A COMPARISON OF THREE NUMERICAL METHODS OF SOLUTIONS OF EQUATIONS DESCRIBING UNSTEADY GAS FLOW AT PIPE BOUNDARIES IN RECIPROCATING COMPRESSOR SYSTEMS

M.H. Mkumbwa
University of Dar es Salaam, Department of Mechanical Engineering,
P.O. Box 35131, Dar es Salaam, Tanzania.

ABSTRACT

A number of finite difference schemes are available to study pressure fluctuation effects in unsteady pipe flows. This paper presents a comparison of the predictions made by three such schemes of unsteady flow effects in a number of reciprocating compressor pipe-work systems. The finite difference schemes considered were;- a first order scheme known as the method of characteristics, two second order schemes which were the Leapfrog method and MacCormack's method. A reciprocating compressor simulation computer program was coupled with equations describing the cylinder thermodynamic processes with the pipe flow equations for steady non-homentropic flow. The comparison presented takes into account both the efficiency of the methods under consideration and their agreement in the prediction of the compressor behaviour. The MacCormack's method was modified to handle processes at pipe boundaries and within gas volumes while the Leapfrog method had to be coupled with the method of characteristics at pipe boundaries. The method of characteristics was also used independently to handle both internal meshes and pipe boundaries. The Leapfrog method was found to be more favourable in terms of computer time followed by the MacCormack's method and lastly the method of characteristics. In terms of accuracy the two second order schemes were found to be superior to the method of characteristics which is a first order accuracy scheme.

INTRODUCTION.

In numerical simulations of the thermodynamic and fluid dynamic processes which occur in compressor systems, a significant proportion of the computational procedures is devoted to calculations relating to unsteady gas flow in the pipes connecting compressor elements. Maclaren et al[1,2] reported the application of the method of characteristics, the Lax-Wendroff finite difference method and the Leapfrog method in studies of reciprocating compressor systems. In both the Lax-

Wendroff and leapfrog cases, the method of characteristics was used at the boundaries. A number of improved numerical methods by Sod[3] and Chu[4] are now available which permit the use of coarser mesh sizes thereby substantially reducing the computer time required. The boundary considerations by Chu and Sereny[5] have allowed the application of methods other than the method of characteristics at the boundaries.

Studies of compressor systems reported in this paper employed an explicit non-centered finite difference scheme at both the internal and the boundary mesh points as an alternative procedure to the previously used[6] characteristics finite difference combination, i.e. finite difference method in internal mesh points and the method of characteristics at the boundaries.

NON-CENTERED FINITE DIFFERENCE APPROACH

The hyperbolic equations governing one dimensional unsteady nonhomentropic flow may be written in the conservation-law form or the normal form as follows;

$$\frac{\partial U}{\partial t} + \frac{\partial G(U)}{\partial x} = B(U) \qquad (1)$$

where the elements of **U** are the dependent variables and **G(U)** is a vector function of **U**. The non-conservative terms relating to heat transfer, friction and area change are included in **B(U)**. The corresponding set of linearized equations is given as;

$$\frac{\partial U}{\partial t} + C\frac{\partial U}{\partial x} = 0 \qquad (2)$$

where C is the Jacobian of **G(U)**.

One of the simplest forms of explicit second order non-centered finite difference schemes which can be applied to the set represented by equation (1), was developed by MacCormack[7]. Its one-dimensional version is reported by Roache[8] and a form suitable for the non-homogeneous set of equations (1) is discussed by Dwyer et al[9].

The scheme itself is executed in two steps;-

First step: The predictor step

$$U_j^{\overline{n+1}} = U_j^n - \frac{\Delta t}{\Delta x}[G(U)^n_{j+1} - G(U)^n_j] + \Delta t\, B(U)^n_j \tag{3}$$

Second step: The corrector step

$$U_j^{n+1} = \frac{1}{2}\left(U_j^{\overline{n+1}} + U_j^n\right) - \frac{1}{2}\frac{\Delta t}{\Delta x}\left(G(U)_j^{\overline{n+1}} - G(U)_{j-1}^{\overline{n+1}}\right) + \frac{1}{2}\Delta t\, B(U)_j^{\overline{n+1}} \tag{4}$$

Figure 1 shows the computational mesh on an x-t plane and indicates the points involved in the different calculations.

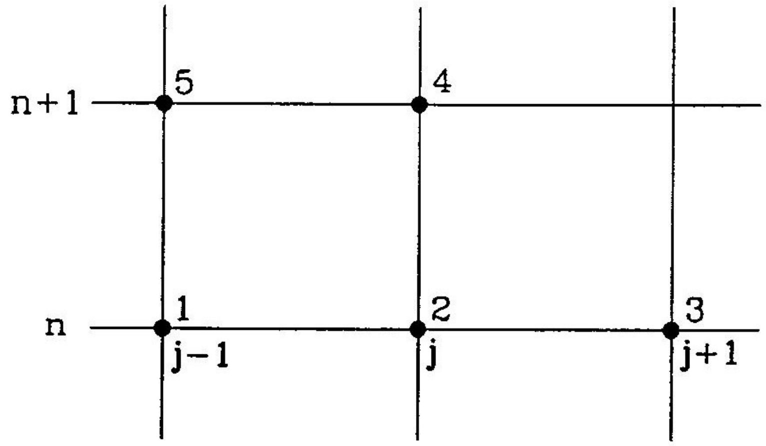

Figure 1 Grid Notation

The first step is regarded as a predictor step while the second step is a corrector step. The method first obtains an approximate value $U_s^{\overline{n+1}}$ at each mesh point using a forward difference scheme to approximate the spatial detrivatives. The approximate solution is then used in the second step to obtain the new corrected value U_s^{n+1} using backward differences. Having done this in the first time step, in the next time step the first equation is solved using a backward difference scheme whilst the second equation is solved using forward differences which, means that for the predictor step, the determination of the temporary values of dependent variables at the time level (n+1) at point 4 requires information from point 2 and 3 at time level n. For the corrector step, the true value of the dependent variables for point 4 is calculated from values of point 2 and 5. When advancing in time step the new dependent variables are then determined by applying the non-centered finite difference scheme in the opposite direction. This treatment is necessary for the increased stability of the method. The alternating difference approach is then used in subsequent time steps.

When the MacCormack procedure is applied to the linearized set of hyperbolic equation (2), it may be reduced to the single step second order Lax-Wendroff scheme[1];

$$U_j^{n+1}=U_j^n-\frac{1}{2}\left(C\frac{\Delta t}{\Delta x}\right)\left(U_{j+1}^n-U_{j-1}^n\right)+\frac{1}{2}\left(C\frac{\Delta t}{\Delta x}\right)^2\left(U_{j+1}^n-2U_j^n+U_{j-1}^n\right) \qquad (5)$$

In this instance its properties, i.e. stability attenuation and phase shift can be considered the same as those evaluated for the Lax-Wendroff method by Maclaren et al[1].

The boundary scheme corresponding to the MacCormack method is provided through two steps;

First step:

$$\overline{U_*^{n+1}}=3U_N^n-3U_{N-1}^n+U_{N-2}^n-\frac{\Delta t}{\Delta x}\left(2G(U)_N^n-3G(U)_{N-1}^n+G(U)_{N-2}^n\right)+\Delta t B(U)_N^n \qquad (6)$$

Second step:

$$U_N^{n+1}=\frac{1}{2}\left(\overline{U_N^{n+1}}+U_N^n\right)-\frac{1}{2}\frac{\Delta t}{\Delta x}\left(G(U)_*^{\overline{n+1}}-G(U)_N^{\overline{n+1}}\right)+\frac{1}{2}\Delta t\, B(U)_N^{\overline{n+1}} \qquad (7)$$

The linearized case gives the following form;

$$U_N^{n+1}=U_N^n-C\frac{\Delta t}{\Delta x}\left(3U_N^n-4U_{N-1}^n+U_{N-2}^n\right)+\frac{1}{2}\left(C\frac{\Delta t}{\Delta x}\right)^2\left(U_N^n-2U_{N-1}^n+U_{N-2}^n\right) \qquad (8)$$

McGuire and Morris[10] showed that the same effect could be obtained by quadratic extrapolation at boundary points in the time level n. Furthermore, a similar analysis can be performed, and the same conclusions deduced for the time level (n+1). It allows the non-centred finite difference scheme to be independently applied not only to all finite difference methods of the Lax-Wendroff type but even to the wider class of suitable explicit internal finite difference mesh methods. If a noncentred finite difference method is applied at boundary points, the boundary values are purely internal field quantities and have to be corrected in the usual manner.

A Von Neumann[11] stability analysis for the boundary scheme applied to the linearised set of equations (2) with the additional restriction C ≡ constant gives an amplification factor ξ of modulus $|\xi|$.

$$|\xi| = \left\{ \left[1 - \frac{1}{2} C\frac{\Delta t}{\Delta x}\left(3 - 4\cos\frac{2\pi}{\lambda}\Delta x + \cos\frac{4\pi}{\lambda}\Delta x\right) + \frac{1}{2}\left(C\frac{\Delta t}{\Delta x}\right)^2 \left(1 - 2\cos\frac{2\pi}{\lambda}\Delta x + \cos\frac{4\pi}{\lambda}\Delta x\right)\right]^2 + \left[-C\frac{\Delta t}{\Delta x}\left(4\sin\frac{2\pi}{\lambda}\Delta x - \sin\frac{4\pi}{\lambda}\Delta x\right) + \frac{1}{2}\left(C\frac{\Delta t}{\Delta x}\right)^2\left(2\sin\frac{2\pi}{\lambda}\Delta x - \sin\frac{4\pi}{\lambda}\Delta x\right)\right]^2 \right\}^{\frac{1}{2}} \quad (9)$$

The numerical solution of equation (9) when plotted against the time/space ratio $C\Delta t/\Delta x$ and the Fourier component wave number $\lambda/\Delta x$ produces Figure 2. The Von Neumann stability criterion requires that $|\xi| \leq 1.0$ if both Δx and Δt approach zero, and it is certainly satisfied if $C\Delta t/\Delta x \leq 1.0$.

The Hirt[12] "heuristic" stability analysis adapted to the MacCormack procedure by Tyler[13], shows some important features of the noncentred boundary schemes as depicted by equation (8). The scheme is consistent with the original set of differential equations, is of second order accuracy and the necessary stability condition is $C\Delta t/\Delta x \leq 1.0$. All stability criteria applied agree with the Courant-Friedrichs Lewy criterion which ensures that the numerical propagation rate does not exceed the physical rate.

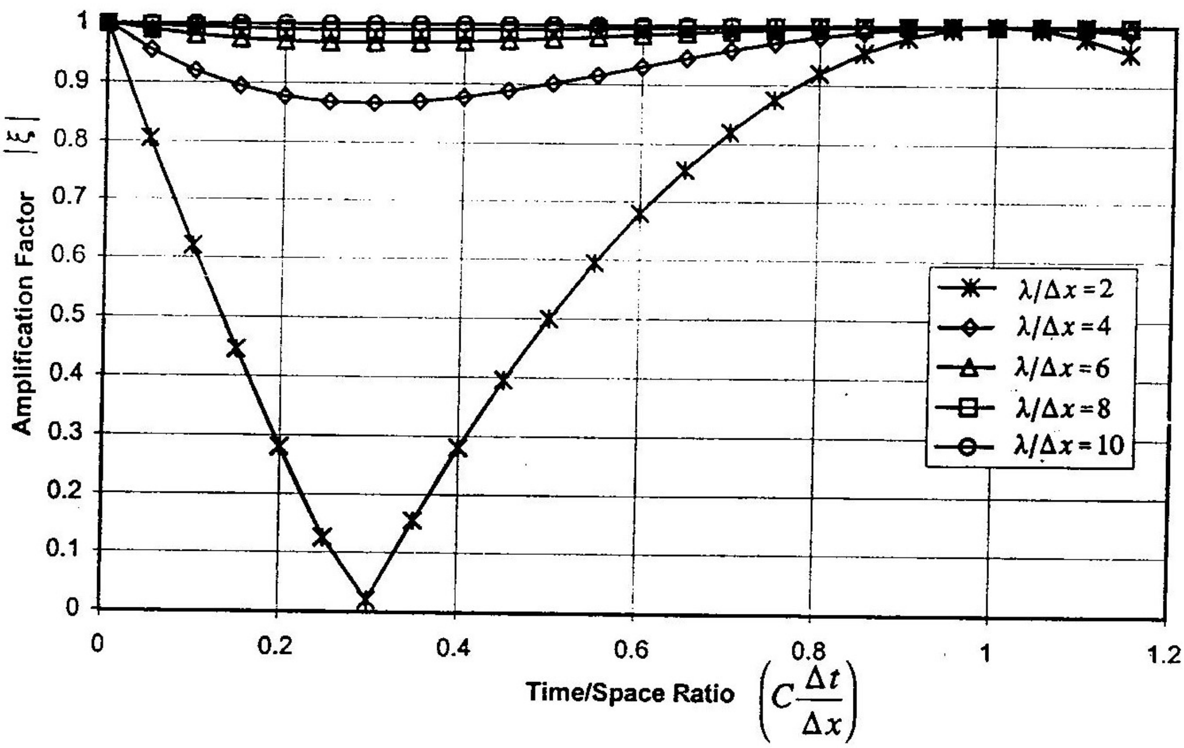

Fig. 2 Amplification Factor vs Mesh Proportion Ratio

NUMERICAL RESULTS

The previous version of the compressor simulation program by Pastrana[6], which employed two finite difference methods coupled with the method of characteristics at the boundary points, was adapted to incorporate the MacCormack finite difference procedure at the internal mesh points and the non-centred finite difference scheme as the replacement of the method of characteristics at the boundaries. The novel boundary approach seems to have some advantages over the method of characteristics - finite difference combination.

- the values of the variables for the initial iterations obtained at the time level n+1 are more accurate than guesses based on the previous time step values the practice used.

- the calculation process is straight forward and avoids any interpolation.

- the overall calculation procedure including the boundary points is second order accurate.

Results presented in Figures 3, 4 and 5 correspond to the fourth simulated cycle. The reason is that it is normally assumed that the dynamic behaviour of a reciprocating compressor could be established satisfactorily by the fourth cycle. Operating conditions for the cases considered are shown in Table 1.

Table 1: Operating Conditions

SPEED (r.p.m)	P_{atm} (bar)	T_{atm} (°C)	P_{dis}/P_{atm}	T_{dis}/T_{atm}	INLET PIPE		DISCHARGE PIPE	
					LENGTH (m)	DIA (mm)	LENGTH (m)	DIA (mm)
552	1.02	530	7.8	1.5	5.75	54.0	4.0	54.0
612	1.02	530	7.8	1.5	5.75	54.0	4.0	54.0
645	1.02	530	7.8	1.5	5.75	54.0	4.0	54.0

Three numerical techniques of solution were used in the simulation program

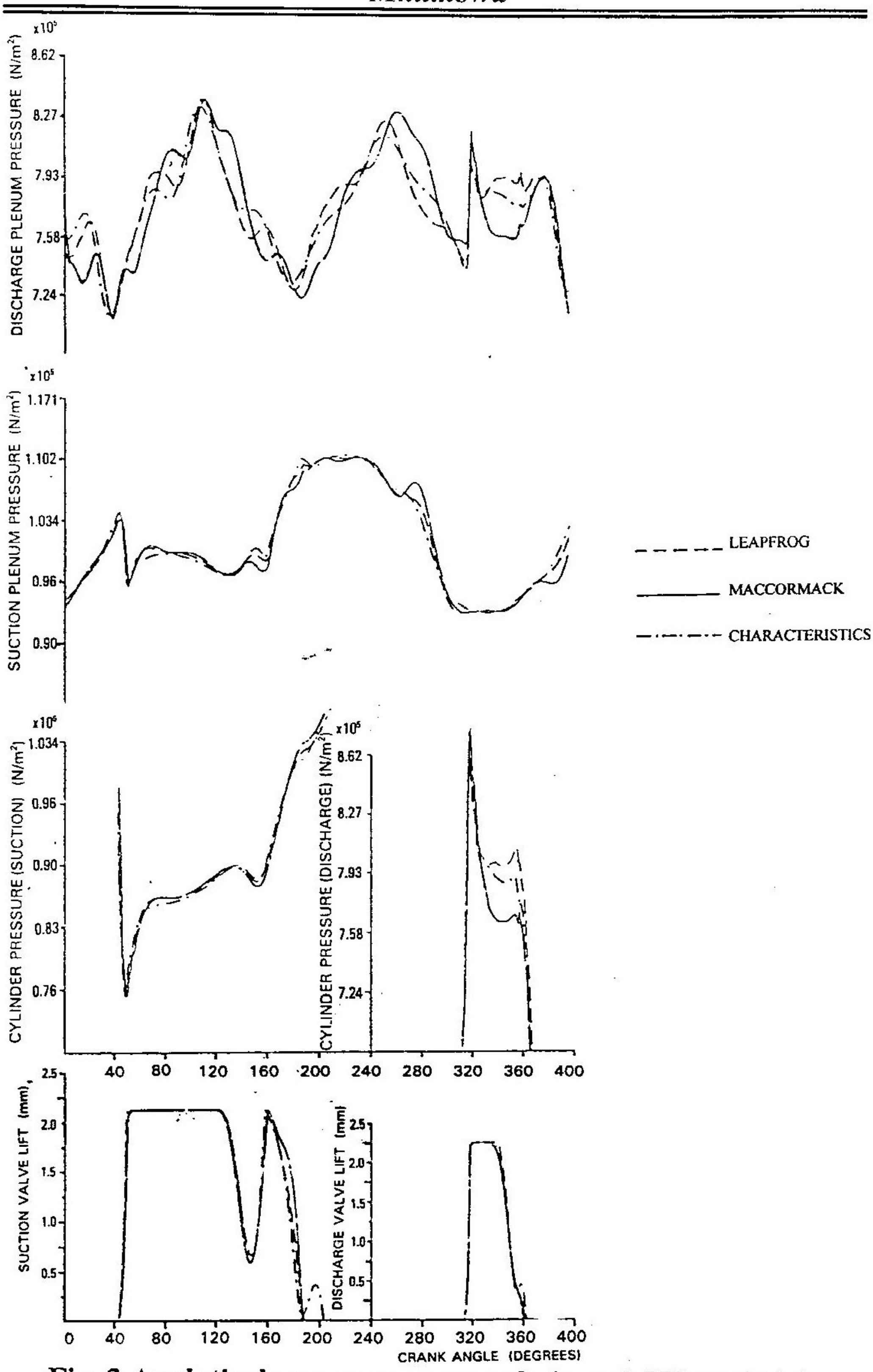

Fig. 3 Analytical compressor records (speed 552 rev/min)

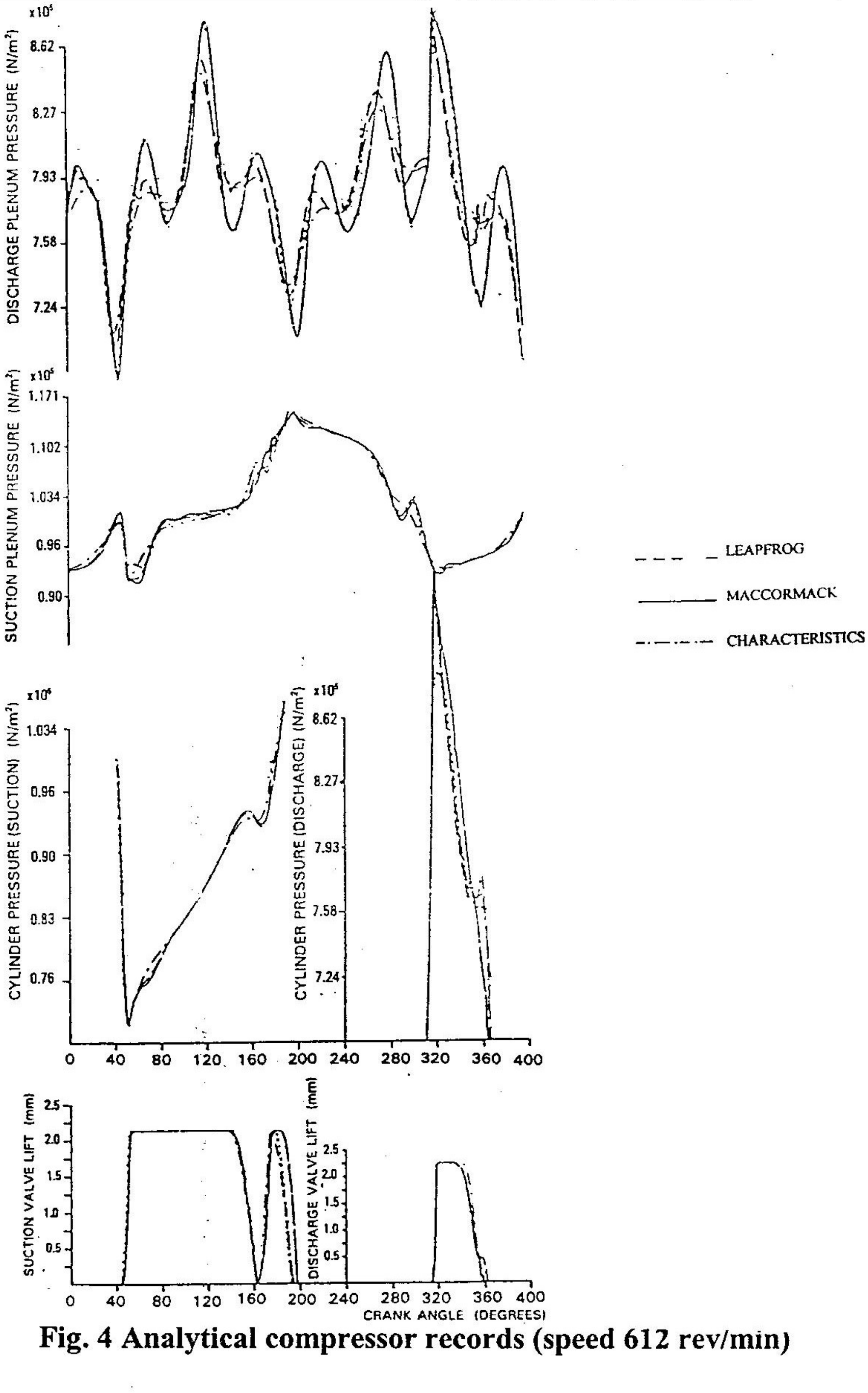

Fig. 4 Analytical compressor records (speed 612 rev/min)

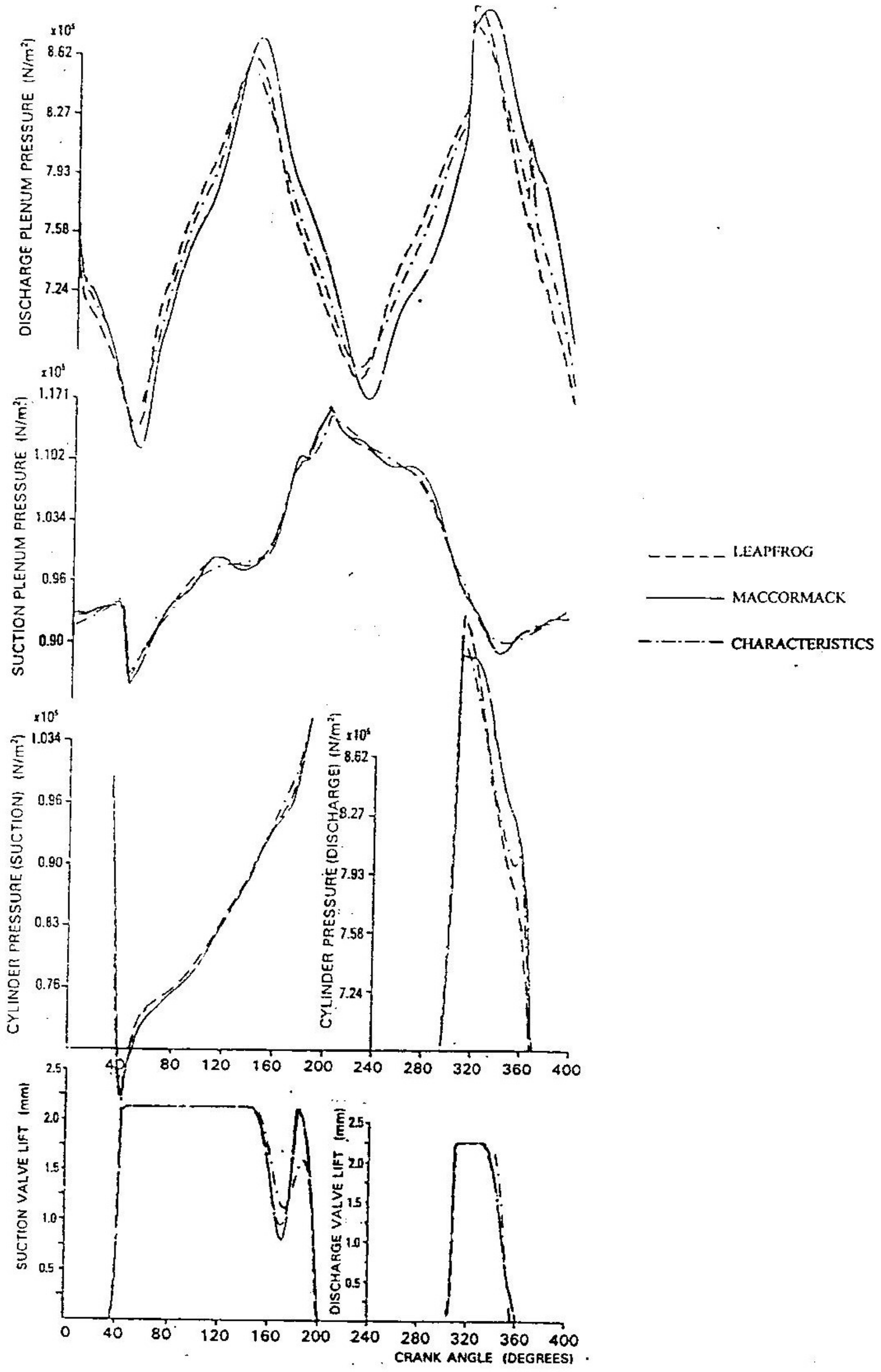

Fig. 5 Analytical compressor records (speed 645 rev/min)

for solving pipe flow equations (Leapfrog, MacCormack and Characteristics). The comparison of all the three schemes is presented in Figures 3, 4 and 5, in terms of the agreement of the methods in the prediction of the compressor behaviour. As it can be seen from the figures, the results obtained for three different compressor speeds, by the various numerical schemes generally show a satisfactory agreement with each other.

Table 2: Computer Time Comparison

SPEED (r.p.m.)	LEAPFROG			MACCORMACK			CHARACTERISTICS		
	MESHES		CPU TIME (sec)	MESHES		CPU TIME (sec)	MESHES		CPU TIME (sec)
	Suction	Disch.		Suction	Disch.		Suction	Disch.	
552	18	14	88	18	14	102	30	24	219
612	18	14	80	18	14	94	30	24	210
645	18	14	74	18	14	85	30	24	203

Table 2 shows that there is an appreciable central processor time reduction when the second order accuracy method is used. This can be explained by the fact that:-

- With these schemes, coarser meshes can be used resulting in fewer mesh points having to be calculated hence less computation.
- Coarser mesh sizes meaning that longer time steps could be used while still satisfying the stability criteria and hence less computation.
- Because differences in the independent variables are taken instead of computation along characteristic directions the need for interpolations and extrapolations is avoided and less calculation is involved in higher order techniques.

From Table 2, it is clearly seen that to produce results which were as close as possible to those produced by the Leapfrog and MacCormack schemes, the computing times needed by the program when using the method of characteristics were generally over twice those required by the two second order of accuracy

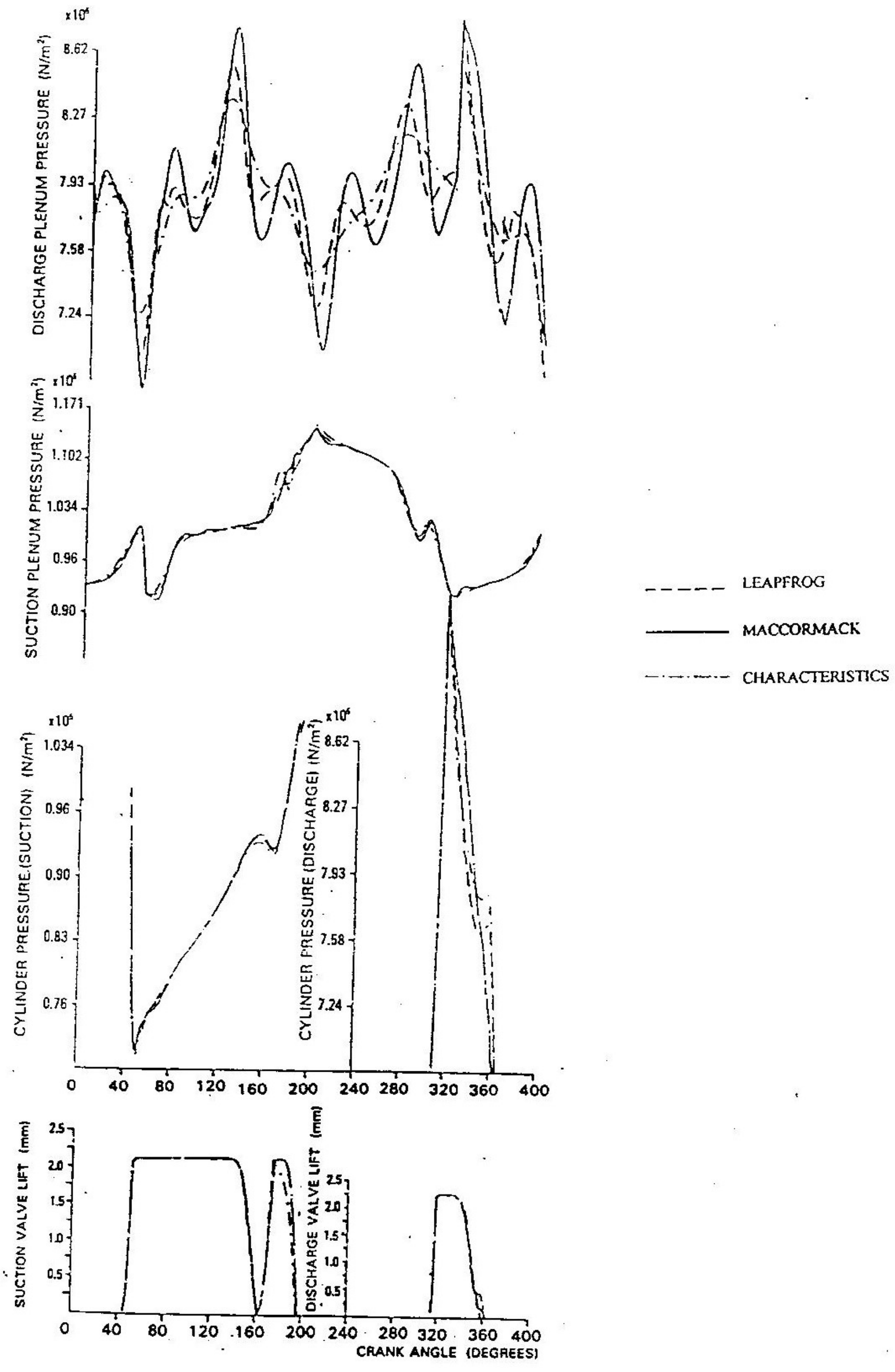

Fig. 6 Analytical compressor records (speed 612 rev/min) (all schemes with same number of meshes)

numerical schemes. In this case the number of meshes for each pipe had to be increased for the method of characteristics thereby not only increasing the computation time but also the computer storage requirements. This is clearly shown in Table 2 where for the same number of meshes in a system calculation the results were poor for the method of characteristics when compared with the other two second order schemes as shown by Figure 6.

CONCLUSION

The MacCormack finite difference procedure and the non-centred finite difference boundary approach when incorporated in the existing compressor simulation program and the unsteady gas flow which occurs in compressor systems, the equations are solved efficiently which is in close agreement with the Leapfrog method.

NOTATION

B	- Vector of terms relating to heat transfer area change and friction.
C	- The Jacobian of G ($\equiv$ constant matrix)
G	- Vector function of U
t	- time
U	- Vector dependent variables
x	- Distance
λ	- Wavelength
ξ	- Amplification factor

Subscripts

j	- Space level
N	- Boundary
*	- Artificial boundary point

Superscripts

n	- Time level

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