be expected as the Lax–Wendroff approximation is conservative in form and, hence, the Rankine–Hugoniot conditions are satisfied across an internal discontinuity.

Reflected shock wave

The boundary conditions at the closed end were approximated by the Courant method in terms of the u, a, a_a variables. For low shock strengths the characteristic method gave good approximations to the exact analytical solution. However, for higher shock strengths these calculations disclosed a discrepancy between the numerical and the exact solutions. This is because characteristic methods provide reasonable solutions to problems containing weak shocks, but for strong shocks the Rankine–Hugoniot conditions must be satisfied across a shock discontinuity and characteristic methods fail to achieve this representation.

The reflection conditions at the closed end boundary suggested by Lax[4] were used also. These conditions, for a closed end at $x = x_J$, take the form:

$$u_{J+1} = -u_{J-1}$$
$$p_{J+1} = p_{J-1} \qquad (29)$$
$$\rho_{J+1} = \rho_{J-1}$$

With these reflection conditions it is now possible to compute values for the unknowns on the boundary solely by the Lax–Wendroff method. These calculations showed that the reflection method, compared with characteristic methods, gave equivalent or greater accuracy over the full range of both weak and strong shocks. This may be illustrated by considering the reflection of the shock wave shown in Fig 3 from the closed end. For these incident values the shock tube problem, to four significant figures, has the exact solution:

$$u = 4.0 \qquad p = 29.0 \qquad \rho = 7.0$$
for $x < 1.0 - 1.8t'$, and (30)
$$u = 0.0 \qquad p = 191.4 \qquad \rho = 22.56$$

for $x > 1.0 - 1.8t'$, where the time, t', is measured from the moment when the shock is reflected from the closed end. From Fig 4, where the calculated values are compared with the exact solution at $t = 0.66$, it is evident that the Lax–Wendroff method with the reflection boundary conditions provides a reasonable approximation to the exact solution. The Lax–Wendroff method with the characteristic boundary conditions, however, provides a reasonable approximation to the pressure but a large error is evident in the calculation of the density in the neighbourhood of the closed end.

Error analysis

The cause of the errors in the characteristic method of solution may be elicited from Eq (15). As the path characteristic RS reduces to the path RA at a closed end, and in addition $\beta \equiv 0$ in Eq (15) for the problem under consideration, the value of the entropy measure variable, a_a, remains unchanged at the closed end both before, during, and after the reflection of the shock wave. However, as is well known, there may well be a significant increase in the entropy of the gas at a closed end after shock reflection, and it is the failure of the characteristic method to account for this increase that results in the errors shown in Fig 4.

Conclusion

This paper has formulated boundary conditions for the Lax–Wendroff method directly in terms of the primitive variables. The necessity for transforming to mixed variables at the boundaries has thus been avoided and it is now possible to solve unsteady gas flow problems solely in terms of the primitive variables, a requirement first called for by MacLaren *et al*[2]. The paper has also presented two test problems for unsteady gas flow, reservoir discharge and shock tube reflection, and has used them to gauge the accuracy of the different formulations.

For the reservoir discharge problem, accurate solutions have been obtained by the Lax–Wendroff method in conjunction with characteristic methods of solution at the boundaries. Further, it has been shown that more accurate results may be obtained by using mixed variables at the boundary in comparison with working solely in terms of the primitive variables.

For the shock reflection problem it has been shown that the Lax–Wendroff method in conjunction with reflected boundary conditions gives results of equivalent or better accuracy, compared with characteristic approximations, and may be recommended, therefore, for flow problems in pipes with closed ends.

Finally it is noteworthy that the Lax–Wendroff method is a useful general purpose tool for the solution of unsteady one-dimensional gas flow problems as it can provide accurate solutions to problems which involve shocks in addition to problems which only involve characteristics. However, as this paper has shown, care is required in the choice of the approximation at the boundary if accurate solutions are required.

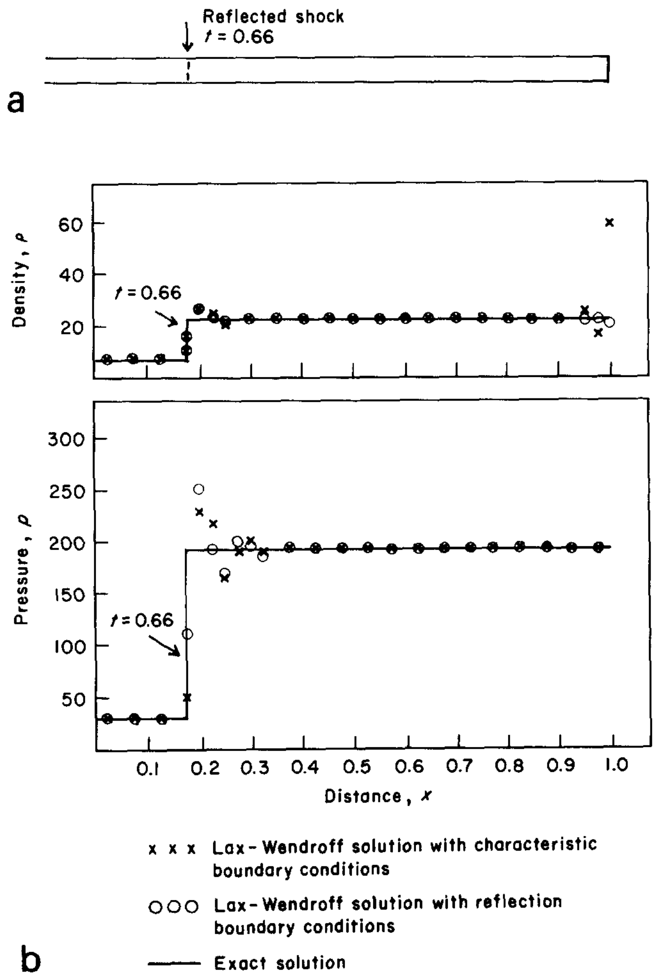

Fig 4 (a) Shock tube (b) Reflected shock wave

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BOOK REVIEW

Developments in Flow Measurement

Ed. R. W. W. Scott

In-depth analyses of several individual meter types combined with a number of excellent surveys of broad aspects of flow measurement make this book very good value. With eight authors who have already written extensively on their subjects in journals and for Conferences it would be surprising if there was much that was new in the book but few will have had the opportunity to follow the dozens of references at the end of each chapter. In consequence collecting together their expertise to produce an overview of the status of flow measurement at the beginning of the 1980's is certainly valuable to all who are involved in the art and science of this subject.

Each chapter has its own distinctive flavour melded together by the editor who has himself contributed a very useful introduction and a detailed appraisal of liquid (mainly water) flowmetering. Similar general studies of petroleum and gas measurement are followed by two detailed examinations of present developments in turbine and electromagnetic flowmeters. Another broad look, this time at open channel flow, leads to the final chapter on assessing the uncertainties which occur in every measurement.

I have purposely left Chapter 2 for special mention. This is by Dr Mattingly of the National Bureau of Standards in the USA and deals with calibration facilities and the dynamic traceability which should be determined between every measurement installation and the eventual national primary standards of mass, length, time, etc. However accurate or inaccurate the actual user wishes to be, it is only by the conscious effort to find out the answer in his case to dynamic traceability that his measurement can have real meaning.

E. A. Spencer

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Modern Compressible Flow

J. D. Anderson

Compressible fluid flow is a subject of considerable interest to students, but one which can easily become an apparently endless parade of equations. The lecturer must enliven the subject by discussing practical applications, experimental results, personal experience and occasionally commenting on the historical development of the subject. This 'filling out' of the subject is not too difficult for a lecturer, but few authors have followed Professor Anderson's approach of including historical and biographical notes in a text book. These notes provide an interesting background to the theory, placing the work in perspective and making the book more readable. The result is a book to which students and teachers can turn without being 'turned off'.

After a general introduction to compressible flow, the governing equations are derived and applied to one-dimensional flows and normal shocks. The Fanno line and Rayleigh line are introduced at this stage, but the flow in nozzles is discussed later. There is a thorough treatment of oblique shocks, shock reflection, shock interaction and expansion waves, with some interesting notes on the development of the subject by Prandtl and Taylor. The chapter on nozzle flows contains an interesting biographical sketch on de Laval and a summary of the pioneering work of Stodola. Linearised compressible flow theory is described and there is a short chapter dealing with the Taylor–Maccoll equation for compressible flow over a cone. The first 259 pages, as outlined here, provide a good treatment of compressible flow theory prior to the development of digital computers.

The remainder of the book, another 200 pages, is an introduction to modern numerical methods in fluid dynamics. The method of characteristics is described, with application to nozzle design. This is followed by finite difference methods and an outline of time-marching techniques, with the last two chapters adding real gas effects with reactions at high