

# A COMPARATIVE STUDY OF SOME FINITE DIFFERENCE SCHEMES IN AN UNSTEADY DISCONTINUOUS COMPRESSIBLE FLOW FIELD

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## ABSTRACT

Analysis of unsteady compressible flow plays an important role in design and performance prediction in many diverse engineering applications. The generated flow fields in most cases involve strong pressure discontinuities, high temperature differences between gas layers and entropy interfaces. Two first order schemes of the modified method of characteristics and three recently developed finite difference schemes, are applied to the one dimensional, frictional and heat transferring gas flow problem. Comparison is made with a shock tube problem, rightly considered as a test tube for flow prediction procedures. The test tube has an analytical solution as well as experimental measurements for comparison and evaluation of friction and heat transfer effects. The earliest and most widely used modified scheme of characteristics [5] is shown to be inadequate to cope with flow discontinuities. The overall implication of analysis of results, proves that the first order scheme, which is based on physical interpretation of the characteristics numerically, have very good ability to deal with discontinuities, showing low computer time as well as simple coding. Despite the accuracy of higher order schemes, they produce non-physical oscillations which should be meditated using artificial damping procedures.

## INTRODUCTION

Good progress has been made in the field of unsteady compressible flow applications in the last three decades. This is credited, in essential part, to the development of numerical techniques suitable to handle the complex unsteady flow problems. Unsteady flow problems in which there are large amplitude variations in the flow properties occur in such applications such as thrust augmenting pulse ejectors, pulsed combustors, pressure exchangers, inlet and exhaust piping of internal combustion engines, propagation of explosion and detonation waves...etc.

The flow fields in such applications always develop pressure, temperature and entropy discontinuities. In addition, to temperature differences between gas layers, or the addition of fluid of non-uniform entropy to the duct in which unsteady flow occurring, waves overtaking each other into shock waves also persist. Friction and heat transfer also add to the change of entropy along particle path lines. For example, unsteady flow in the exhaust pipe of supercharged I.C.E. reported by [1] and flow in pulsed combustor

by [2], the temperature differences between gas layers of exhaust gas and fresh charge may exceed 1000 °C and pressure ratios may be more than 4.

The finite difference approach may be divided into two categories. In the first, the method of characteristics in which the finite difference approximations are derived using the properties of characteristic directions which have real slopes if the system of differential equations is hyperbolic. In the second category, which for the purpose of the present work shall be called straight forward finite difference terms replace partial derivatives with little premanipulation of the equations.

The one dimensional unsteady gas flow requires the use of special techniques to solve the describing hyperbolic partial system of differential equations. The flow properties at each point of the flow field depend on those properties in finite region of upstream flow and independent of properties downstream. Hence, a characteristic concept is defined as the path of physical disturbance and the partial D.E. can be reduced into

total derivatives along characteristics [3]. Practical unsteady flow calculations in supercharging I.C.E. came into use more than 30 years ago by Jenny [4]. These hand calculations are extremely tedious and time consuming. The first application of computer using numerical technique to solve the unsteady flow problem is reported by Benson [5,6]. It is a first order scheme modifying the method of characteristics to suit coding by computer. The method has been widely used and can cope with friction and heat transfer by modifying the homentropic solution. However, the present study shows that the method fails to handle the presence of discontinuities. Spalding [7] introduced a first order discretization scheme based on physical interpretation in the integration of the differential equations along characteristics in hybrid method. Marzouk [8] applied the first order technique of characteristics to pulse ejector problem without taking heat transfer and friction into account and pulse pressure ratio was low.

Recent stage of development is represented by application of straight forward finite difference methods, by expanding equations in Taylor series with respect to time and replacing time derivatives by space derivatives approximated by central, forward and backward differences. Lax [9] introduced a first order accurate finite difference explicit scheme. The work by [10] is a study to compare some numerical methods to guide specialists to choose the appropriate scheme. However, this work was based on shock free flow without friction and heat transfer effects. Also the order of discretization of the higher order schemes also changed at the boundaries which makes this comparison inadequate. Morsy [11] applied Lax-Windroff second order scheme [13] to study the behaviour of pressure waves in variable area ducts. The order of discretization also changed at boundaries and the wave pressure ratio is low such that the flow is basically homentropic.

The present study gives researchers the opportunity to select appropriate technique when the unsteady flow field develops strong discontinuities. Five numerical techniques are tested. Comparison is made with a shock tube problem, rightly considered as a "test tube" for unsteady compressible flow prediction procedures. This allows the generation of as strong shock waves as required and high temperature differences between gas layers of non-homentropic flow. The problem has an

analytical solution [15] and experimental measurements for comparison and evaluation of friction and heat transfer effects.

## THE MATHEMATICAL MODEL

The one dimensional unsteady viscous and heat transferring flow is described by the system of differential equations of mass, momentum and energy, in constant area pipe. It is represented vectorially with right hand side includes perturbation terms of friction and heat transfer [14,15]

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho(e + \frac{u^2}{2}) \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u(e + \frac{u^2}{2} + \frac{p}{\rho}) \end{pmatrix} = \begin{pmatrix} 0 \\ -f \\ q \end{pmatrix} \quad (1)$$

Since the gas pressure and temperature are far from the critical values, the state and caloric equations take the form.

$$p = \rho RT \quad (2)$$

$$e = C_v T \quad (3)$$

Equations (1), (2) and (3) are used to reduce the system of conservation laws as follows:

$$\frac{\partial}{\partial t} W + \frac{\partial}{\partial x} F = S \quad (4)$$

where  $W$ ,  $F$ , and  $S$  are vectors of dimension 3.

$$w_1 = \rho, w_2 = \rho u, w_3 = \frac{p}{\gamma - 1} + \frac{\rho u^2}{2}$$

$$F_1 = \rho u, F_2 = p + \rho u^2, F_3 = u \left( \frac{\gamma p}{\gamma - 1} + \frac{\rho u^2}{2} \right)$$

and

$$S_1 = 0, S_2 = -f, S_3 = q$$

in which,

$$f = \frac{4C_f}{2d} \rho u^2 \frac{u}{|u|},$$

represents the friction force per unit volume and

$$q = S_t \frac{4\rho C_p u (T_w - T)}{d}$$

presents the heat transfer per unit volume per unit time.

The values of friction coefficient and Stanton number  $C_f$  and  $S_t$  are estimated from boundary layer theory or may be taken as functions of non-dimensional parameters like Reynolds number.

*Mathematical and Finite Difference Procedures:*

1. THE MODIFIED METHOD OF CHARACTERISTICS OF BENSON [5,6]:

The method of characteristics is based on the transformation of the non linear PDE into ordinary differential equations along characteristic curves. The conservation equations (1), may be written as follows in the dependent variables  $p, \rho$  and  $u$ , along the characteristics.

$$\frac{dp}{dt} \pm \rho a \frac{du}{dt} - (\gamma - 1)(q + uf) \pm af = 0 \text{ along } \frac{dx}{dt} = u \pm a \quad (5)$$

and

$$\frac{dp}{dt} - a^2 \frac{d\rho}{dt} - (\gamma - 1)(q + uf) = 0 \text{ along } \frac{dx}{dt} = u \quad (6)$$

where

$$a = \sqrt{\frac{\gamma p}{\rho}}$$

Benson [5,6] introduced a first order numerical technique modifying the hand calculation procedure by [4]. It employs a rectangular grid in space and time. The solution is obtained at each node of the grid by integrating the equations along the two Reimann characteristics and the particle path line homentropically and then adding friction, heat transfer and entropy modifying terms.

If  $a_A$  represents sonic speed at entropy level  $s_A$  of a reference pressure, the change in Reimann variables and entropy level,  $\lambda$ ,  $\beta$  and  $a_A$  (taken as main dependent variables), are obtained through finite differences along the characteristics having slopes

$$\frac{dx}{dt} = u \pm a, \quad \frac{dx}{dt} = u$$

in the form:

$$d\lambda, d\beta = d\left(a \pm \frac{\gamma - 1}{2} u\right) = a \frac{da_A}{a_A} + \frac{(\gamma - 1)^2}{2\rho a} (q + uf) dt \mp \frac{(\gamma - 1)}{2} \frac{f}{\rho} dt \quad (7)$$

along  $\lambda$ ,  $\beta$  characteristics and,

$$\frac{da_A}{a_A} = \frac{(\gamma - 1)}{2\rho a^2} (q + uf) \quad (8)$$

along particle path.

Equation (7) and (8) are integrated along the respective characteristics to obtain the difference equations and march the solution provided that the condition of stability  $\frac{\Delta t}{\Delta x} \leq \frac{1}{|u| + a}$ , is satisfied.

In this method, it is considered that the change in Reimann variables and entropy along their relevant characteristics, is solely due to friction and heat transfer, i.e. the flow is non-homentropic from the point of view of entropy change along the path line. This is not the case when the flow field generates shock waves, temperature and entropy discontinuities where the reimann variables  $\lambda$ ,  $\beta$  vary along their relevant characteristics due to change of entropy level across such discontinuities. For problems with low pressure ratio, such as those studied by [4,6], the entropy discontinuity has minor effects on the solution. However, for high pressure ratios, they would be highly influential. This is the basic reason for failure of this procedure to cope with the discontinuity when it is applied, in the present study, to even an adiabatic frictionless shock tube problem with pressure ratio of 10 and initial uniform temperature.

2. THE MODIFIED METHOD OF CHARACTERISTICS OF SPALDING [7]

This modified version is a first order technique that combines the use of characteristics with rectangular grid. Though the following characteristic equations can be shown to be the same as (7), (8), they are presented in the new dependent variables  $p, u$  and  $s$  to demonstrate the difficulties that must be encountered in dealing with discontinuities. For concise presentation the dependent variables are taken as

$$P = (p)^\frac{\gamma - 1}{\gamma}, \quad U = \frac{\gamma - 1}{2} u, \quad \sigma = \exp\left(\frac{\gamma - 1}{2} s\right)$$

Hence Equation (7), (8) take the form.

$$d(P\sigma \pm U) = D dt \pm E \frac{\partial s}{\partial x} dt \mp G dt \text{ along } \frac{dx}{dt} = u \pm a \quad (9)$$

$$d\sigma = \sigma F \quad \text{along} \quad \frac{dx}{dt} = u \quad (10)$$

where

$$D = \left(\frac{\gamma-1}{2}\right) \frac{a}{p} (q + uf), \quad E = \left(\frac{\gamma-1}{2}\right) a^2$$

$$F = \left(\frac{\gamma-1}{2\gamma}\right) \frac{q + uf}{p}, \quad G = \left(\frac{\gamma-1}{2\gamma}\right) \frac{a^2 f}{p}$$

and

$$E \frac{\partial s}{\partial x} dt = \pm P d\sigma \mp \frac{1}{\gamma} D dt$$

The term  $P_{d\sigma}$  in the last equation does not vanish for a discontinuity along Reimann variable characteristics. The problem is that the dependent variables are not known in advance to set a solution so that an iterative procedure may be applied. Based on physical interpretation of a shock tube flow, the pressure in the integral is shown to be equal to the new pressure level  $P_I$  [7]. The subscripts M, N and R denote crossing points of the reimann and path lines characteristics from point I at the new time level as shown in figure (1).

Hence the solution is obtained in explicit form as:

$$P_I = \frac{\frac{1}{2}P_N(\sigma_I + \sigma_N) + \frac{1}{2}P_M(\sigma_I + \sigma_M) + U_N - U_M + \left[\frac{\gamma-1}{\gamma}D - G\right]_{NI} \Delta t + \left[\frac{\gamma-1}{\gamma}D + G\right]_{MI} \Delta t}{\sigma_I + \frac{1}{2}(\sigma_M + \sigma_N)} \quad (11)$$

$$U_I = \frac{\left[\frac{1}{2}P_N - \frac{1}{2}P_M\right] + \frac{U_N}{\sigma_N + \sigma_I} + \frac{U_M}{\sigma_M + \sigma_I} + \frac{\left[\frac{\gamma-1}{\gamma}D - G\right]_{NI} \Delta t}{\sigma_N + \sigma_I} - \frac{\left[\frac{\gamma-1}{\gamma}D + G\right]_{MI} \Delta t}{\sigma_M + \sigma_I}}{\frac{1}{\sigma_N + \sigma_I} + \frac{1}{\sigma_M + \sigma_I}} \quad (12)$$

$$\sigma_I = \frac{2 + F_{SI} \Delta t}{2 - F_{SI} \Delta t} \sigma_S \quad (13)$$

$$\frac{\Delta t}{\Delta x} \leq \frac{1}{|u| + a}$$

Subscripts MI, NI and SI denote average values over the relevant characteristics. The method is also stable provided that

$$\frac{\Delta t}{\Delta x} \leq \frac{1}{|u| + a}$$

MI, NI, RI Characteristics conveying information of fluid from M, N, R.

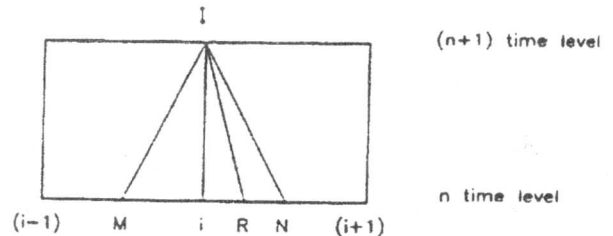


Figure 1. Illustration of the method of computation for the modified method of characteristics.

### 3- THE LAX SCHEME [9]

This is an explicit first order method. It is well known for its large dissipation error. It is used to show clearly the main features of a first order accurate scheme. The method takes the following form with reference to equation (4).

$$W_i^{n+1} = .5 \left( W_{i+1}^n + W_{i-1}^n - \frac{\Delta t}{\Delta x} [F_{i+1}^n - F_{i-1}^n] + \Delta t [S_{i+1}^n + S_{i-1}^n] \right) \quad (14)$$

The method is stable provided that the following condition is satisfied:

### 4- THE SINGLE STEP LAXWENDROFF SCHEME [12]

This is a second order scheme both in time and space, i.e., the truncation errors are  $O(\Delta t^2, \Delta x^2)$ . It is generated by developing eq.(4) into a Taylor series

with respect to time and replacing the time derivatives by space derivatives approximated by central differences. The method takes the following form:

$$W_i^{n+1} = W_i^n - \frac{1}{2} \frac{\Delta t}{\Delta X} (F_{i+1}^n - F_{i-1}^n) + \Delta t S_i^n + \frac{1}{4} \left( \frac{\Delta t}{\Delta X} \right)^2 [(F'_{i+1}^n + F'_{i-1}^n)(F_{i+1}^n - F_{i-1}^n) - (F'_{i+1}^n - F'_{i-1}^n)(F_i^n - F_{i-1}^n)] \quad (15)$$

where  $F'$  is the Jacobian matrix and is defined as :

$$F' = \begin{pmatrix} 0 & 1 & 0 \\ \frac{\gamma-1}{2} u^2 & (3-\gamma)u & \gamma-1 \\ \left( \frac{\gamma-2}{2} u^3 - \frac{\gamma}{\gamma-1} \frac{up}{\rho} \right) & \left( \frac{3-2\gamma}{2} u^2 + \frac{\gamma-1}{\gamma} \frac{p}{\rho} \right) & \gamma u \end{pmatrix} \quad (16)$$

The method is stable provided that the Courant-Friedrich-Lewy condition is satisfied as follows:

$$\frac{\Delta t}{\Delta x} \leq \frac{1}{|u| + a}$$

## 5- THE EXPLICIT MACCORMACK METHOD [13]

The explicit MacCormack scheme is second order accurate in space and in time. It has a predictor-corrector explicit algorithm as follows:

$$W_i^{\bar{n}+1} = W_i^n - \frac{\Delta t}{\Delta X} (F_{i+1}^n - F_i^n) + \Delta t S_i^n \quad (17)$$

$$W_i^{n+1} = \frac{1}{2} \left[ W_i^n + W_i^{\bar{n}+1} - \frac{\Delta t}{\Delta X} (F_i^{\bar{n}+1} - F_{i-1}^{\bar{n}+1}) + \Delta t S_i^{\bar{n}+1} \right] \quad (18)$$

The two step process consists of evaluating derivatives by one-sided differences taken in opposite directions during alternate steps for symmetric calculations. The first equation calculates a temporary predicted values of  $W$  and  $F$  vectors. The corrector equation provides

the final value at the time level  $n+1$ . The method is stable provided that the product  $q \| \lambda_{\max} \| < 1$ , where  $q = \Delta t / \Delta x$  and  $\lambda_{\max}$  is the maximum eigenvalue in the Jacobian matrix  $F'$ .

## TEST PROBLEM

The shock tube problem as shown in Fig. (2) is investigated and two cases are considered

*Case 1:* A tube of pressure ratio 10 across the diaphragm and uniform initial temperature excluding the effect of friction and heat transfer is considered. This case is compared with the analytical solution [16] to basically distinguish the performance characteristics of each numerical scheme.

*Case 2:* A tube of pressure ratio 9.8 and uniform initial temperature with 1 3/8 inch inner diameter. This tube is so selected in order to compare with the available experimental results [17]. The problem is solved analytically and numerically with and without the friction and heat transfer effects. For both cases the tube length is selected such that no interaction between the schemes and the boundary conditions is accomplished and thus all schemes maintain their order of discretization. Based on properties predicted for the adiabatic frictionless flow field, fixed average values of the friction factor and Stanton number are taken to be 0.00175 and 0.00125 respectively.

## RESULTS AND DISCUSSION

Computations were carried out using five coded computer programs written in C language on an IBM personal computer. The results of case 1 after .5 ms are presented in Figures (3) to (6) in which the numerical solution without friction and heat transfer, is compared with the analytical frictionless adiabatic solution.

Figure (3) represents the results of the modified characteristics according to Spalding. The corners at the end points of the rarefaction waves are rounded. This may be attributed to the interpolation that must be used with any numerical technique. The constant state between the contact discontinuity and the shock wave is fully realized. There is a slight deviation from the analytical solution in the smooth regions. However, all the internal features of the shock wave events are preserved.

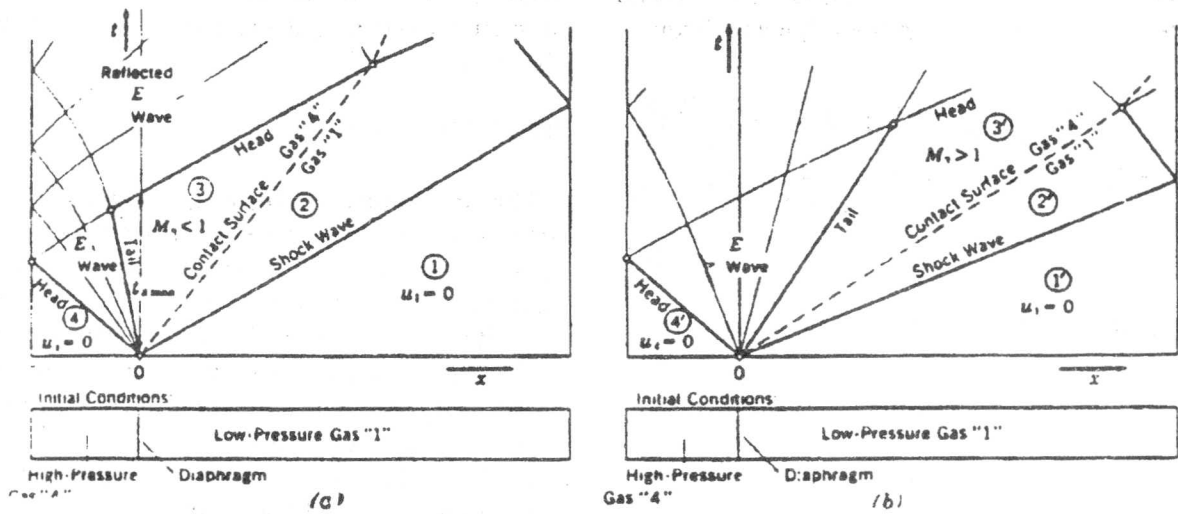


Figure 2. Wave pattern in a shock tube closed at ends a- for mach number  $M_2 < 1$  b- for mach number  $M_3 > 1$ .

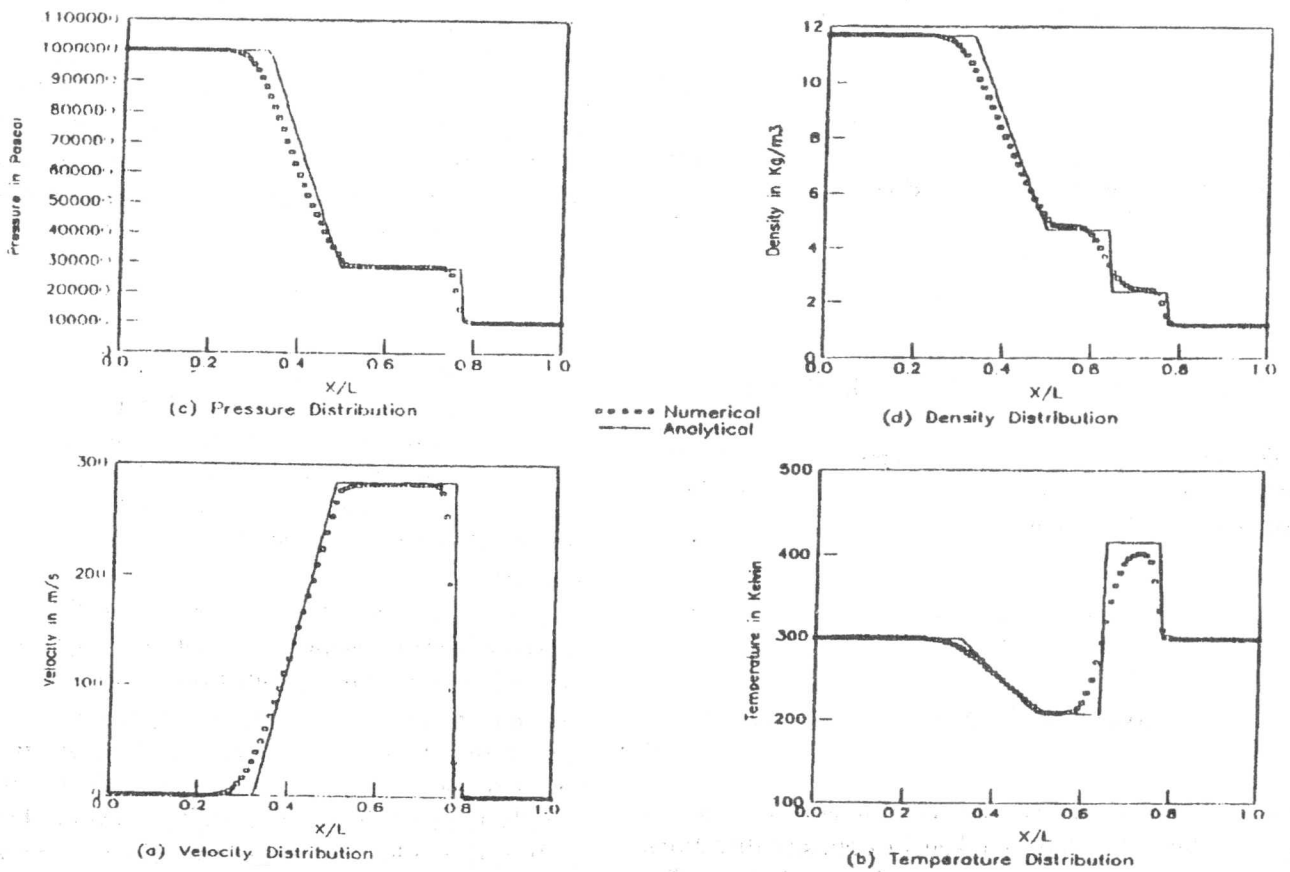


Figure 3. Prediction of the modified method of spalding after 5 MS.

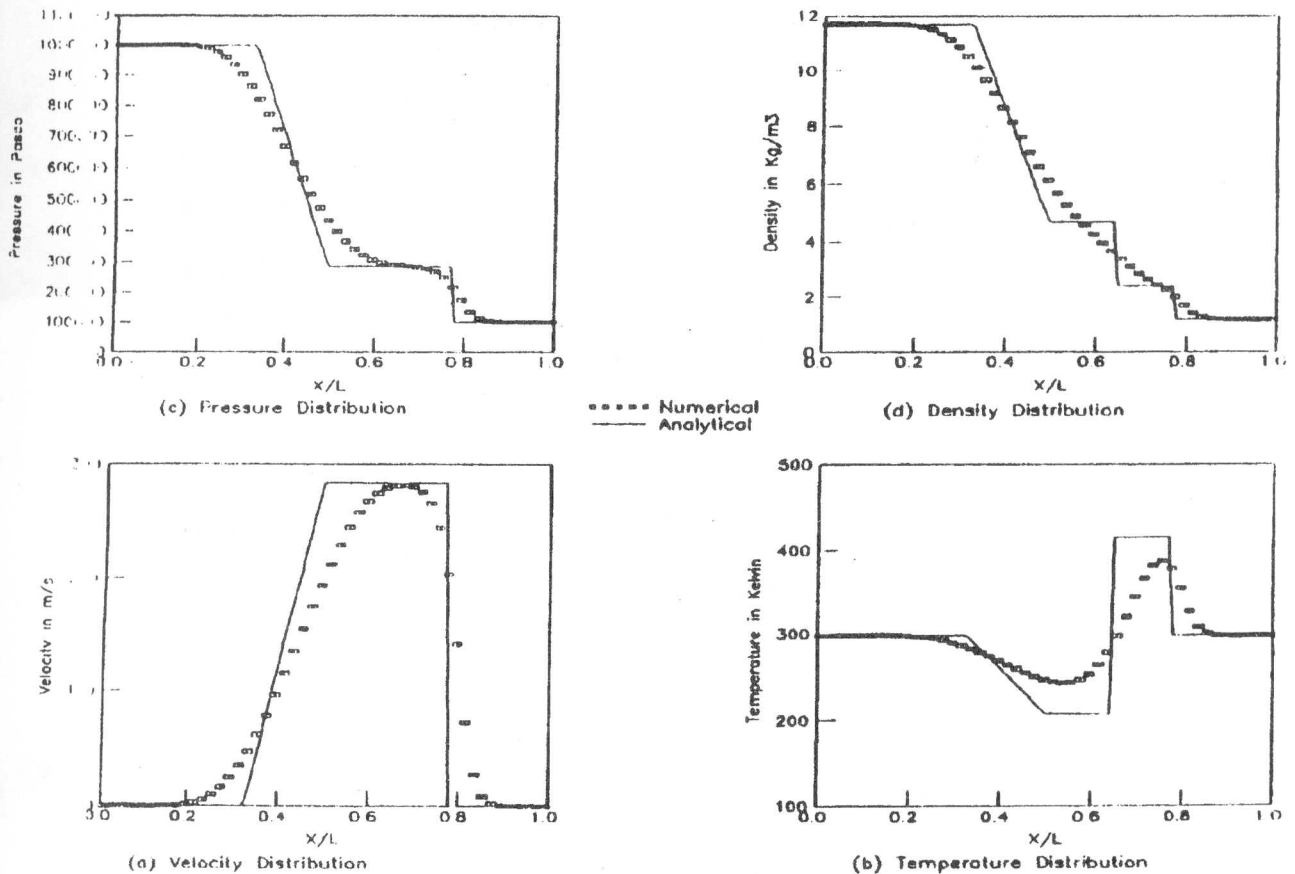


Figure 4. Prediction of lax method after .5 MS.

Figure (4) illustrates the results using Lax method. The contact discontinuity is barely visible in the density profile. The corners at the end points of the rarefaction waves are highly rounded. The constant state between the contact discontinuity and the shock wave is barely existent. It is clear that this scheme entails extremely high dissipative errors.

Figure (5) shows the results of the Lax and Wendroff scheme. There are slight overshoots at the shock wave and more noticeable overshoots at the contact discontinuity. The rarefaction waves are predicted accurately. The corners at the end points of the rarefaction waves are only slightly rounded.

Figure (6) represents the results of the MacCormack Method. There are certain overshoots at the contract discontinuity and the shock wave. The rarefaction waves are very accurate. The end points of the rarefaction waves are only slightly rounded. It may be

observed that results of figure (6) are quite similar to those of figure (5).

From the previous analysis it is evident that all methods produce one of two error patterns. First order methods show an inaccuracy in the solution at regions far from steep gradients. Also smearing in the solution at steep gradients are always exhibited. Higher order methods despite their accuracy in smooth regions and prediction of steep gradients without smearing, produce non-physical oscillations at sharp gradients. The methods have to be incorporated with damping procedures to suppress the oscillations. The phoenical flux correction method, to suppress the oscillation, has been used for all higher order schemes.

The computation's time duration is primarily a function of the numerical method itself and efficiency of the computer program and these are the time duration of each scheme for case 1:

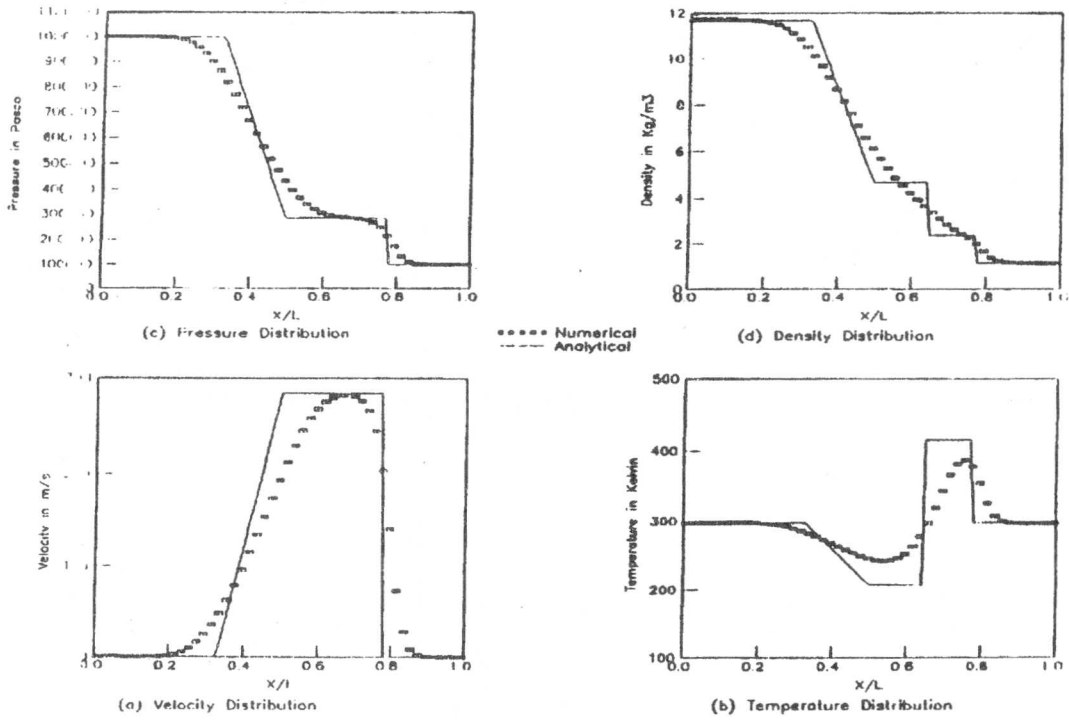


Figure 5. Prediction of Laxwendorff method after .5 ms.

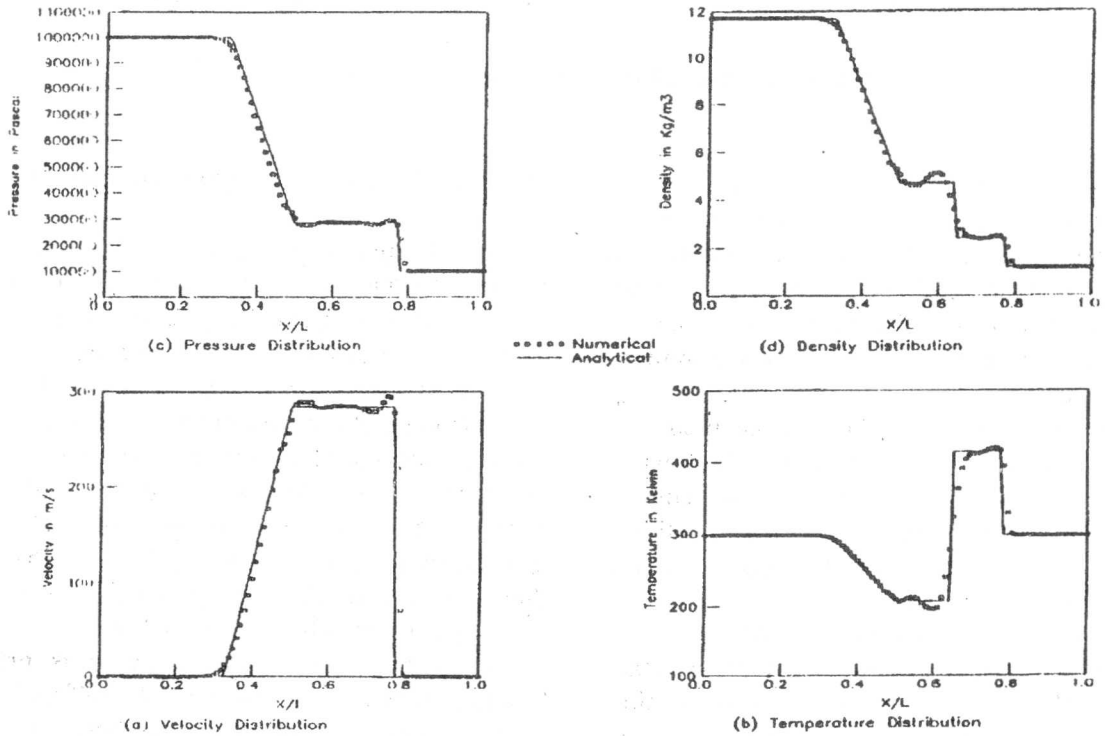


Figure 6. Prediction of maccormack method after .5 MS.



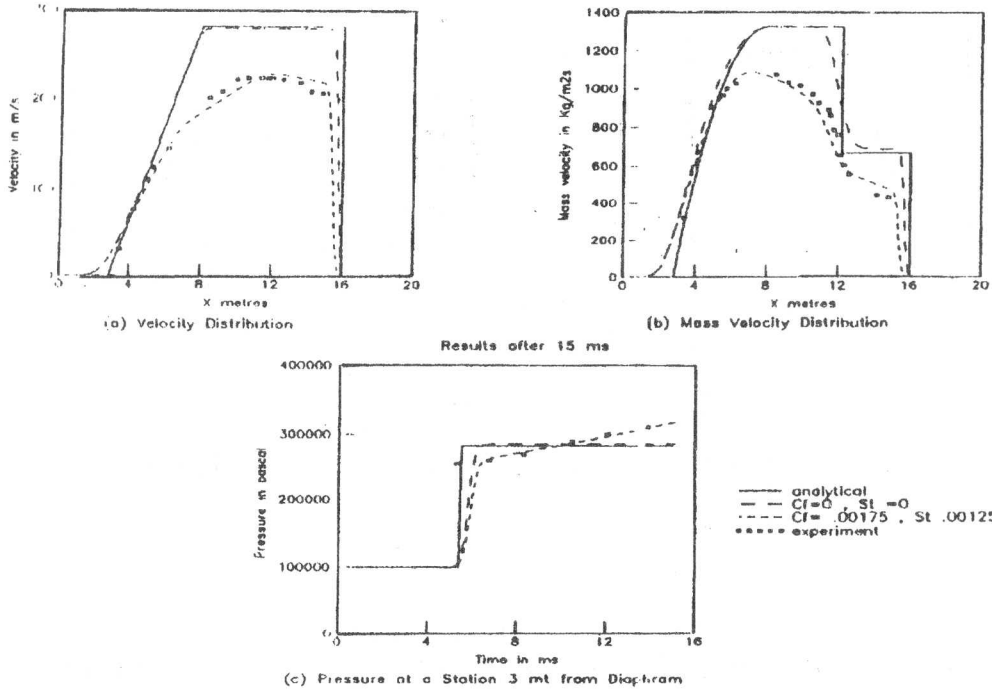


Figure 7. Numerical simulation modified method of spalding with analytical solution and experimental measurements.

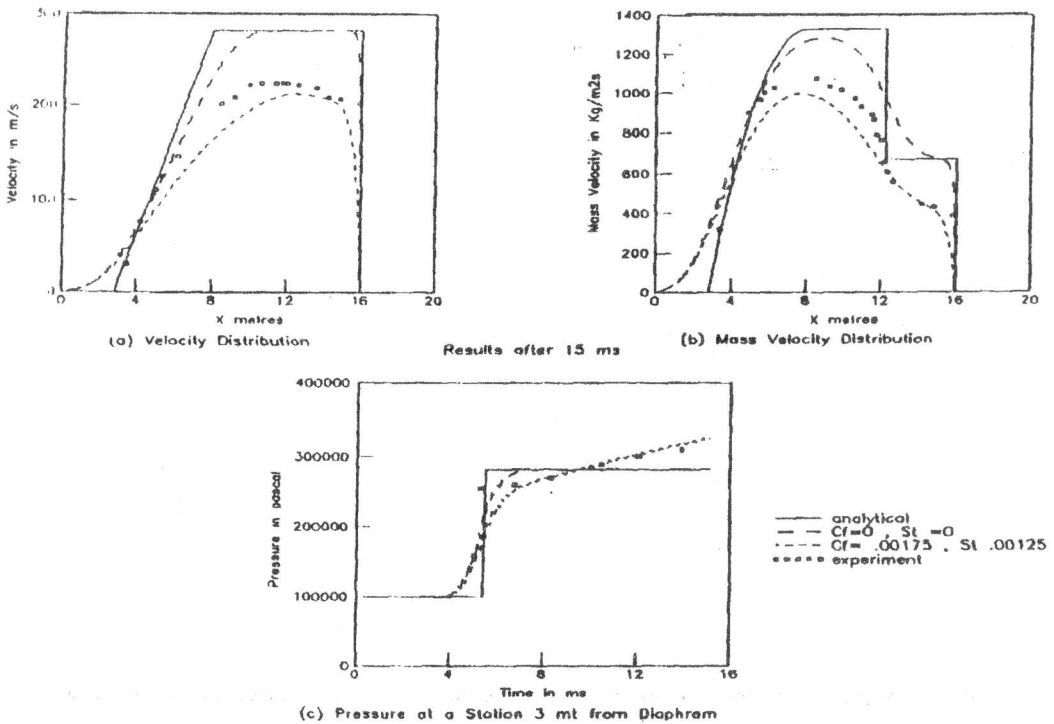


Figure 8. Numerical simulation. ax method with analytical solution and experimental measurements.

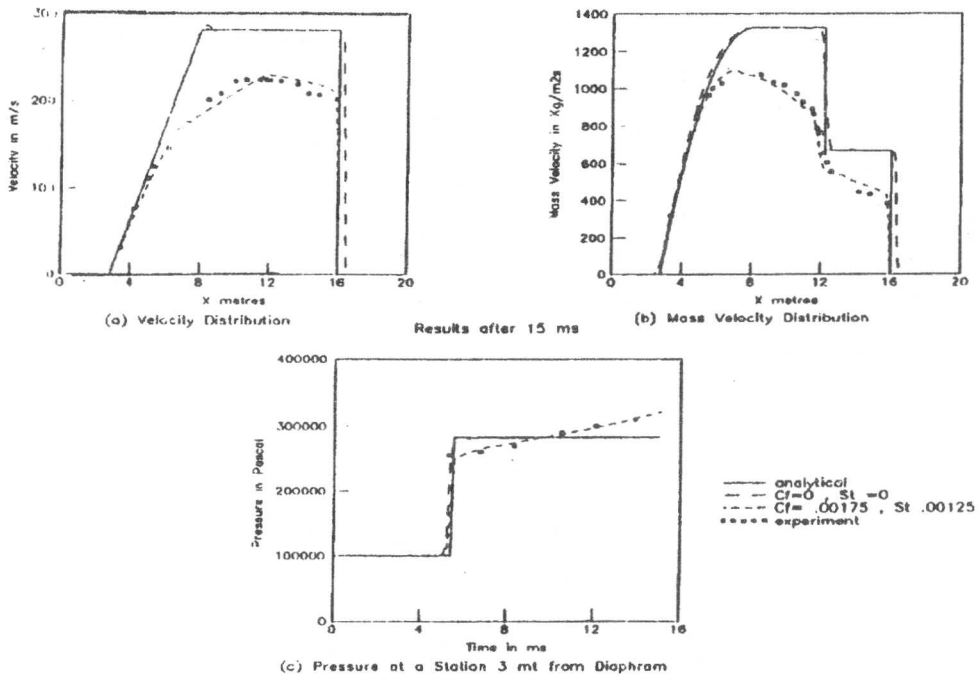


Figure 9. Numerical simulation laxwendroff method with analytical solution and experimental measurements.

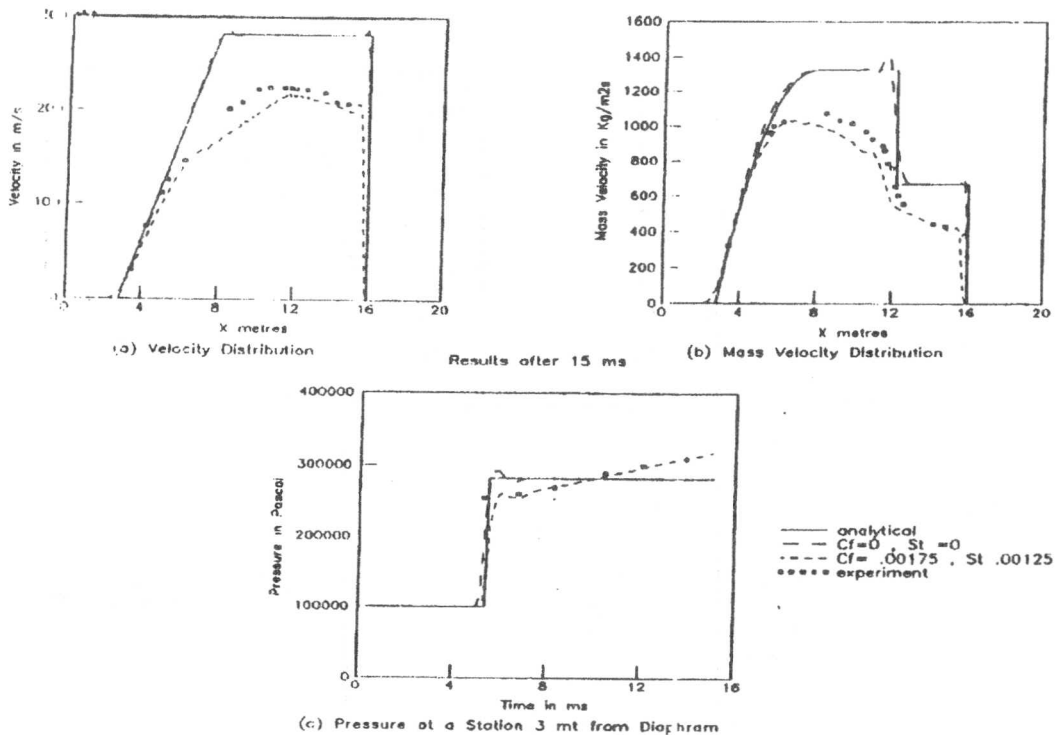


Figure 10. Numerical simulation maccormack method with analytical solution and experimental measurements.

Scheme	CPU time, sec.
Lax Scheme	15
Modified Method of Characteristics of Spalding	59
Explicit MacGormack scheme	96
Single Step LaxWendroff Scheme	98

The results of case 2 are presented in figure (7) to (10) in which the algebraic frictionless adiabatic solution is compared to the numerical solution without friction and heat transfer and to the numerical solutions with friction and heat transfer and the previous results are compared to the experimental results. The comparison is performed after 15 ms from the rupture of the diaphragm .

Figure (7) represents the results of the modified method of characteristics of Spalding. The method predicts the velocity and pressure distributions for the frictionless adiabatic flow fairly accurate, but that the sharp corners are rounded.

Figure 8 shows the results of the Lax method the scheme entails high inaccuracy. The smearing effect and the friction effect have produced a solution far from true not only from the analytical view point but also from the comparison with experimental results.

Figure 9 shows the results of the Lax and wendroff method. The method shows very good velocity and pressure distributions for both the ideal and actual cases but the numerical shock is somewhat faster than the analytical one. The method exhibits a very good resemblance with the experimental results .

Figure 10 represents the results of the MacCormack method. The scheme is quite accurate when comparing the analytical solution with the numerical solution without friction and heat transfer except for a slight overshoot at the contact discontinuity . However, the numerical solution with friction and heat transfer is quite inaccurate in the velocity and mass velocity profiles.

It may be concluded that the first order method of Spalding shows the least smearing and high accuracy. The higher order methods are generally more accurate but with unrealistic spikes and ravines that appear with discontinuities . One higher order method that exhibited the least oscillations after the application of the damping method is the Laxwendroff second order method.

## CONCLUSIONS

The modified method of characteristics of Benson fails to handle the shock tube problem. It can not deal with problems of high entropy gradients because it is not incorporated with entropy modifying terms i.e.it adopts the homentropic flow cases of low pressure ratios.

Lax scheme proved to be the fastest in obtaining a solution but at the expense of accuracy as it shows large dissipation errors. The other methods showed comparable CPU times in both the frictionless adiabatic and the actual cases but with different performance characteristics.

From the accuracy point of view , the methods except Lax highly dissipative scheme, showed relatively comparable error levels but with first order methods showing some smearing at the end points of sharp gradients while higher order method showing certain dispersive errors in the form of spikes and ravines at sharp gradients which had to be damped in order to obtain stable solutions

The modified method of characteristics of Benson and Lax scheme are not recommended for the study of high pressure ratio unsteady flow phenomena since the first scheme fails to handle the entropy discontinuities and the second produce high dissipation errors.

The higher order methods are ideally suited for unsteady flow problems where no sharp gradients can appear. The solution becomes oscillation free and superior to first order methods from the accuracy view point.

The first order method of characteristics of spalding is one method that is superior to higher order methods due to its oscillation free solution, especially at sharp gradients and low error levels but at the expense of some smearing of the sharp gradients.

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## NOMENCLATURE

$a$	:	Gas sonic speed
$a_A$	:	Sonic speed at $S_A$ and reference pressure.
$C_p, C_v$	:	Specific heats at constant pressure and constant volume.
$C_f$	:	Friction factor.
$d$	:	Duct diameter.
$e$	:	Specific internal energy
$f$	:	Friction force per unit fluid volume
$i, (i+1)$	:	Spatial grid points
$n, (n+1)$	:	Time level steps.
$p$	:	Gas pressure
$q$	:	Heat transfer per unit fluid volume
$R$	:	Gas constant
$s$	:	Specific entropy
$S_t$	:	Stanton number
$t$	:	Time
$T_w$	:	Wall temperature
$u$	:	Gas velocity
$x$	:	Space coordinate
$\gamma$	:	Specific heat ratio
$\rho$	:	Gas density
$\sigma$	:	Non-dimensional entropy, ( $\exp(\frac{\gamma - 1}{2}s)$ ) where $s = s/R$ .
$\lambda, \beta$	:	Reimann variables.