MATHEMATICS DEPARTMENT

A COMPARISON OF THE DIRECTIONAL DIFFERENCE SCHEME AND ROE'S SCHEME FOR THE APPROXIMATE SOLUTION OF TRANSIENT FLOW OF AN IDEAL GAS IN A PIPE

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Numerical Analysis Report 2/90

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Abstract

Two finite difference schemes for the solution of the Euler equations of gas flow are compared. One is based on the use of pseudo-characteristic variables and is used in the Gas Industry, and the other is based on an approximate (linearized) Riemann solver. The schemes are contrasted theoretically and also applied to a number of test problems for comparison of the results.

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1. Introduction

This report presents two schemes for the solution of the equations of gas flow in a pipe. In a network of gas pipes, it is often necessary to be able to model the behaviour of the dynamics. Transient behaviour in a gas network can have a typical timescale of hours, associated with the fluctuations in the demand for gas on a daily basis, and can also have a timescale of minutes or seconds when associated with the operation of equipment in the gas network, or the failure of some component. The schemes described here attempt to model well this rapid transient behaviour.

Attempts to model gas flow in the networks (see [1]) are based on the solution of the equations of gas flow in a single pipe. Chapter 2 describes the equations chosen to model this flow, and the simplifications and assumptions made. The two schemes used are also outlined in that chapter, but given in detail in chapter 3. One of the schemes is a recent scheme by Roe, and the other is a scheme that is used in the gas industry. The schemes' properties and a comparison between the two schemes are investigated at the end of chapter 3. Chapter 4 details the test cases and gives results, and chapter 5 draws conclusions and summarizes the findings.

2. Statement of the problem

The Euler Equations

The equations governing the flow of gas in a pipeline under the assumptions that the gas is inviscid but compressible are the Euler equations [1]. Under the further assumptions that the flow is one-dimensional, irrotational and homogeneous, and that the pipeline is straight, level, and has a constant circular cross-section, those equations become:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0 \tag{2.1}$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(p+\rho u^2) = -\frac{2f\rho u|u|}{d} \tag{2.2}$$

$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial x}(u(e+\rho)) = \Omega \tag{2.3}$$

where ρ,u,e,p are, respectively, the density, velocity, total energy and pressure of the gas. The friction term on the right-hand side of (2.3) involves the Fanning friction factor f [1] and the pipe diameter d. The heat per unit length into the pipe is given by Ω.

Equations (2.1)-(2.3) are not sufficient to find the four unknown quantities ρ,u,e,p; a further equation relating these must be provided. The equation of state for the gas provides this relationship. Equation (2.4) is a version of the ideal gas equation with a factor Z providing variable compressibility to allow some departure from the ideal (see[1]).

$$p = \frac{ZRT}{M}\rho \tag{2.4}$$

The following form (written for an ideal gas) can also be used:

$$e = \frac{p}{\gamma-1} + \frac{1}{2}\rho u^2 \quad , \tag{2.5}$$

where $\gamma = C_p/C_v$, the ratio of specific heats for the gas.

The set of equations (2.1)-(2.3), taken with an equation of state such as (2.4) or (2.5), will be called the full system of Euler equations, or the 3-system, with the appropriate assumption of equation of state.

The Adiabatic Approximation

The assumption is often made, especially for rapid transients where the dynamic effects are on a shorter timescale than heat transfer effects, that the effective heat input $\Omega = 0$. In this case, equation (2.3) and the equation of state are replaced by an equation of state for adiabatic conditions, or an adiabatic law. For ideal gases, this is

$$\rho = k(s)p^{1/\gamma} \tag{2.6}$$

where $k(s)$ is a function of the entropy, s . If friction is negligible, the isentropic assumption holds, i.e.

$$\rho = kp^{1/\gamma} \tag{2.7}$$

where k is constant. Equation (2.7) is often taken even when friction is present.

The set of equations (2.1), (2.2) with (2.7) or (2.6) will be called the Euler equations under the adiabatic or isentropic

assumptions, or the 2-system, for an ideal (real) gas.

The Isothermal Approximation

For slow transients, the flow may be assumed isothermal, as heat transfer effects may be taken to even out the temperature distribution on a shorter timescale than the dynamic effects. In this case, equations (2.1) & (2.2) can be taken along with the following equation of state (for an ideal gas)

$$\rho = k(T)p \ , \tag{2.8}$$

where $k(T)$ is a function of the temperature, T . This set is also described as the 2-system, under the isothermal assumption. The partial differential equations are the same, and the equation of state differs only in prescribed values of constants.

The Schemes Used

Two numerical schemes are used here for computing solutions to the gas flow equations.

The Directional Difference Scheme [2] stems from a method of characteristics approach, and uses pseudo-characteristic variables, denoted by α and β . The 2-system equations are put into a form of 2 PDEs, each of which is written largely in terms of derivatives of a single variable but involves derivatives of the other:

$$\frac{\partial \alpha}{\partial t} = c_{11} \frac{\partial \alpha}{\partial x} + c_{12} \frac{\partial \beta}{\partial x} + s_1$$

$$\frac{\partial \beta}{\partial t} = c_{21} \frac{\partial \beta}{\partial x} + c_{22} \frac{\partial \alpha}{\partial x} + s_2 \ ,$$

where the c_{ij}, s_i, $i,j = 1,2$ are functions of the conserved variables not involving derivatives.

Each equation is derived largely from one of the two characteristic equations and is discretized by upwinding in the direction of the respective characteristics. Difficulties with the scheme arise from the incompleteness of the decoupling.

Roe's scheme [3],[4] can be applied to either the 2-system or the 3-system (indeed, to any system of conservation laws) and seeks locally linear solutions to the equation between nodes. The scheme is an approximate Riemann solver in that it solves approximately the Riemann problem

$$\underline{u}_t + \underline{f}_x = \underline{h}$$

$$\underline{u}(x,0) = \underline{u}_o = \begin{cases} \underline{u}_L & x < x_o \\ \underline{u}_R & x > x_o \end{cases}$$

within each cell (between nodes). Here, $\underline{u} = (\rho, \rho u)^T$ is the vector of conserved variables, and $\underline{u}_L, \underline{u}_R$ the initial values to the left and right of $x = x_o$. The vectors $\underline{f}$ and $\underline{h}$ are the vectors of flux quantities and source terms respectively. The first of these equations can be written in terms of the Jacobian matrix $A = \partial \underline{f} / \partial \underline{u}$:

$$\underline{u}_t + A\underline{u}_x = \underline{h}$$

The matrix system can be analysed into a system of eigenvectors and eigenvalues associated with each of the wave disturbances of the physical system. An approximation, $\tilde{A}$, to the matrix A can be found

as a linear function of the two initial states : $\tilde{A} = A(\underline{u}_L, \underline{u}_R)$. The eigenvectors and eigenvalues of this matrix are used to find the approximate disturbances associated with each wave, then each wave is upwinded separately.

The Directional Difference and Roe's schemes, each with its refinements, are detailed in the next chapter and a more thorough comparison of the two schemes is given.

3. The Two Schemes

In this chapter, both the Directional Difference Scheme and Roe's scheme as applied to the 2-system are derived, and in the final section the schemes are analysed for comparison of their approaches and features.

3.1. The Directional Difference Scheme

The Euler 2-system equations of mass conservation and momentum conservation for gas flow in one dimension (2.1) and (2.2), with friction, can be written (not in conservation form) [2]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0 \qquad (3.1a)$$

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} = \frac{-2f\rho u|u|}{d} \quad . \qquad (3.1b)$$

The adiabatic law relating pressure and density for an ideal gas is taken to replace the energy equation and the ideal equation of state. Although friction is present, the isentropic form of this law is assumed:

$$\rho = kp^{1/\gamma} \qquad (2.7)$$

Since $\rho = \rho(p)$, the derivatives take the form

$$\rho_t = \left[\frac{\partial \rho}{\partial p}\right]_s p_t$$

and

$$\rho_x = \left[\frac{\partial \rho}{\partial p}\right]_s p_x$$

But the adiabatic sound speed is (see [1])

$$c^2 = \left[\frac{\partial p}{\partial \rho}\right]_s = \frac{\gamma p}{\rho} \tag{3.2}$$

and therefore

$$c^2 \rho_t = p_t \tag{3.3a}$$

$$c^2 \rho_x = p_x \tag{3.3b}$$

Using (3.3a) in (3.1), the Euler equations can be written in matrix form:

$$\frac{\partial}{\partial t}\begin{bmatrix} p \\ u \end{bmatrix} + \begin{bmatrix} u & \rho c^2 \\ \rho^{-1} & u \end{bmatrix} \frac{\partial}{\partial x}\begin{bmatrix} p \\ u \end{bmatrix} + \begin{bmatrix} 0 \\ 2fu|u|/d \end{bmatrix} = \underset{\sim}{0} \tag{3.4}$$

These can be converted into pseudo-characteristic form by pre-multiplication by the matrix

$$\begin{bmatrix} 1 & \rho c \\ 1 & -\rho c \end{bmatrix}$$

which is the matrix of right eigenvectors of the Jacobian matrix (see section 3.3). This gives the equations

$$(p_t+\rho c u_t) + (u+c)(p_x+\rho c u_x) + \rho c(2fu|u|/d) = 0 \tag{3.7a}$$

$$(p_t-\rho c u_t) + (u-c)(p_x-\rho c u_x) - \rho c(2fu|u|/d) = 0 \ . \tag{3.7b}$$

In the scheme the variables α, β are defined as

$$\alpha = p + \rho c u \tag{3.8a}$$

$$\beta = p - \rho c u \tag{3.8b}$$

The equations (3.7) can be reworked (see Appendix A) into forms relating α_t to α_x,β_x, and β_t to α_x,β_x. Each equation has cross terms involved, so they are not decoupled. These equations are (A.8):

$$\alpha_t = \left[-(u+c) + \frac{u^2(\gamma+1)^2}{8c}\right] \alpha_x + \frac{u(\gamma+1)}{2}\left[1 + \frac{u(\gamma+1)}{4c}\right]\beta_x - F \qquad (3.9a)$$

$$\beta_t = \left[-(u+c) - \frac{u^2(\gamma+1)^2}{8c}\right] \beta_x + \frac{u(\gamma+1)}{2}\left[1 - \frac{u(\gamma+1)}{4c}\right]\alpha_x + F \qquad (3.9b)$$

where

$$F = \frac{2fpcu|u|}{d} . \qquad (3.10)$$

The directional difference scheme discretizes the space derivative terms in each of (3.9) according to the original characteristic equation from which it is derived. Thus, for (3.9a), which is derived from (3.7a), the characteristic wave travels forward and therefore backward differences are used. For (3.9b), derived from the backward travelling characteristic equation (3.7b), forward differences are used.

For example, with first order differences, equation (3.9a) is used with the following approximations:

$$\left.\begin{aligned} \alpha_t &\simeq (\alpha_j^{n+1} - \alpha_j^n)/\Delta t \\ \alpha_x &\simeq (\alpha_j^n - \alpha_{j-1}^n)/\Delta t \\ \beta_x &\simeq (\beta_j^n - \beta_{j-1}^n)/\Delta t \end{aligned}\right\} \qquad (3.11a)$$

and equation (3.9b) is used with the approximations:

$$\left.\begin{aligned} \beta_t &\simeq (\beta_j^{n+1} - \beta_j^n)/\Delta t \\ \alpha_x &\simeq (\alpha_{j+1}^n - \alpha_j^n)/\Delta t \\ \beta_x &\simeq (\beta_{j+1}^n - \beta_j^n)/\Delta t \end{aligned}\right\} \qquad (3.11b)$$

with all other terms evaluated at time level n, node j.
The solution variables are recovered from α and β at each point by inverting (3.8):

$$p = \tfrac{1}{2}(\alpha+\beta) \qquad (3.12a)$$

$$u = \frac{(\alpha-p)}{\rho c} = \frac{(p-\beta)}{\rho c} \qquad (3.12b)$$

Note that in (3.12b), ρc is a function of p so the inversion is nonlinear.

Boundary Conditions

Let the pipe be modelled by N nodes numbered $j = 1...N$, at positions spaced regularly with spacing Δx, where $(N-1)\Delta x$ is the length of the pipe.

Then use of (3.11a) enables α to be evaluated at the new time level at nodes $2...N$, and (3.11b) enables β to be evaluated at nodes $1...N-1$:

α	o	x	x	.	.	.	x	x	x
β	x	x	x	.	.	.	x	x	o
node no.	1	2	3	.	.	.	N-2	N-1	N

Therefore the boundary condition at the inlet (node 1) must specify α , and that the outlet (node N), β . The values of β at the inlet and α at the outlet are given by the difference scheme.

If p is specified at either end, then u can be found from whichever form of (3.12b) is appropriate:

$$u = \frac{p-\beta}{\rho c} \qquad \text{at inlet, as } \beta \text{ is known here, or}$$

$$u = \frac{\alpha-p}{\rho c} \qquad \text{at outlet, as } \alpha \text{ is known here.}$$

(N.B. ρc is a function of p).

If u is specified at either end, the appropriate form of (3.12b) has to be iterated to find p :

$$(\rho c)_j = \rho c(p_j)$$

$$p_{j+1} = \beta + (\rho c)_j u \qquad \text{at inlet, as } \beta \text{ is known here, or}$$

$$p_{j+1} = \alpha - (\rho c)_j u \qquad \text{at outlet, as } \alpha \text{ is known here.}$$

The first iterate, p_o, can be taken as β or α (depending on whether the condition is at the inlet or outlet, respectively).

Second Order

Higher order approximations to the derivatives may be used in place of (3.11a) and (3.11b). Approximations that are one-sided can be used to preserve the directional differencing. Where second order

differences are shown in the results, the following approximations have been made (see [2]).

Backward spatial differences (replacing (3.11a))

$$\eta_x \simeq (3\eta_i - 4\eta_{i-1} + \eta_{i-2})/2\Delta x \qquad (3.13a)$$

Forward spatial differences (replacing 3.11b))

$$\eta_x \simeq -(3\eta_i - 4\eta_{i+1} + \eta_{i+2})/2\Delta x \qquad (3.13b)$$

where η is either of α or β. The approximations to the time derivatives remain the same. First order differences are used at nodes next to the boundary.

3.2. Roe's Scheme

The scheme outlined here is based on the approach by Roe in [3] & [4]. Applied to the reduced set of Euler equations subject to the adiabatic approximation it is very similar to the scheme used by Glaister for the shallow water equation (see [6],[7]).

The Euler equations of mass conservation and momentum conservation for gas flow in one dimension, with friction, (2.1),(2.2) & (2.7), can be written:

$$\underline{u}_t + \underline{f}_x = \underline{h} \tag{3.14}$$

where

$$\underline{u} = (\rho, \rho u)^T \tag{3.15}$$

$$\underline{f}(\underline{u}) = (\rho u, p+(\rho u)^2/\rho)^T \tag{3.16}$$

$$\underline{h} = (0, \ -2f\rho u|u|/d)^T \tag{3.17}$$

The Jacobian matrix $A = \partial \underline{f}(\underline{u})/\partial \underline{u}$, its eigenvalues λ_i and corresponding right eigenvectors $\underline{r}_i$, i = 1,2, are found to be

$$A = \begin{bmatrix} 0 & 1 \\ c^2-u^2 & 2u \end{bmatrix} \tag{3.18}$$

$$\lambda_1 = u + c \tag{3.19a}$$

$$\lambda_2 = u - c \tag{3.19b}$$

$$\underline{r}_1 = \begin{bmatrix} 1 \\ u+c \end{bmatrix} \tag{3.20a}$$

$$\underline{r}_2 = \begin{bmatrix} 1 \\ u-c \end{bmatrix} \tag{3.20b}$$

where

$$c^2 = \left[\frac{\partial p}{\partial \rho}\right]_s = \frac{\gamma p}{\rho} \tag{3.21}$$

is the adiabatic sound speed squared from equation (3.2).

The Approximate Riemann Problem

The Riemann problem is the following: given the system of equations governing the flow (3.14), suppose that up to time $t = 0$, the following states are maintained by a membrane at $x = 0$:

$$\underline{u}_L = (\rho_L, \rho_L u_L)^T \qquad x < 0$$

$$\underline{u}_R = (\rho_R, \rho_R u_R)^T \qquad x > 0$$

which are constant states. Suppose further that the membrane is removed at $t = 0$; then the problem is to find the resulting fluid flow.

The approximate Riemann solver is constructed by solving problems of the above type approximately in the region

$$[x_L, x_R] \times (t_n, t_{n+1}) .$$

This cell, between two grid points with abscissae x_L and x_R, has initial data (at $t = t_n$)

$$\underline{u} = \begin{cases} \underline{u}_L = \underline{u}(x_L, t_n) & x < x_L + \Delta x/2 \\ \underline{u}_R = \underline{u}(x_R, t_n) & x > x_R - \Delta x/2 \end{cases} \tag{3.22}$$

where Δx is the spacing between x_L and x_R .

Equation (3.14) can be written

$$\underline{u}_t + A(\underline{u})\underline{u}_x = \underline{h} \ .$$

It is possible [3] to find a locally linear approximation to A , called $\tilde{A}$, in the cell, such that the following hold:

$$\Delta\underline{u} = \Sigma\, \tilde{\alpha}_k\, \tilde{\underline{r}}_k \tag{3.23}$$

$$\Delta\underline{f} = \Sigma\, \tilde{\alpha}_k\, \tilde{\lambda}_k\, \tilde{\underline{r}}_k \tag{3.24}$$

for some numbers $\tilde{\alpha}_k$, where $\Delta(.) = (.)_R - (.)_L$, and $\tilde{\lambda}_k$, $\tilde{\underline{r}}_k$ $(k = 1,2)$ are the eigenvalues and eigenvectors of the approximate matrix $\tilde{A}$. This provides a unique decomposition of the flux difference $\Delta\underline{f}$ into the eigenvectors of $\tilde{A}$ (provided that they are independent). The update at t_{n+1} is made by following each component of $\Delta\underline{f}$ to the right or left, according as the sign of the associated eigenvalue is positive or negative .

To obtain the approximate Jacobian matrix $\tilde{A}(\underline{u}_L, \underline{u}_R)$, or equivalently, the $\tilde{\lambda}_k$ and $\tilde{\underline{r}}_k$, and to obtain the coefficients $\tilde{\alpha}_k$, the expressions (3.23), (3.24) are first satisfied for states $\underline{u}_L, \underline{u}_R$ which are close to each other. Then average values in the cell are sought to make the expressions correct for arbitrary states.

Decomposition for Close States

Consider two states $\underline{u}_L = (\rho_L, \rho_L u_L)^T$, $\underline{u}_R = (\rho_R, \rho_R u_R)^T$, both close

to an average state $\underline{u} = (\rho, \rho u)^T$. It is required to satisfy (3.23) and (3.24) to within $O(\Delta^2)$. Here we take $\tilde{A} = A(u)$. Specifically, we require

$$\Delta \underline{u} = \sum_{k=1}^{2} \alpha_k \underline{r}_k \tag{3.25}$$

$$\Delta \underline{f} = \sum_{k=1}^{2} \alpha_k \lambda_k \underline{r}_k \ . \tag{3.26}$$

where the $\underline{r}_k$ and the λ_k are given by (3.19) & (3.20). Then, from (3.15) & (3.16), we have to find α_1 and α_2 that satisfy

$$\Delta\rho = \alpha_1 + \alpha_2 \tag{3.25a}$$

$$\Delta(\rho u) = \alpha_1(u+c) + \alpha_2(u-c) \tag{3.25b}$$

$$\Delta(\rho u) = \alpha_1(u+c) + \alpha_2(u-c) \tag{3.26a}$$

$$\Delta(p+\rho u^2) = \alpha_1(u+c)^2 + \alpha_2(u-c)^2 \ . \tag{3.26b}$$

Equation (3.26a) is the same as (3.25b). Solving (3.25a) and (3.25b) for α_1, α_2 gives

$$\alpha_1 = \tfrac{1}{2}\Delta\rho + \frac{1}{2c}\left(\Delta(\rho u) - u\Delta\rho\right) \tag{3.27a}$$

$$\alpha_2 = \tfrac{1}{2}\Delta\rho - \frac{1}{2c}\left(\Delta(\rho u) - u\Delta\rho\right) \tag{3.27b}$$

To within $O(\Delta^2)$,

$$\Delta p = c^2 \Delta \rho$$

$$\Delta(\rho u^2) = u^2 \Delta \rho + 2\rho u \Delta u$$

Hence, to first order,

$$\Delta(p+\rho u^2) = c^2 \Delta \rho + u^2 \Delta \rho + 2\rho u \Delta u$$

and therefore, also to first order,

$$\begin{aligned}
&(\alpha_1 + \alpha_2)(u^2+c^2) + (\alpha_1 - \alpha_2)2uc \\
&= (u^2+c^2)\Delta\rho + 2u(\Delta(\rho u) - u\Delta\rho) \\
&= c^2 \Delta p + u^2 \Delta p + 2\rho u \Delta u \\
&= \Delta(p+\rho u^2) \ .
\end{aligned}$$

So, equation (3.26b) is satisfied by the choice of α_1, α_2 given in (3.27), and therefore, all of the equations (3.25) & (3.26), are satisfied to within $O(\Delta^2)$.

Decomposition for general $\underline{u}_L, \underline{u}_R$

It is now required to find an average $\tilde{A}(\underline{u}_L, \underline{u}_R)$ such that (3.23) and (3.24) hold for arbitrary states $\underline{u}_L, \underline{u}_R$. In fact an average state $\tilde{\underline{u}}$ is sought such that $\tilde{A} = A(\tilde{\underline{u}})$. Specifically the relations

$$\Delta \underline{u} = \sum_{k=1}^{2} \tilde{\alpha}_k \, \tilde{\underline{r}}_k \qquad (3.28)$$

$$\Delta \underline{f} = \sum_{k=1}^{2} \tilde{\alpha}_k \, \tilde{\lambda}_k \, \underline{\tilde{r}}_k \tag{3.29}$$

are required to be satisfied by some $\underline{\tilde{u}} = (\tilde{\rho}, \tilde{\rho u})^T$ where

$$\tilde{\lambda}_1 = \tilde{u} + \tilde{c} \quad , \quad \tilde{\lambda}_1 = \tilde{u} - \tilde{c} \tag{3.30}$$

$$\underline{\tilde{r}}_1 = \begin{bmatrix} 1 \\ \tilde{u}+\tilde{c} \end{bmatrix} \quad , \quad \underline{\tilde{r}}_2 = \begin{bmatrix} 1 \\ \tilde{u}-\tilde{c} \end{bmatrix} \tag{3.31}$$

$$\tilde{\alpha}_1 = \tfrac{1}{2}\Delta\rho + \frac{1}{2\tilde{c}} (\Delta(\rho u) - \tilde{u}\Delta\rho) \tag{3.32a}$$

$$\tilde{\alpha}_2 = \tfrac{1}{2}\Delta\rho + \frac{1}{2\tilde{c}} (\Delta(\rho u) - \tilde{u}\Delta\rho) \tag{3.32b}$$

$$\Delta(.) = (.)_R - (.)_L$$

and $\tilde{c} = \tilde{c}(\underline{\tilde{u}})$ in some manner.

Equations (3.28) and (3.29) are, with the help of (3.30) and (3.31), in full:

$$\Delta\rho = \tilde{\alpha}_1 + \tilde{\alpha}_2 \tag{3.33a}$$

$$\Delta(\rho u) = \tilde{\alpha}_1(\tilde{u} + \tilde{c}) + \tilde{\alpha}_2(\tilde{u} - \tilde{c}) \tag{3.33b}$$

$$\Delta(\rho u) = \tilde{\alpha}_1(\tilde{u} + \tilde{c}) + \tilde{\alpha}_2(\tilde{u} - \tilde{c}) \tag{3.33c}$$

$$\Delta(p+\rho u^2) = \tilde{\alpha}_1(\tilde{u} + \tilde{c})^2 + \tilde{\alpha}_2(\tilde{u} - \tilde{c})^2 \ . \tag{3.33d}$$

Equations (3.33b) and (3.33c), which are identical, and equation (3.33a), are automatically satisfied by any averages, where the $\tilde{\alpha}$'s are given by (3.32). Equation (3.33d) gives (by 3.32)

$$\Delta p + \Delta(\rho u^2) = (\tilde{\alpha}_1 + \tilde{\alpha}_2)(\tilde{u}^2 + \tilde{c}^2) + 2\tilde{u}\tilde{c}\,(\tilde{\alpha}_2 - \tilde{\alpha}_2)$$

$$= (\tilde{u}^2 + \tilde{c}^2)\Delta\rho + 2\tilde{u}(\Delta(\rho u) - \tilde{u}\Delta\rho)$$

or

$$\tilde{u}^2\Delta\rho - 2\tilde{u}\Delta(\rho u) + \Delta(\rho u^2) = \tilde{c}^2\Delta\rho - \Delta p \ . \tag{3.34}$$

Values for $\tilde{u}$ and $\tilde{c}$ to satisfy this equation can be found by setting both sides to zero. Thus

$$\tilde{c}^2 = \frac{\Delta p}{\Delta\rho} = \frac{p_R - p_L}{\rho_R - \rho_L} \tag{3.35}$$

and the appropriate solution of the remaining quadratic for $\tilde{u}$ in (3.34) is

$$\tilde{u} = \frac{\Delta(\rho u) - \sqrt{(\Delta(\rho u))^2 - \Delta\rho\Delta(\rho u^2)}}{\Delta\rho} \tag{3.36}$$

which reduces to

$$\tilde{u} = \frac{\Delta(\rho u) - \sqrt{\rho_R\rho_L}\ \Delta u}{\Delta\rho}$$

and

$$\tilde{u} = \frac{\rho_R^{1/2}\, u_R + \rho_L^{1/2}\, u_L}{\rho_R^{1/2} + \rho_L^{1/2}} \ . \tag{3.37}$$

Note that:

$$\Delta(\rho u) - \tilde{u}\Delta\rho = \sqrt{\rho_R \rho_L}\,\Delta u$$

and that equations (3.32) can be simplified to

$$\alpha_1 = \tfrac{1}{2}\Delta\rho + \tfrac{1}{2}\frac{\tilde{\rho}}{\tilde{c}}\Delta u \tag{3.38a}$$

$$\alpha_2 = \tfrac{1}{2}\Delta\rho - \tfrac{1}{2}\frac{\tilde{\rho}}{\tilde{c}}\Delta u \tag{3.38b}$$

if $\tilde{\rho}$ is defined as

$$\tilde{\rho} = \sqrt{\rho_R \rho_L}\ . \tag{3.39}$$

In the case where $\Delta\rho = 0$, $\tilde{c}^2$ can not be defined using (3.35). Instead, it is defined as

$$\tilde{c}^2 = \frac{\gamma\tilde{p}}{\tilde{\rho}} = \frac{\gamma p_L}{p_L} = \frac{\gamma p_R}{p_R} \tag{3.40}$$

as $\rho = \rho_L = \rho_R$, $p = p_L = p_R$. Note that the right hand side of (3.34) is identically zero and so the result for $\tilde{u}$ is not affected.

In summary, we have found that for the problem (3.22), the equations

$$\Delta\underline{u} = \Sigma\, \tilde{\alpha}_k \underline{\tilde{r}}_k \tag{3.22}$$

$$\Delta\underline{f} = \Sigma\, \tilde{\alpha}_k \tilde{\lambda}_k \underline{\tilde{r}}_k \tag{3.23}$$

hold, where

$$\lambda_{1,2} = \tilde{u} \pm \tilde{c} \tag{3.41}$$

$$\underline{e}_{1,2} = (1, \tilde{u} \pm \tilde{c})^T \tag{3.42}$$

$$\alpha_{1,2} = \tfrac{1}{2}\Delta\rho \pm \tfrac{1}{2} \frac{\tilde{\rho}}{\tilde{c}} \Delta u \tag{3.43}$$

$$\Delta(.) = (.)_R - (.)_L$$

$$\tilde{u} = \frac{\rho_R^{1/2} u_R + \rho_L^{1/2} u_L}{\rho_R^{1/2} + \rho_L^{1/2}} \tag{3.44}$$

$$\tilde{\rho} = (\rho_R \rho_L)^{1/2} \tag{3.45}$$

$$\tilde{c}^2 = \begin{cases} \Delta p / \Delta \rho & \Delta\rho \neq 0 \\ \gamma p_R / \rho_R & \Delta\rho = 0 \end{cases} . \tag{3.46}$$

Source term

The source term is similarly decomposed onto the eigenvectors:

$$\underline{h} = \sum_{k=1}^{2} \tilde{\beta}_k \underline{r}_k \quad . \tag{3.47}$$

In this case, with $\underline{h}$ given as per (3.17), we seek $\tilde{\beta}_1$ and $\tilde{\beta}_2$ such that

$$0 = \tilde{\beta}_1 + \tilde{\beta}_2 \tag{3.48}$$

$$F = -2f\rho u|u|/d = \tilde{\beta}_1(\tilde{u}+\tilde{c}) + \tilde{\beta}_2(\tilde{u}-\tilde{c})$$

$$= (\tilde{\beta}_1+\tilde{\beta}_2)\tilde{u} + (\tilde{\beta}_1+\tilde{\beta}_2)\tilde{c} \qquad (3.49)$$

therefore

$$F/\tilde{c} = \tilde{\beta}_1 - \tilde{\beta}_2 \ . \qquad \text{by (3.48)}$$

and

$$\tilde{\beta}_1 = -\tilde{\beta}_2 = \frac{F}{2\tilde{c}} \ . \qquad (3.50)$$

The term F can be any average value for the cell. As $F = F(\underline{u})$, convenient choices are $F = \frac{1}{2}(F(\underline{u}_L) + F(\underline{u}_R))$ and $F = F(\tilde{\underline{u}})$, where $\tilde{\underline{u}} = (\tilde{\rho}, \tilde{\rho}\tilde{u})^T$ is given by (3.44) and (3.45). Here the choice $F = F(\tilde{\underline{u}})$ is taken.

The Scheme

Referring to Figure 1, the values of $\underline{u}$ at each point $(i\Delta x)$ at time level n are assumed to define a piecewise constant state

$$\underline{u} = \underline{u}_i^n \qquad x \in ((i-\tfrac{1}{2})\Delta x, (i+\tfrac{1}{2})\Delta x) \ , \quad t = t_n \ , \quad \forall i \qquad (3.51)$$

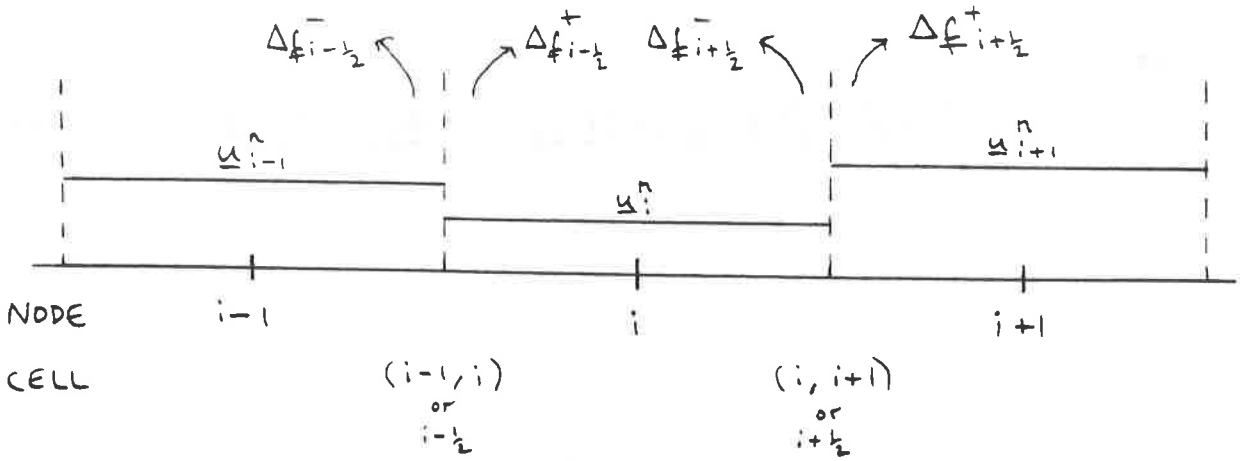

Fig. 1.

At each node, the equation (3.14) is discretized in the following way: The decomposition of the flux differences $\Delta \underline{f}$ is performed in each cell $(i,j+1)$, giving these differences as the sum of two terms

$$\Delta \underline{f}^{-} = \sum_{\substack{k=1 \\ \tilde{\lambda}_k < 0}}^{2} \tilde{\alpha}_k \, \tilde{\lambda}_k \, \tilde{\underline{r}}_k$$

$$\Delta \underline{f}^{+} = \sum_{\substack{k=1 \\ \tilde{\lambda}_k < 0.}}^{2} \tilde{\alpha}_k \, \tilde{\lambda}_k \, \tilde{\underline{r}}_k$$

If these flux differences in the cell $(i,i+1)$ are denoted by the subscript $i + \frac{1}{2}$, i.e. $\Delta \underline{f}_{i+\frac{1}{2}}$, $\Delta \underline{f}^{+}_{i+\frac{1}{2}}$, $\Delta \underline{f}^{-}_{i+\frac{1}{2}}$, then the flux contribution to the node i is that travelling rightwards from the cell $(i-1,i)$ and leftwards from the cell $(i,i+1)$, that is, $\Delta \underline{f}^{+}_{i-\frac{1}{2}}$ and $\Delta \underline{f}^{-}_{i+\frac{1}{2}}$. The source term at each node can be produced similarly, so the update is given by

$$\frac{\underline{u}_i^{n+1} - \underline{u}_i^{n}}{\Delta t} = - \frac{(\Delta \underline{f}^{+}_{i-\frac{1}{2}} + \Delta \underline{f}^{-}_{i+\frac{1}{2}})}{\Delta x} + \underline{h}^{+}_{i-\frac{1}{2}} + \underline{h}^{-}_{i+\frac{1}{2}}$$

or

$$\underline{u}_i^{n+1} = \underline{u}_i^{n} - \frac{\Delta t}{\Delta x} (\Delta \underline{f}^{+}_{i-\frac{1}{2}} + \Delta \underline{f}^{-}_{i+\frac{1}{2}}) + \Delta t(\underline{h}^{+}_{i-\frac{1}{2}} + \underline{h}^{-}_{i+\frac{1}{2}}) \qquad (3.52)$$

Boundary terms

Taking the boundary to be at node 1, say, and with reference to figure 2, it can be seen that the boundary node receives a contribution only from cell (1,2) from the left-moving eigenvector. To balance this, a wave from outside the computational region is assumed to contribute to node 1 also.

The wave is assumed to be proportional to the right eigenvector of the Jacobian matrix, as are the flux differences and source terms of all rightward travelling waves in all other cells. The right eigenvector can be evaluated at node 1 directly or over the cell (0,1) by the decomposition of equations (3.42), (3.44) and (3.46) where the value of $\underline{u}$ at node 0 is obtained by some extrapolation. Here it is evaluated at node 1 directly.

The steps in the calculation of the new boundary values are: first, the contributions from the flux and source terms from the cell (1,2) are added to $\underline{u}_i^n$, giving an intermediate value at the boundary, which we denote by $\underline{u}_1^*$. If the boudary condition to be satisfied is at time level $n + 1$

$$\underline{y}(\underline{u}_1^{n+1}) = 0 \tag{3.53}$$

then (3.53) has to be solved along with

$$\underline{u}_1^{n+1} = \underline{u}_1^* + \xi \tilde{\underline{r}}_1 \tag{3.54}$$

where $\tilde{\underline{r}}_1$ is the right eigenvector of the approximate Jacobian, and ξ is an unknown determining the 'strength' of the incoming wave.

Equation (3.54) then gives the value of $\underline{u}_1^{n+1}$ at the new time level. The system (3.53) and (3.54) may or may not require iteration, depending on the form of the boundary condition (3.53).

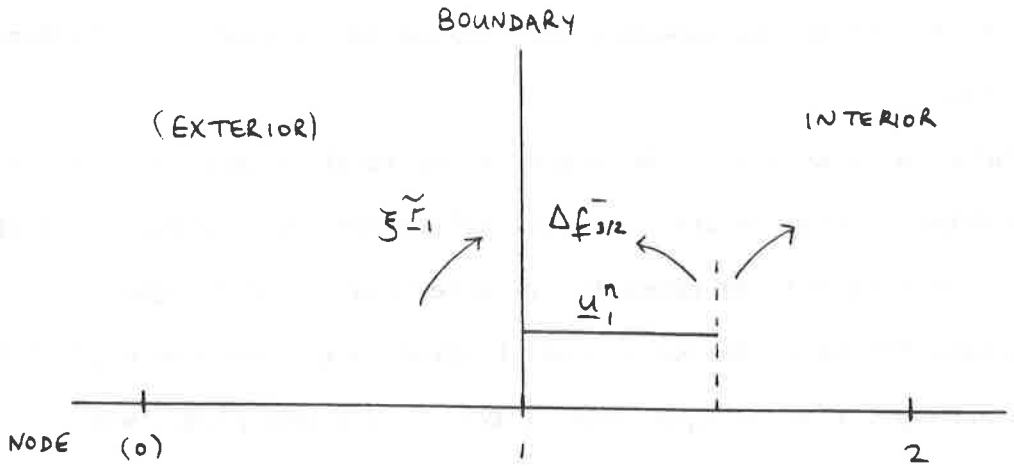

Fig. 2.

At the right hand boundary the system to be solved is

$$z(\underline{\tilde{u}}^{n+1}) = 0 \tag{3.55}$$

$$\underline{u}_N^{n+1} = \underline{u}_N^* + \eta\tilde{\underline{r}}_2 \tag{3.56}$$

where (3.55) is the boundary condition, N is the boundary node, $\underline{u}_N^*$ the intermediate value, and $\tilde{\underline{r}}_2$ the leftward travelling eigenvector of some approximate Jacobian and η is an unknown again determining the 'strength' of the incoming wave. Equation (3.56) gives the new boundary value $\underline{u}_N^{n+1}$.

Second Order

For second order schemes, the method of flux limiters can be

applied. For a discussion and details of these, the reader is referred to [13]. The limiters used here are the minmod and superbee limiters. 'No Limiter' in the results refers to the basic first-order scheme.

An entropy correction

The Roe's scheme can in rare situations give solutions to the conservation equations that are non-physical, i.e. entropy violating. A modification is used here to ensure that the solutions do not violate the entropy condition. For discussion and details see [4],[8].

3.3. Comparison of Schemes

The Euler equations (2.1)-(2.3) can be written in a variety of ways. The form used as the basis for a particular numerical scheme can to some extent determine the properties of that scheme. This section attempts to show how the features of the two schemes discussed in this report arise from the form of the Euler equations chosen as a basis for each scheme, and compares the schemes. For a general discussion and basic ideas, see [5].

The Euler equations are derived from physical conservation laws, and the following form (ignoring friction) is called the conservative form:

$$\underline{u}_t + \underline{f}(\underline{u})_x = \underline{0} \ . \tag{3.57}$$

Here, the components of $\underline{u}$ are the conserved variables and the components of $\underline{f}$ are the flux quantities arising from the physical law. One desirable property of a numerical scheme is that it mimics an integrated form of (3.57) over a control volume, that is, the total amount of (each of) the conserved variables within the computational region increases at each time step by the net numerical flux into the region in that time step. Such a scheme is called conservative, and has the additional properties that for shocks, the shock speeds and positions will be correct.

By writing

$$A = \partial \underline{f} / \partial \underline{u}$$

the equation (3.57) can be transformed into matrix form:

$$\underline{u}_t + A\underline{u}_x = \underline{0} \ . \tag{3.58}$$

The Jacobian matrix A has left eigenvectors $\underline{l}_i$, right eigenvectors $\underline{r}_i$, and eigenvalues λ_i that satisfy

$$A\underline{r}_i = \lambda_i \underline{r}_i \tag{3.59}$$

$$\underline{l}_i A = \lambda_i \underline{l}_i \ . \tag{3.60}$$

For the Euler equations, the λ_i are distinct. The left eigenvectors can be normalized such that

$$\underline{l}_i \cdot \underline{r}_j = \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \ . \tag{3.61}$$

The following matrices can be defined; the matrix of left eigenvectors

$$L = \begin{bmatrix} \underline{l}_1 \\ \vdots \\ \underline{l}_N \end{bmatrix} \ ,$$

the matrix of right eigenvectors

$$R = (\underline{r}_1 \ \ldots\ldots \underline{r}_N) \ ,$$

and the diagonal matrix of eigenvalues

$$\Lambda = \text{diag}\ (\lambda_1\ ,\ldots,\lambda_N)$$

where N is the number of equations in (3.57). With these definitions and equations (3.59)-(3.61), the following hold:

$$\left.\begin{aligned} &LA = \Lambda L \\ &AR = R\Lambda \\ &LR = I \\ &\Lambda LR = LR\Lambda = \Lambda \\ &A = R\Lambda L \end{aligned}\right\} \qquad (3.62)$$

(I is the identity matrix).

Roe's Scheme

Roe's Scheme requires that a discrete form of the relation

$$\underline{f}_x = A\underline{u}_x$$

(cf. (3.57),(3.58)) is satisfied in each cell (between nodes) where the terms $\underline{f}_x$, $\underline{u}_x$ are discretized as $(.)_x = \Delta(.)/\Delta x$, and $\Delta(.) = (.)_R - (.)_L$. This is done by finding an approximation to the Jacobian A, i.e. $\tilde{A}$, such that

$$\Delta\underline{f} = \tilde{A}\Delta\underline{u} \ . \qquad (3.63)$$

Denoting the eigenvalues and eigenvectors of $\tilde{A}$ by $\tilde{\lambda}_i, \tilde{\underline{l}}_i$ and $\tilde{\underline{r}}_i$ we can find the projections $\tilde{\alpha}_i$ of $\Delta\underline{u}$ onto the right eigenvectors $\tilde{\underline{r}}_i$ via

$$\Delta\underline{u} = \sum \tilde{\alpha}_i \, \tilde{\underline{r}}_i \tag{3.64}$$

since

$$\tilde{\underline{l}}_j \cdot \Delta\underline{u} = \sum \tilde{\alpha}_i \, \tilde{\underline{l}}_j \cdot \tilde{\underline{r}}_i$$

$$= \sum \tilde{\alpha}_i \, \underline{\delta}_{ij}$$

$$= \tilde{\alpha}_j$$

i.e. the projection strengths are

$$\tilde{\alpha}_j = \tilde{\underline{l}}_j \cdot \Delta\underline{u} \tag{3.65}$$

Using (3.63),(3.64) gives

$$\Delta\underline{f} = \sum \tilde{\alpha}_i \, A\tilde{\underline{r}}_i$$

$$= \sum \tilde{\alpha}_i \, \tilde{\lambda}_i \, \tilde{\underline{r}}_i \, . \tag{3.66}$$

This equation gives the flux difference in the cell as being split into components belonging to each wave motion (characteristic direction), enabling upwinding to be carried out. Therefore updating the solution

in time may be done in such a way as to ensure that information passes in the correct direction, but the total update is the flux difference, keeping the conservation property.

Specifically, the update $\underline{Eu}_k = \underline{u}_k^{n+1} - \underline{u}_k^n$ to node k depends on flux difference components from the cells to the left and right (denoted by $k - \frac{1}{2}$ and $k + \frac{1}{2}$ respectively), where

$$\underline{Eu}_k = -\frac{\Delta t}{\Delta x}\left((\Delta f)^+_{k-\frac{1}{2}} + (\Delta f)^-_{k+\frac{1}{2}}\right)$$

$$= -\frac{\Delta t}{\Delta x}\left[\sum_{\lambda>0}(\tilde{\lambda}_i\tilde{\alpha}_i\tilde{\underline{r}}_i)_{k-\frac{1}{2}} + \sum_{\lambda<0}(\tilde{\lambda}_i\tilde{\alpha}_i\tilde{\underline{r}}_i)_{k+\frac{1}{2}}\right]$$

$$= -\frac{\Delta t}{\Delta x}\sum(\tilde{\lambda}_i(\tilde{\underline{l}}_i\cdot\Delta\underline{u})\tilde{\underline{r}}_i)^{\text{UPWIND}} \qquad (3.67)$$

Directional Difference Scheme

This scheme treats the matrix A in (3.58)

$$\underline{u}_t + A\underline{u}_x = 0$$

by premultiplication by the matrix of left eigenvectors L:

$$L\underline{u}_t + LA\underline{u}_x = 0$$

$$L\underline{u}_t + \Lambda L\underline{u}_x = 0 \qquad \text{(from 3.62)}$$

i.e.

$$\underline{l}_i\cdot\underline{u}_t + \lambda_i\underline{l}_i\cdot\underline{u}_x = 0 \qquad i = 1\ldots N\,. \qquad (3.68)$$

The scheme then takes pseudo-characteristic variables which are here denoted by α_i :

$$\alpha_i = \underline{l}_i . \underline{u} .$$

Substituting into (3.68):

$$(\alpha_i)_t + \lambda_i(\alpha_i)_x = (\underline{l}_i)_t . \underline{u} + \lambda_i(\underline{l}_i)_x . \underline{u} . \qquad (3.69)$$

The terms on the right-hand sides that are time derivatives can be eliminated in terms of space derivatives to give a set of equations:

$$(\alpha_i)_t + \lambda_i(\alpha_i)_x = g_i((\alpha_1)_x, \ldots, (\alpha_N)_x) \ , \quad i = 1 \ldots N \ . \qquad (3.70)$$

(See Appendix A, equation (A.12) to see how this is done.)
The scheme then discretizes and solves these equations for each α_i in an upwind manner, that is, at node k , the update $E(\alpha_i)_k$ defined as

$$E(\alpha_i)_k = (\alpha_i)_k^{n+1} - (\alpha_i)_k^n \ ,$$

is given by

$$E(\alpha_i)_k = \frac{\Delta t}{\Delta x}(- \lambda_i \Delta^{\pm}(\alpha_i)_k + g_i(\Delta^{\pm}(\alpha_1)_k, \ldots, \Delta^{\pm}(\alpha_N)_k)) \ , \ i = 1 \ldots N. \qquad (3.71)$$

$\Delta^{\pm}$ denotes an upwind difference which depends on the sign of λ_i and is the same in all occurrences in each equation, that is, all of the difference terms in g_i are differenced in a forward or backward manner according as λ_i is negative or positive, and irrespective of the direction associated with the pseudo-characteristic variable being

differenced. The existence of the g_i (i.e. the cross terms or non-diagonal terms) arises because the α_i are not true characteristic variables. The scheme has the following properties:

i) the scheme does not use proper characteristic variables, but pseudo-charactertistic variables, therefore

(a) boundary conditions are easy to implement, although the information will not be on exactly the correct variables;

(b) there is 'upwinding' in the cross terms that is not in the correct direction (which is to some extent mitigated by the small size of the terms in typical gas problems),(see below).

ii) The scheme does not deal with fluxes, and it can be shown that conservation is not respected.

iii) the scheme is consistent with the Euler equations.

If the cross terms in (3.69) can be neglected, by neglecting derivatives of the vectors $\underline{l}_i$, then in the differences the corresponding terms can also be neglected, i.e.

$$\Delta(\alpha_i) = \Delta(\underline{l}_i . \underline{u}) = \underline{l}_i . \Delta\underline{u}$$

(where Δ denotes finite differencing in time or space), and the scheme becomes (from (3.71) with the terms g_i omitted)

$$\underline{l}_i . E\underline{u}_k = \frac{\Delta t}{\Delta x}(- \lambda_i \underline{l}_i . \Delta^{\pm}\underline{u}_k) \quad , \quad i = 1 \ldots N \ .$$

These equations can be solved for $E\underline{u}_k$, giving

$$E\underline{u}_k = - \frac{\Delta t}{\Delta x} (\lambda_i (\underline{l}_i . \Delta^{\pm} \underline{u}_k) \underline{r}_i) \qquad (3.72)$$

The λ_i , $\underline{l}_i$, $\underline{r}_i$ are all evaluated functions of $\underline{u}_k^n$. We call this the simplified Directional Difference Scheme.

Comparing (3.72) with the Roe Scheme, (3.67), we observe the similarities of the schemes. The differences are:

i) The λ_i , $\underline{l}_i$, $\underline{r}_i$ are evaluated at nodes in the Directional Difference Scheme, and as cell averages in the appropriate adjacent cells in the Roe Scheme.

ii) The use of particular cell averages in Roe's Scheme ensures conservation. Such a property does not hold for the Directional Difference Scheme.

iii) The simplified Directional Difference Scheme is not consistent with the Euler equations. The schemes are similar in that both upwind correctly, but, the simplified directional difference scheme differs from the full version in that the cross terms have been eliminated. If they had not been eliminated, then the eigenvectors $\underline{l}_i$ would also be differenced in (3.71). Solving for $E\underline{u}_k$ from $E(\alpha_i)$ would involve inversion of the matrix L at both the old and new time levels, so an expression such as (3.72) could not be arrived at in the full case.

In the case of the gas equations the simplified Directional Difference Scheme can be thought of as intermediate between two distinct

orders of approximation of the full scheme. The full equations to be discretized are (writing $\alpha = \alpha_1$, $\beta = \alpha_2$, and neglecting friction)

$$\alpha_t = \left[- (u+c) + \frac{u^2(\gamma+1)^2}{8c} \right]\alpha_x + \frac{u(\gamma+1)}{2} \left[1 + \frac{u(\gamma+1)}{4c}\right]\beta_x \qquad \text{(from 3.9)}$$

$$\beta_t = \left[- (u-c) - \frac{u^2(\gamma+1)^2}{8c} \right]\beta_x + \frac{u(\gamma+1)}{2} \left[1 - \frac{u(\gamma+1)}{4c}\right]\alpha_x$$

These contain terms of order 1, (u/c), and $(u/c)^2$. If $u \ll c$, the 1st order approximation is:

$$\alpha_t = - (u+c)\alpha_x + \frac{u(\gamma+1)}{2} \beta_x \qquad (3.73)$$

$$\beta_t = - (u-c)\beta_x + \frac{u(\gamma+1)}{2} \alpha_x$$

which still contains cross terms. The 0'th order approximation is

$$\alpha_t = -c\alpha_x$$

$$\beta_t = c\beta_x \qquad (3.74)$$

which are the wave equations for α and β . The simplified scheme (3.72) corresponds to an upwind discretization of

$$\alpha_t + (u+c)\alpha_x = 0$$
$$\beta_t + (u-c)\beta_x = 0$$

which contains some of the terms of (3.73) and includes all terms of (3.74). In many cases $u \ll c$ applies, and therefore the simplified

scheme is approximately what is being solved. The resemblance of the solutions of the directional difference and Roe schemes at first order for small u is therefore expected.

Here, we have treated only the homogeneous case. In fact, it appears that the modelling within the schemes of the friction terms is crucial to the behaviour of the schemes, and a difference between the rates of convergence in test problem 3 should be noted.

A scheme akin to the Directional Difference Scheme using Riemann Invariants.

The directional difference scheme attempts to transform the Euler equations (3.58)

$$\underline{u}_t + A\underline{u}_x = 0$$

by premultiplication by the matrix L, i.e.

$$L\underline{u}_t + LA\underline{u}_x = 0 \qquad (3.75)$$

such that the resulting set of equations (3.75) is a diagonal set,

$$\underline{w}_t + \Lambda\underline{w}_x = 0 \qquad (3.76)$$

in a new set of variables $\underline{w}$. The diagonal matrix contains the physical wavespeeds as entries and is therefore the matrix Λ of eigenvalues associated with A. The directional difference scheme takes

$$\underline{w} = L\underline{u}$$

and finds that (3.76) does not hold exactly. If instead we take

$$\underline{w} = \underline{w}(\underline{u})$$

and let

$$L = \partial \underline{w} / \partial \underline{u}$$

we obtain

$$\underline{w}_x = L\underline{u}_x$$
$$\underline{w}_t = L\underline{u}_t \ .$$

Therefore (3.75) is

$$\underline{w}_t + LAL^{-1} \underline{w}_x = 0$$

i.e.

$$\underline{w}_t + A\underline{w}_x = 0$$

Now

$$L = (l_{ij}) = \left(\frac{\partial w_i}{\partial u_j}\right) = \begin{bmatrix} \underline{\nabla} w_1 \\ \vdots \\ \underline{\nabla} w_N \end{bmatrix}$$

where $$\underline{\nabla} = \left(\frac{\partial}{\partial u_1} \ , \ldots , \frac{\partial}{\partial u_N}\right)$$

and $R = (\underline{r}_1, \ldots \underline{r}_N)$. But

$$LR = (\underline{r}_i \cdot \underline{\nabla} w_j)$$

is diagonal so the Riemann invariants satisfy

$$\underline{r}_i \cdot \underline{\nabla} w_j = 0 \qquad \text{if} \quad i \neq j \ .$$

The w_j are the Riemann invariants (see [9]). For the reduced Euler equations:

$$w_{1,2} = \frac{u}{2} \pm \frac{c}{\gamma - 1} \ , \qquad (\text{where} \quad \lambda_{1,2} = u \pm c) \tag{3.77}$$

are the Riemann invariants.

The method of directional differencing can then be applied to (3.76), and will suffer from neither problem associated with pseudo characteristic variables outlined in note (i) above, but will still be non-conservative. This scheme, as opposed to the simplified directional difference scheme, will be consistent with the Euler equations. Similar schemes using Riemann Invariants but with more complicated discretisations exist, see [11],[12].

4. Test Problems and Results

Three test problems are used, namely, Sod's shock tube problem, which is a theoretical problem with an analytical answer, and two model problems from the gas industry, the flow increase problem and the load rejection problem, the latter of which has experimental results available for comparison. All graphs are in Appendix C.

4.1. Sod's Shock Tube Problem [10]:

This is essentially the Riemann problem for gas in a pipeline. Gas is held in two parts of a tube separated by a membrane, at different states. At t=0 , the membrane is removed and the motion observed. The problem can be modelled by the 3-system or the 2-system, but friction and heat input are taken as zero. The analytical solution for the 2-system case is given in appendix B.

Initial condition:

$\rho = \rho_L$	$\rho = \rho_R$
$u = u_L$	$u = u_R$
$(p = p_L)$	$(p = p_R)$

$x = x_o$

Fig. 3.

In the results presented here, the intial values taken are $\rho_L = p_L = 1.0$, $p_r = 0.1$, $u_L = u_R = 0.0$. The gas is modelled by the adiabatic approximation with $\gamma = 1.3$.

Results: Graphs 1-8 give the distributions of pressure (top) and velocity (bottom) along the tube at a time 0.14s after the membrane is

removed. The numerical solution is found using 51 nodes, and plotted as points. The analytical solution is represented by the line. The time step used is 0.01s except where stated.

Graphs 1-3 show Roe's scheme applied with no limiter (1st order), and with the minmod and Superbee limiters respectively (see [13]). The accuracy of the solution, especially the shock position and the lack of oscillations are to be noted, with the 2nd order schemes improving on the 1st order.

Graphs 4-7 show the results from the Directional Difference scheme with 1st order differences, both in its full version (Graph 4) and in the various levels of simplification mentioned in section 3.3. Smaller time steps are necessary to obtain any solution at all at t = 0.14s for the full version and the $0(u/a)$ version (Graph 5). These solutions are unstable and would break down if run to a later time. Graphs 6 and 7 both used simplified schemes which have no non-diagonal terms (see section 3.3) and are both stable although inaccurate. Comparing Graphs 4 and 5 with 6 and 7 demonstrates well the difficulties that the non-diagonal terms present.

Graphs 8 show the results using the Directional Difference scheme with the Riemann Invariants (characteristic variables) as opposed to the pseudo-characteristic variables, as suggested in section 3.3. The results are not particularly accurate but the solution is stable, as in the diagonal versions of the ordinary Directional Difference scheme (graphs 6 and 7).

4.2. Flow Increase Problem

A pipeline of 500ft, diameter 6in, has gas flowing though initially

at a rate of 10,000 SCFH. The inlet pressure is 14.78psi and the outlet pressure 14.70psi. The flow is increased at the inlet to 20,000 SCFH (at time 0.174s) causing a wave to travel down the pipe. In the simulation the pressure at the outlet is held constant. In this case, the wave is reflected up and down the pipe several times. Comparisons of the pressures and flows obtained by the various schemes are shown. The graphs show the variation in time of the pressures and flows at an upstream and a downstream node each. Solutions use 21 nodes each. Friction is added to the Roe's scheme by projection onto the eigenvectors (see section 3.2).

Graphs 9 (pressures and flows) compares the two schemes at 1st order.

Graphs 10 (pressures and flows) contrasts the use of flux limiters in Roe's scheme and the basic scheme. In this case the pressure rises as the wave passes are sharper in both 2nd order schemes, but the Superbee tends to predict overshoots in pressures and flows.

Graphs 11 (pressures and flows) shows the presence of large oscillations in the solutions obtained by the use of 2nd order differences in the Directional Difference scheme (see section 3.1), even with a small time step in comparison to the other sets of results.

Graph 12 (pressures, using Roe's scheme/minmod limiter) and Graph 13 (flows, using Roe's scheme/Superbee limiter) demonstrate the convergence to a solution as the time step is reduced.

4.3. Load Rejection Problem

A pipeline of length 43.1 miles and diameter 34.75 inches has gas flowing through initially at a rate of 56 MSCFH. The inlet pressure is initially 942.7psi and the outlet pressure 635.7psi. The flow taken

from the outlet is reduced to zero over the next 30s. The flow into the pipe is also reduced between times 430s and 900s by 16.67 MSCFH (see Graph 14 for flows in and out).

The pressures at the inlet and outlet are found and plotted. Experimental results are also available and plotted. The friction term in Roe's scheme is added by projection onto eigenvectors, as a preliminary run showed addition of a point value to be inappropriate (see section 3.2).

Graphs 15 demonstrate that the isothermal model gives results closer to the experimental results than an adiabatic model with $\gamma = 1.3$; subsequently, the isothermal model is taken.

Graphs 16 show results obtained by the various approximations to the Directional Difference scheme when the gas velocity is small and the non-diagonal terms in the scheme are relatively unimportant. Note the similarity of the full version of the scheme to the simplifications which include only terms of $O(u/a)$ and $O(1)$. The scheme which omits only non-diagonal terms omits some, but not all terms of $O(u/a)$, which explains its inaccuracy. See section 3.3.

Graphs 17 (Roe's scheme), Graphs 18 (Directional Difference scheme) and Graphs 19 (Directional Difference scheme using Riemann Invariants) scheme, show the convergence of the schemes on this problem using smaller time steps with a fixed ratio of time and space steps.

Graphs 20 demonstrate the similarity of the results obtained by the three schemes at the smallest time step. The three are expected to be similar as the gas velocity is small. The Roe scheme may exhibit greater accuracy due to the treatment of the source terms, as has been mentioned. The inaccuracy at large time steps of the two Directional

Difference Schemes could be due to implementation of boundary conditions or source terms. It is strongly suspected that the treatment of source terms is responsible, by analogy with a variant of Roe's method with a different treatment of friction which shows comparable convergence behaviour to the Directional Difference method.

5. Concluding Remarks

In chapter 3, section 3, it was noted that Roe's scheme was expected to produce better results than the Directional Difference scheme. Roe's scheme is conservative, and this leads to accuracy in the shock position in problem 4.1. The Directional Difference scheme suffers from using pseudo-characteristic variables which cannot be differenced in an upwind manner consistently everywhere in the scheme, and that this presents severe difficulties, especially at high gas speeds, (e.g. at pipebreaks), is again demonstrated in problem 4.1. The more stable behaviour of less accurate versions of this scheme which neglect the terms differenced in the wrong direction, can be improved upon by the use of proper characteristic variables as suggestion in section 3.3. However, the existence of easily calculable characteristic variables for systems of equations which model the gas thermodynamics in a different manner is not certain.

Roe's scheme upwinds correctly by the use of an approximate linearized solution in each cell. The flux differences are decomposed onto eigenvectors associated with each wave component of the motion, and these eigenvectors can also be used in the implementation of boundary conditions and the addition of friction and other right-hand side terms. Second order methods can be used by Roe's scheme which are more refined than the use of second order spatial derivatives in the Directional Difference scheme.

In conclusion, whilst the two schemes have certain similarities of approach and give similar solutions at low gas speeds, the theoretical advantages of Roe's shceme and its better ability to produce good

results with rapid transients and high gas speeds would seem preferable. The questions of implementation of boundary conditions and friction terms are still quite open and more work may be needed to find a good resolution of these questions for the particular problems of gas pipeline modelling.

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Appendix A

Deriving the Directional Difference Equations from the Characteristic Form of the Euler Equations

Here, equations (3.3) are used:

$$c^2 \rho_t = p_t \qquad \text{(A.1a)}$$

$$c^2 \rho_x = p_x \qquad \text{(A.2b)}$$

From (3.2),

$$c^2 = \frac{\gamma p}{\rho} \,, \qquad \text{(3.2)}$$

the following partial derivatives of c can also be derived:

$$2cc_t = \frac{\gamma p_t}{\rho} - \frac{\gamma p}{\rho^2} \rho_t$$

$$= \frac{\gamma}{\rho^2} \left(\rho p_t - \frac{p p_t}{c^2}\right)$$

$$= \frac{\gamma p_t}{\rho} \left(1 - \frac{1}{\gamma}\right)$$

$$c_t = \left[\frac{\gamma-1}{2\rho c}\right] p_t \qquad \text{(A.2)}$$

and (from A.1a, A.2)

$$(\rho c)_t = \rho c_t + c \rho_t$$

$$= \frac{\gamma-1}{2c} p_t + \frac{1}{c} p_t$$

so

$$(\rho c)_t = \left[\frac{\gamma+1}{2c}\right] p_t \quad . \tag{A.3a}$$

and similarly,

$$(\rho c)_x = \left[\frac{\gamma+1}{2c}\right] p_x \quad . \tag{A.3b}$$

Now, the Euler equations have been transformed into the equations (3.7):

$$(p_t + \rho c u_t) + (u + c)(p_x + \rho c u_x) + F = 0 \tag{A.4a}$$

$$(p_t - \rho c u_t) + (u - c)(p_x - \rho c u_x) - F = 0 \tag{A.4b}$$

where

$$F = 2f\rho cu|u|/d \quad . \tag{A.5}$$

Defining variables α, β as in (3.8):

$$\alpha = p + \rho cu \tag{A.6a}$$

$$\beta = p - pcu \tag{A.6b}$$

allows (A.4a) to be written as

$$[\alpha_t - (\rho c)_t u] + (u + c)[\alpha_x - (\rho c)_x u] + F = 0$$

Using (A.3a)

$$\alpha_t - u\frac{(\gamma+1)}{2c} p_t = - (u + c)[\alpha_x - (\rho c)_x u] - F \quad .$$

and using the first equation (component) of (3.4), an equation for the time derivative of α alone is found:

$$\alpha_t = \left[\frac{-u(\gamma+1)}{2c}\right](up_x + \rho c^2 u_x) - (u+c)\,[\alpha_x - (\rho c)_x u] - F \ . \qquad (A.7)$$

With the definitions of α,β (A.6) and also with (A.3b), the following hold:

$$p_x = \frac{1}{2}(\alpha_x + \beta_x)$$

$$(\rho c)_x = \left[\frac{\gamma+1}{2c}\right] \frac{\alpha_x + \beta_x}{2}$$

$$\rho c u_x = \frac{\alpha_x - \beta_x}{2} - (\rho c)_x u$$

$$= \frac{\alpha_x - \beta_x}{2} - \frac{u(\gamma+1)}{2c}\left[\frac{\alpha_x + \beta_x}{2}\right]$$

Substituting these into (A.7) and collecting the terms in α_x,β_x, gives

$$\alpha_t = \left[-(u+c) + \frac{u^2(\gamma+1)^2}{8c}\right]\alpha_x + \frac{u(\gamma+1)}{2}\left[1 + \frac{u(\gamma+1)}{4c}\right]\beta_x - F \ . \qquad (A.8a)$$

Using a similar method, it can be found that

$$\beta_t = \left[-(u-c) + \frac{u^2(\gamma+1)^2}{8c}\right]\beta_x + \frac{u(\gamma+1)}{2}\left[1 - \frac{u(\gamma+1)}{4c}\right]\alpha_x + F \ . \qquad (A.8b)$$

Appendix B

The Exact Solution to Test Problem 1.

The first test problem is just the Riemann problem for the Euler equations in the adiabatic form given in chapter 2 without friction, that is,

$$\underline{u}_t + \underline{f}(\underline{u})_x = \underline{0}$$

where

$$\underline{u} = (\rho, \rho u)^T$$

$$\underline{f} = (\rho u, p+\rho u^2)^T$$

and

$$p = k\rho^{\gamma} \qquad \text{(B.1)}$$

where the initial data consists of two constant states either side of a position $x = x_o$ (denoted by L and R), that is,

$$\underline{u}(x,0) = \begin{cases} \underline{u}_L, & x < x_o \\ \underline{u}_R, & x > x_o \end{cases}.$$

The values for the problem considered in chapter 4 are $\rho_L = p_L = 1.0$, $p_R = 0.1$, $u_L = u_R = 0.0$. The other densities can be found by using equation (B.1), with γ taken as 1.3.

The exact solution in $t > 0$ to this problem can be found and has the following form.

The left-hand state $\underline{u}_L$ is connected to an intermediate state, $\underline{u}_o$, say, by an expansion in the (u-a)-field, that is, the solution

$\underline{u}(x,t)$ in the expansion satisfies

$$\lambda_2(\underline{u}) = (x-x_o)/t$$

$$\lambda_2(\underline{u}_L) \leq \lambda_2(\underline{u}) \leq \lambda_2(\underline{u}_o)$$

$$w_1(\underline{u}) = w_1(\underline{u}_L)$$

where the wavespeed $\lambda_2 = u-c$, the Riemann Invariant w_1, given by $w_1 = \frac{1}{2}u + c/(\gamma-1)$, and the sound speed is c as given in chapter 3 above (equations (3.19a), (3.77), (3.2)).

Also, the intermediate state $\underline{u}_o$ is connected to the right-hand state $\underline{u}_R$ by a shock, that is, the solution jumps between $\underline{u}_o$ and $\underline{u}_R$ at a point moving with speed s, and where jump conditions hold:

$$s = [\underline{f}(\underline{u})]/[\underline{u}]$$

where $[.] = (.)_R - (.)_o$.

These conditions allow the full solution at a time $t > 0$ to be calculated; full details on these conditions and for methods of obtaining the solution will be presented elsewhere. For these initial conditions, then, the solution is, in terms of $\xi = (x-x_o)/t$,

$$\underline{u}(x,t) = \underline{u}(\xi) = \begin{cases} \underline{u}_L, & \xi \leq \lambda_2(\underline{u}_L) \\ \underline{u}_E, & \lambda_2(\underline{u}_L) < \xi < \lambda_2(\underline{u}_o) \\ \underline{u}_o, & \lambda_2(\underline{u}_o) \leq \xi < s \\ \underline{u}_R, & \xi > s \end{cases}$$

where $\underline{u}_L, \underline{u}_R$ are as given initially, $\underline{u}_o = (0.428,\ 0.389)^T$, $\lambda_2(\underline{u}_L) = -1.140$, $\lambda_2(\underline{u}_o) = -0.010$, $s = 1.505$, and the states in the expansion are given by $\underline{u}_E = (\rho_E, \rho_E u_E)$, where

$$\rho_E(\xi) = \left[\frac{(w_1(\underline{u}_L) - \xi).(\frac{\gamma-1}{2})}{\left[\frac{\gamma+1}{2}\right] . \sqrt{\gamma}}\right]^{\left[\frac{2}{\gamma-1}\right]}$$

$$= (0.1144(7.601 - \xi))^{6.667}$$

$$u_E(\xi) = u_L + \frac{(\xi-\lambda_2(\underline{u}_L))}{(\lambda_2(\underline{u}_o)-\lambda_2(\underline{u}_L))}(u_o - u_L)$$

$$= 0.803(\xi + 1.140) .$$

For the solutions plotted, $x_o = 0.5$ and $t = 0.14$. All answers here are to 3 decimal places.

Appendix C

Graphs of Results

TEST PROBLEM 1 - RESULTS

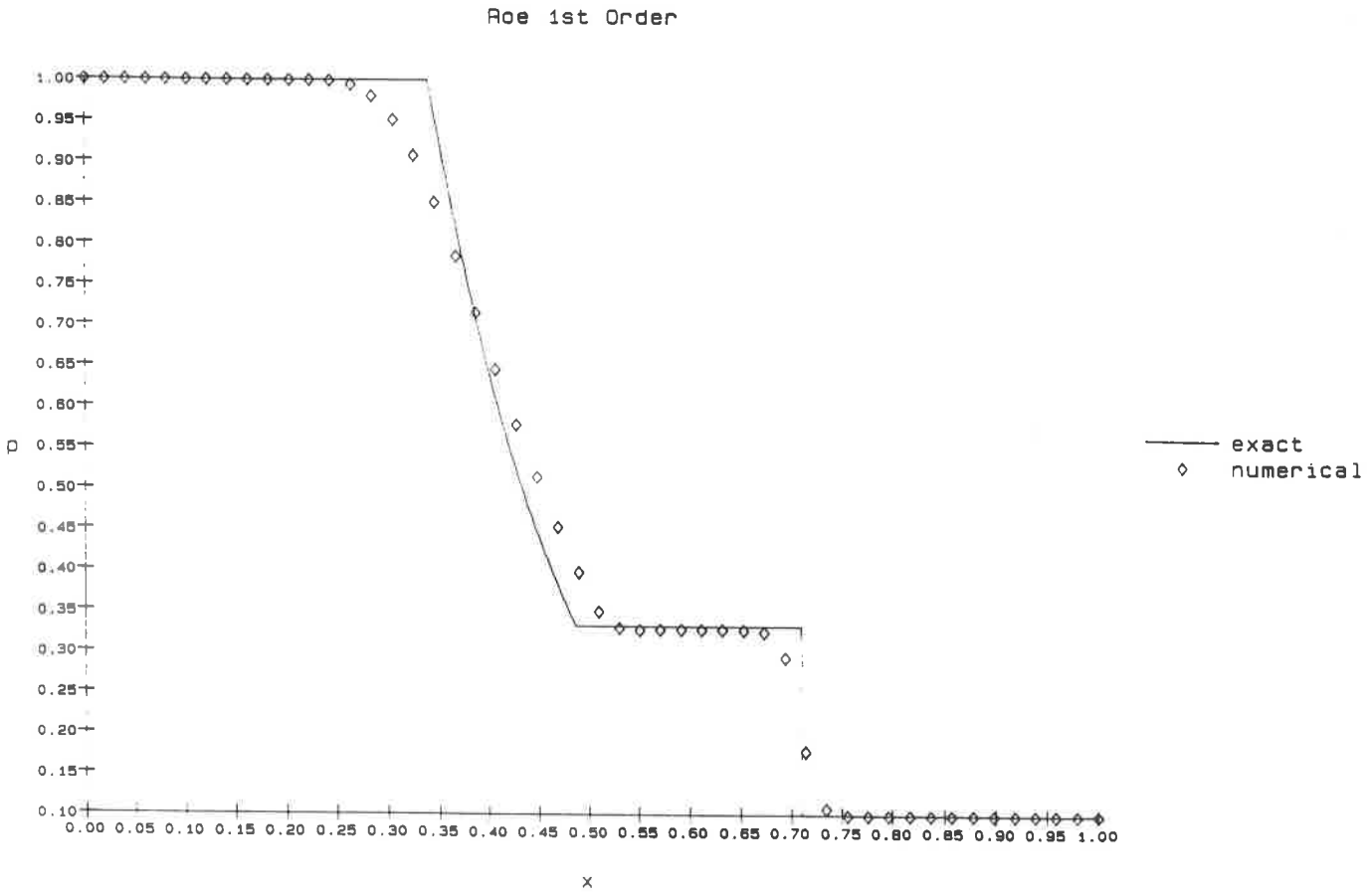
Graphs of pressure vs. x and velocity vs. x at time 0.14s

Time step 0.01s (unless stated).

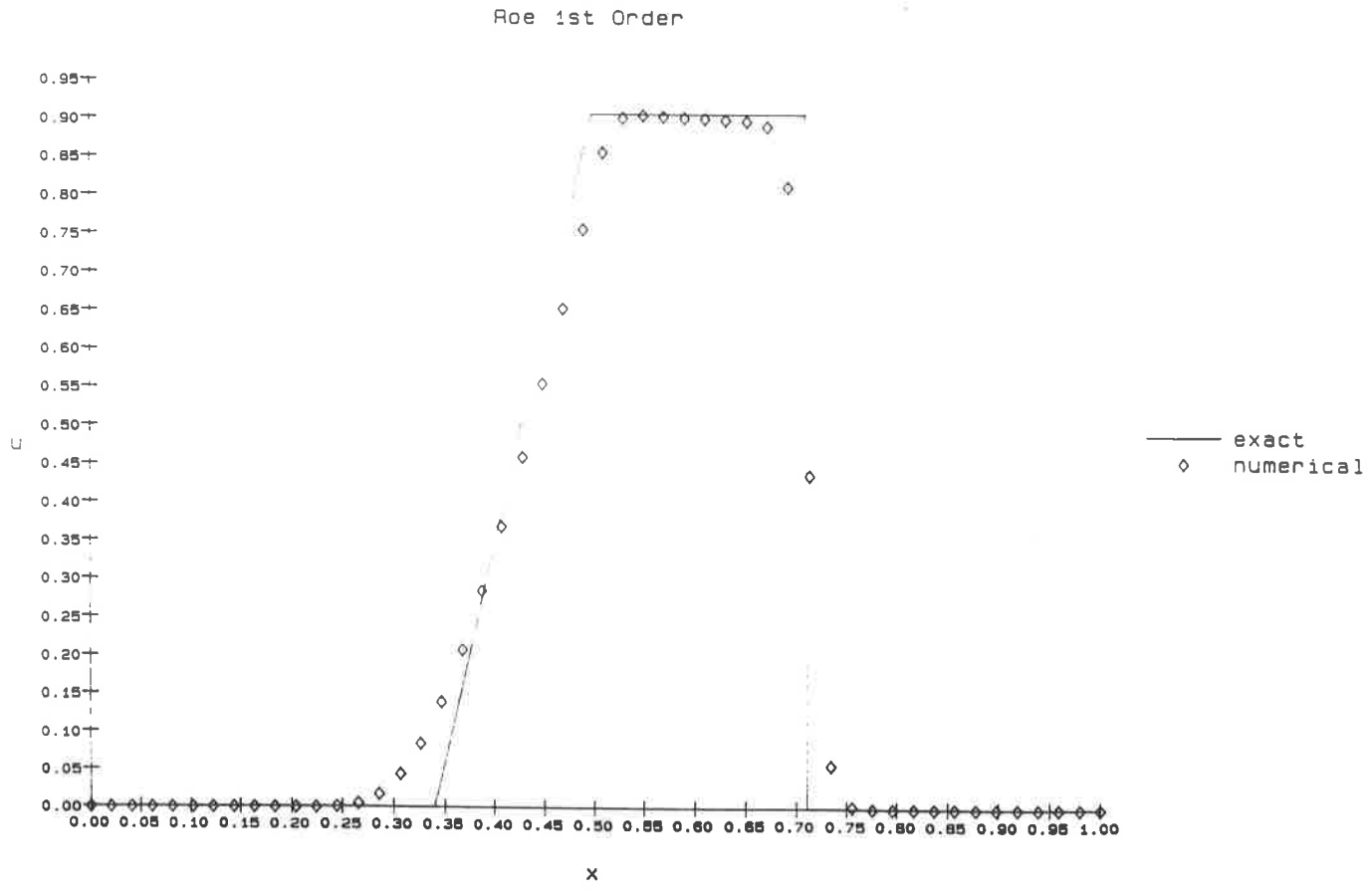
50 nodes used.

Analytical and numerical results.

GRAPH_1A



GRAPH_1B



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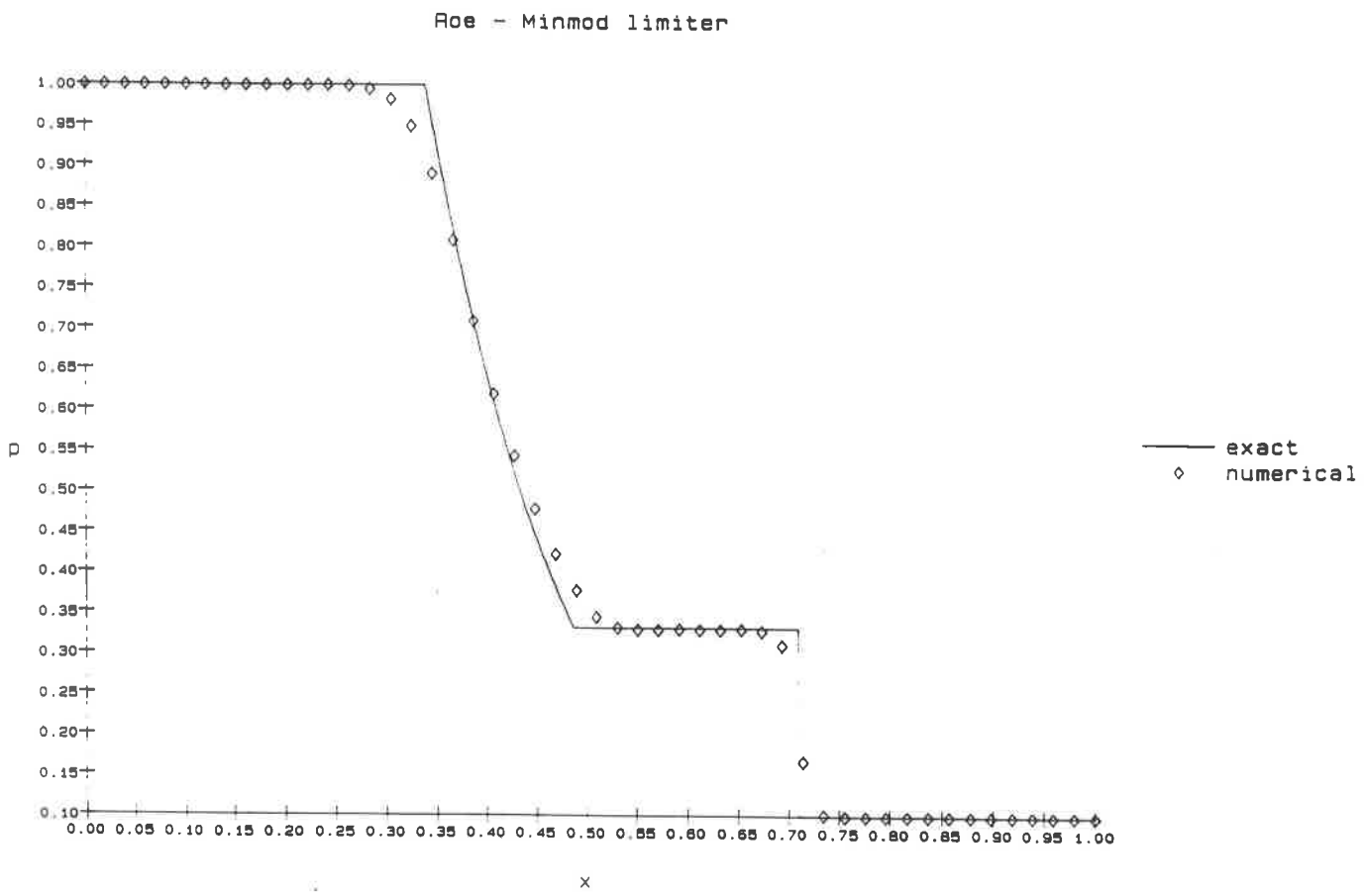
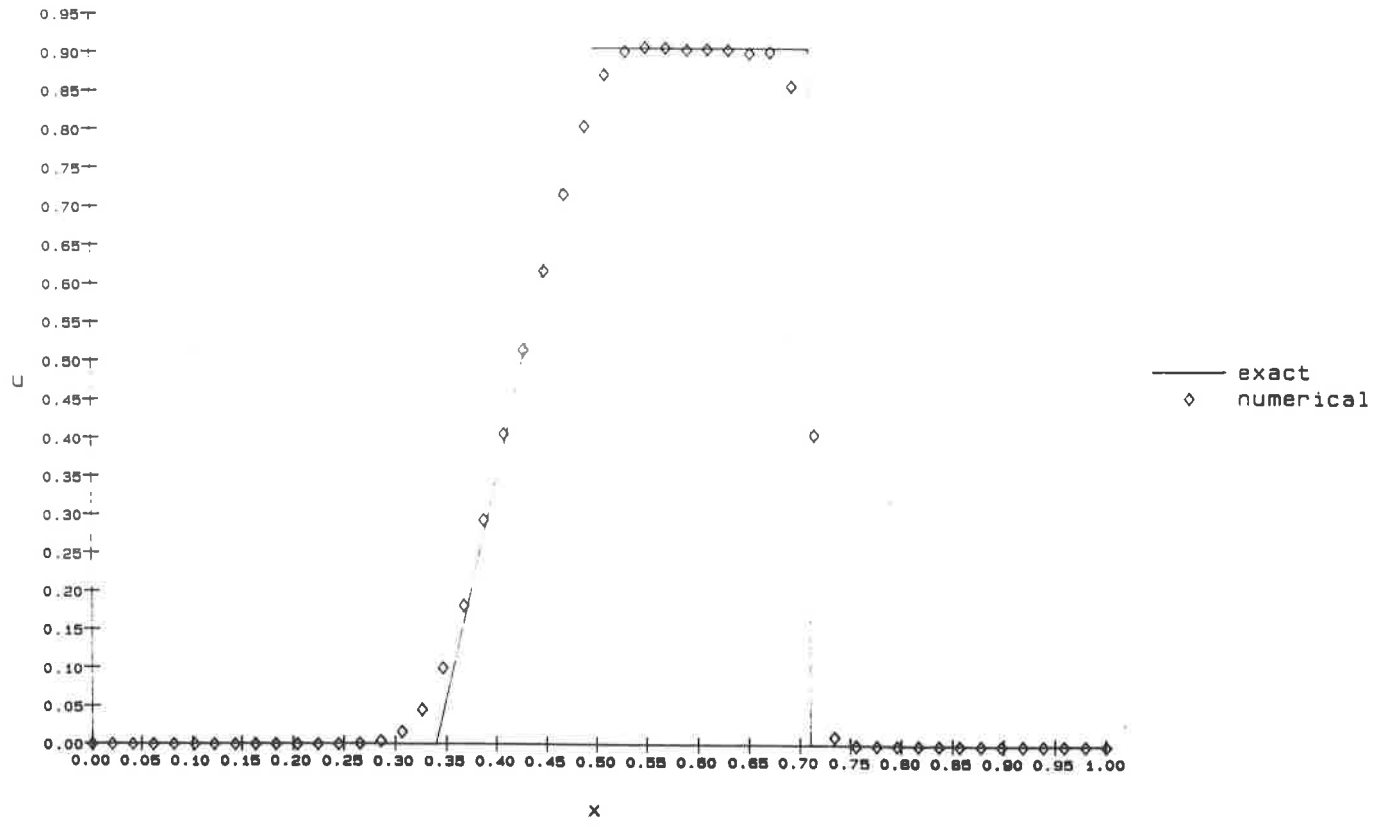


GRAPH_2B



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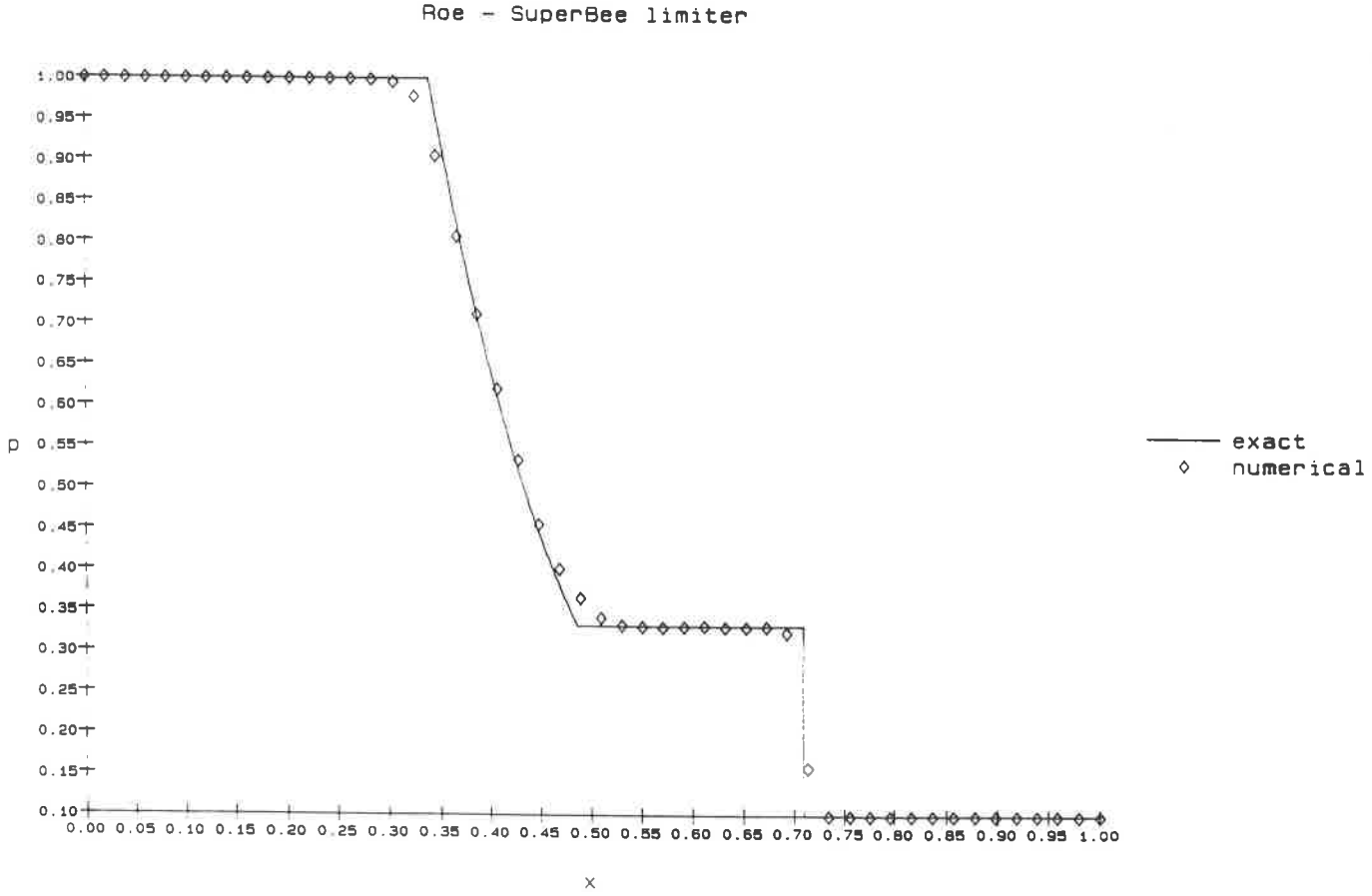
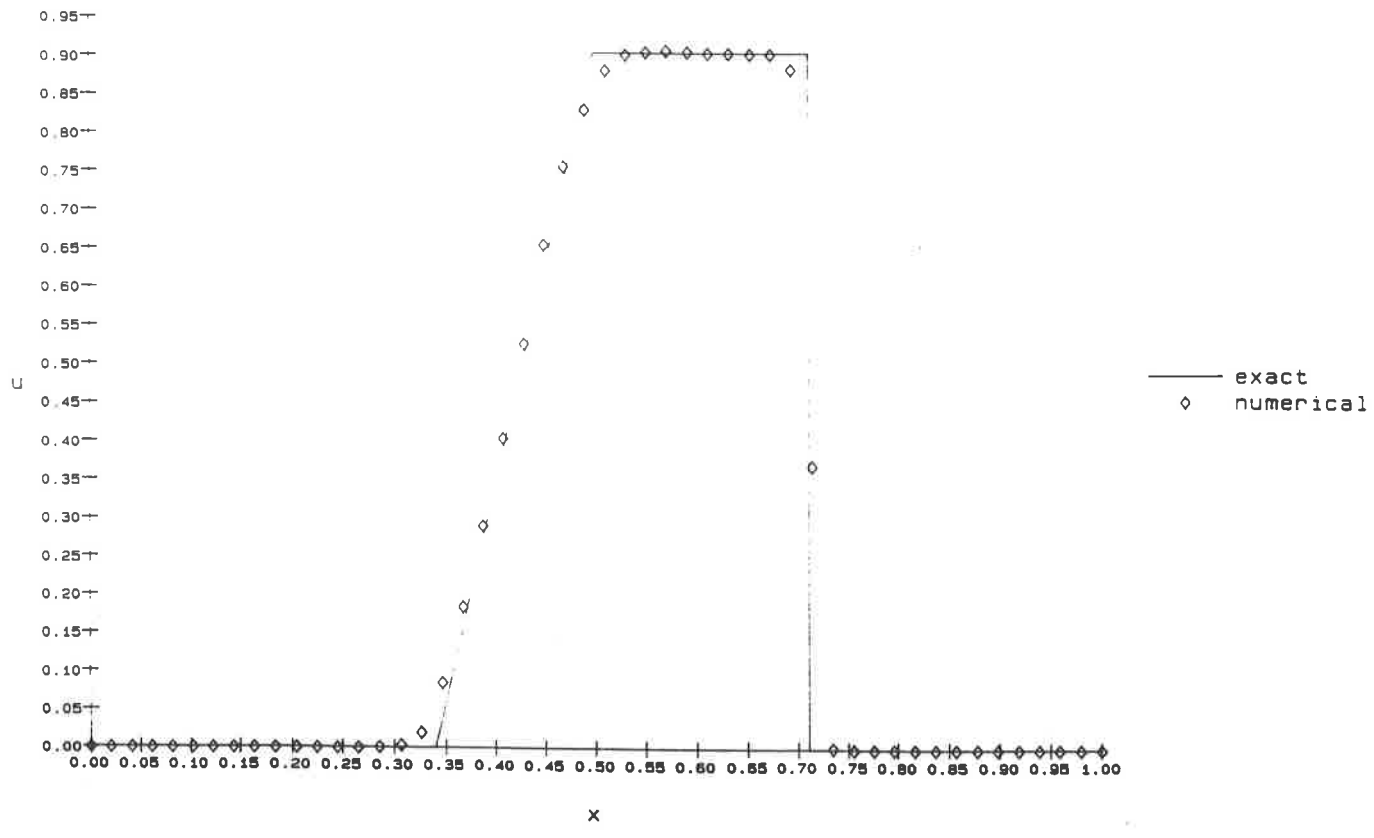
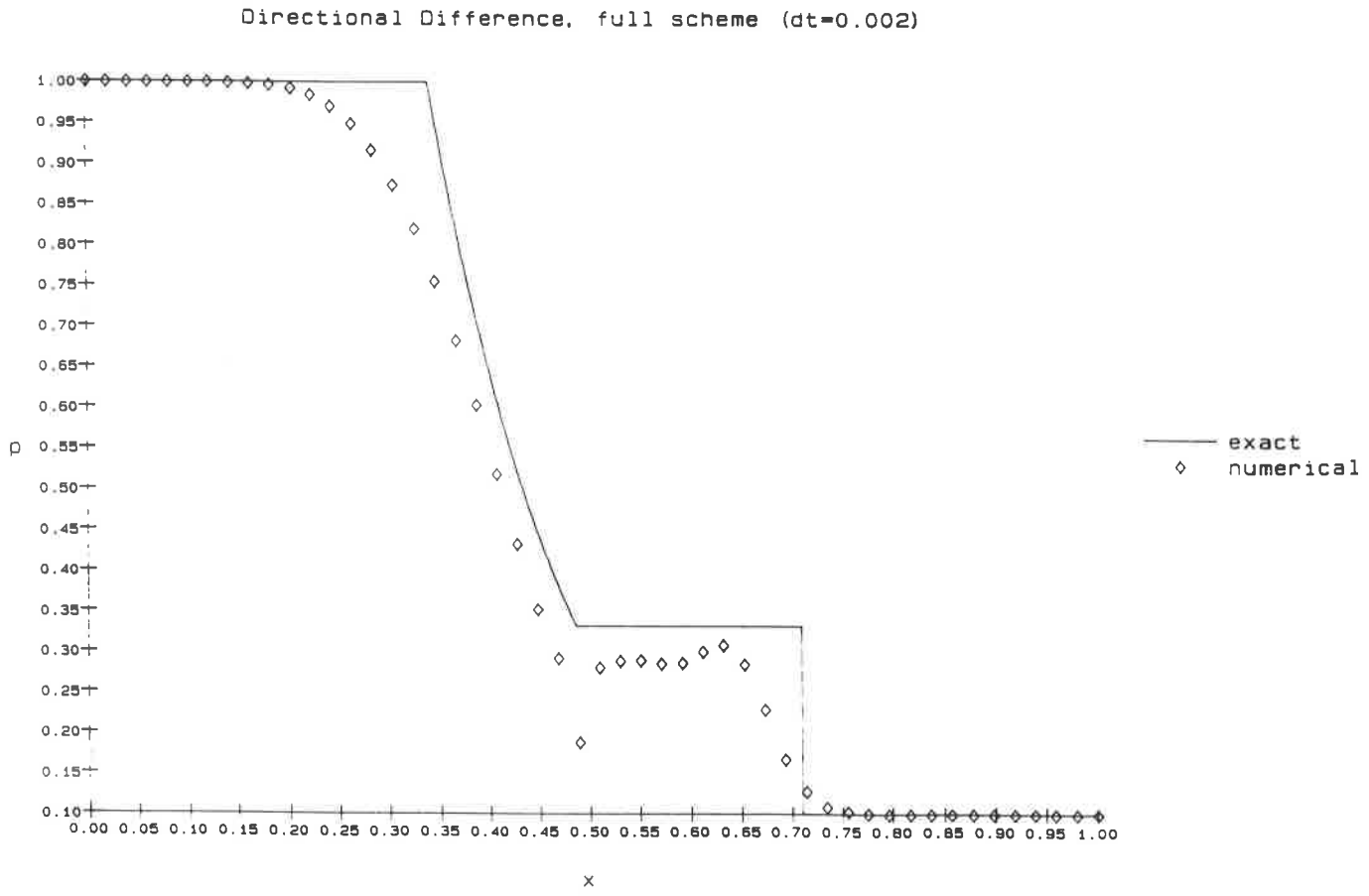


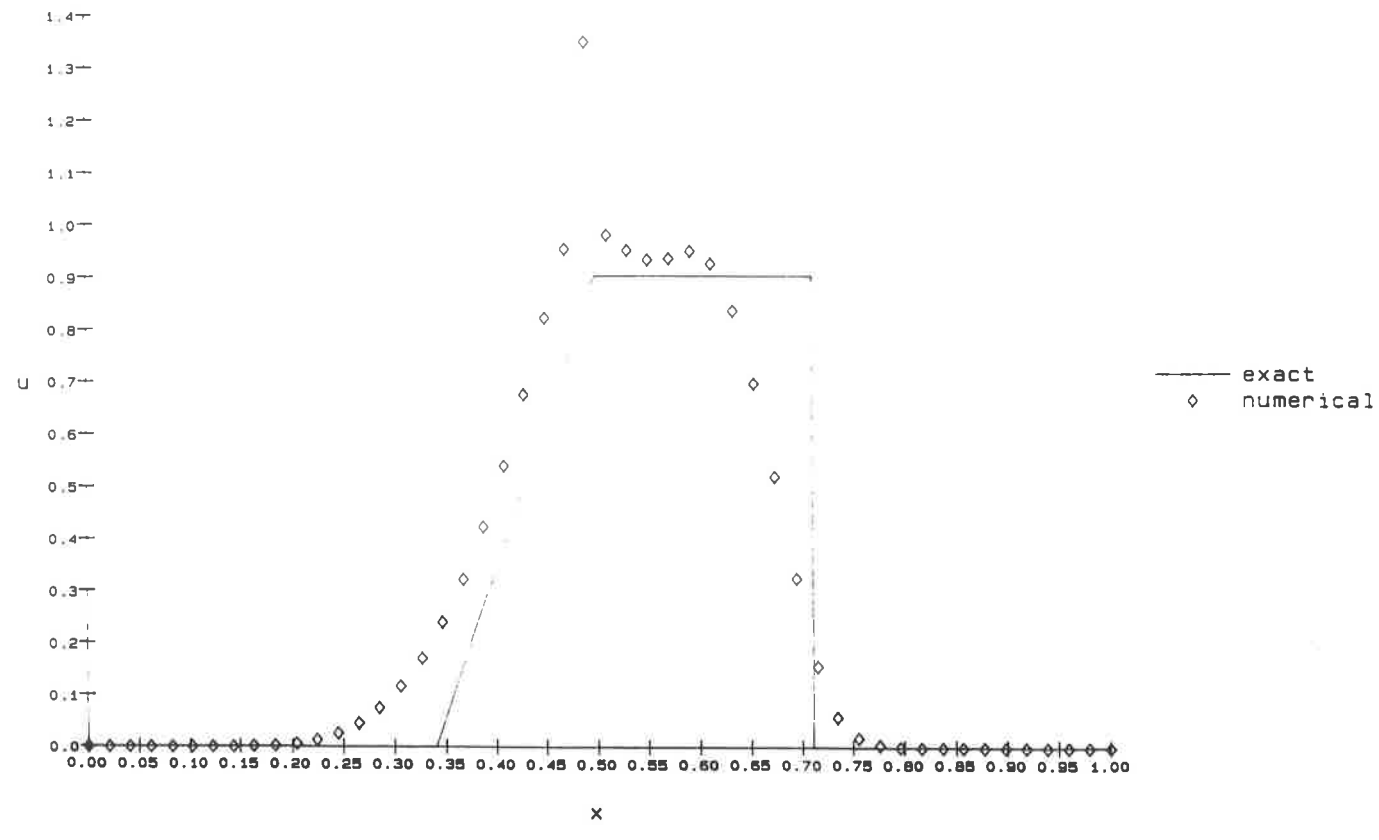
GRAPH_3B



GRAPH_4A



GRAPH_4B



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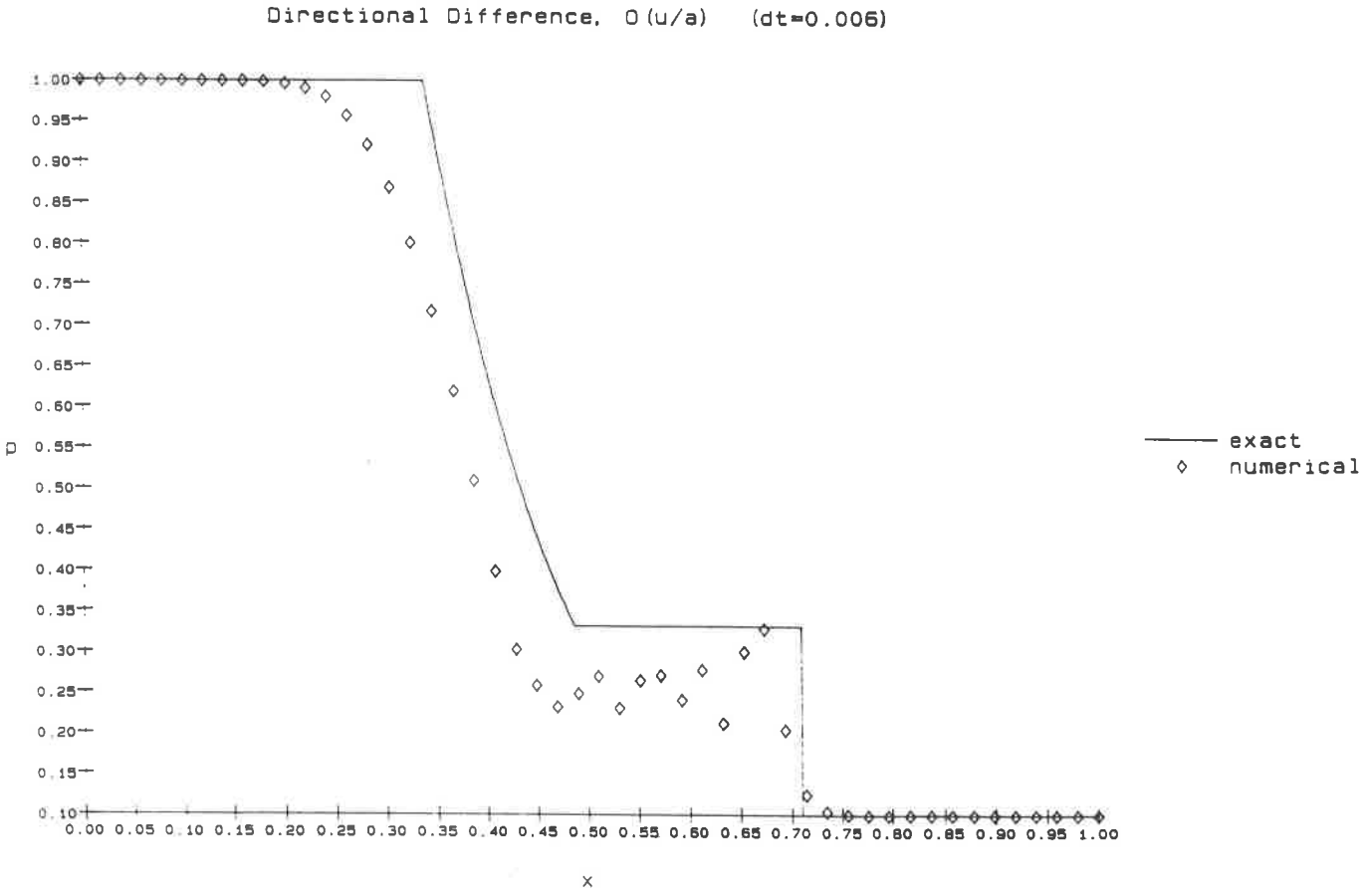
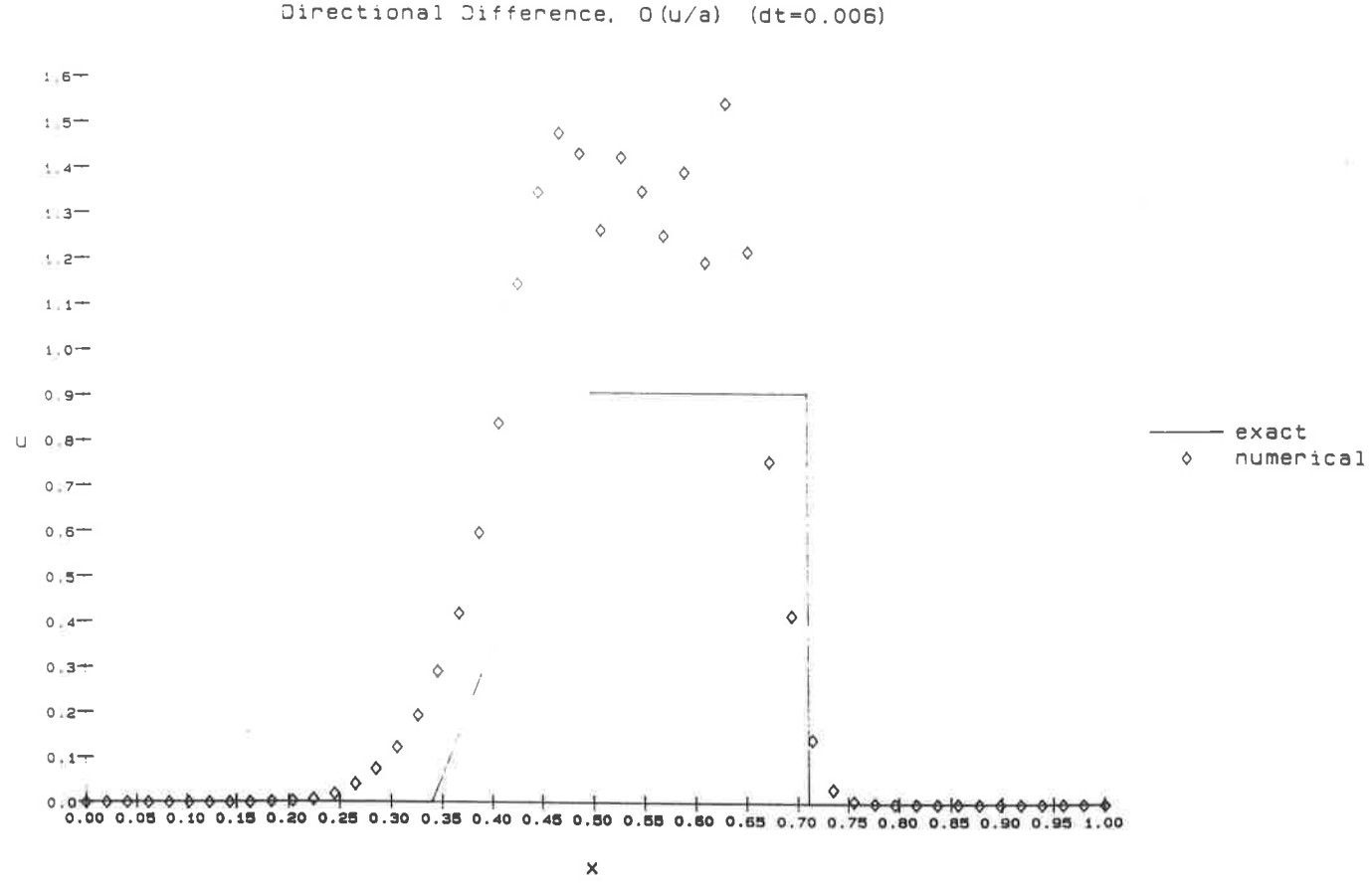


GRAPH_5B



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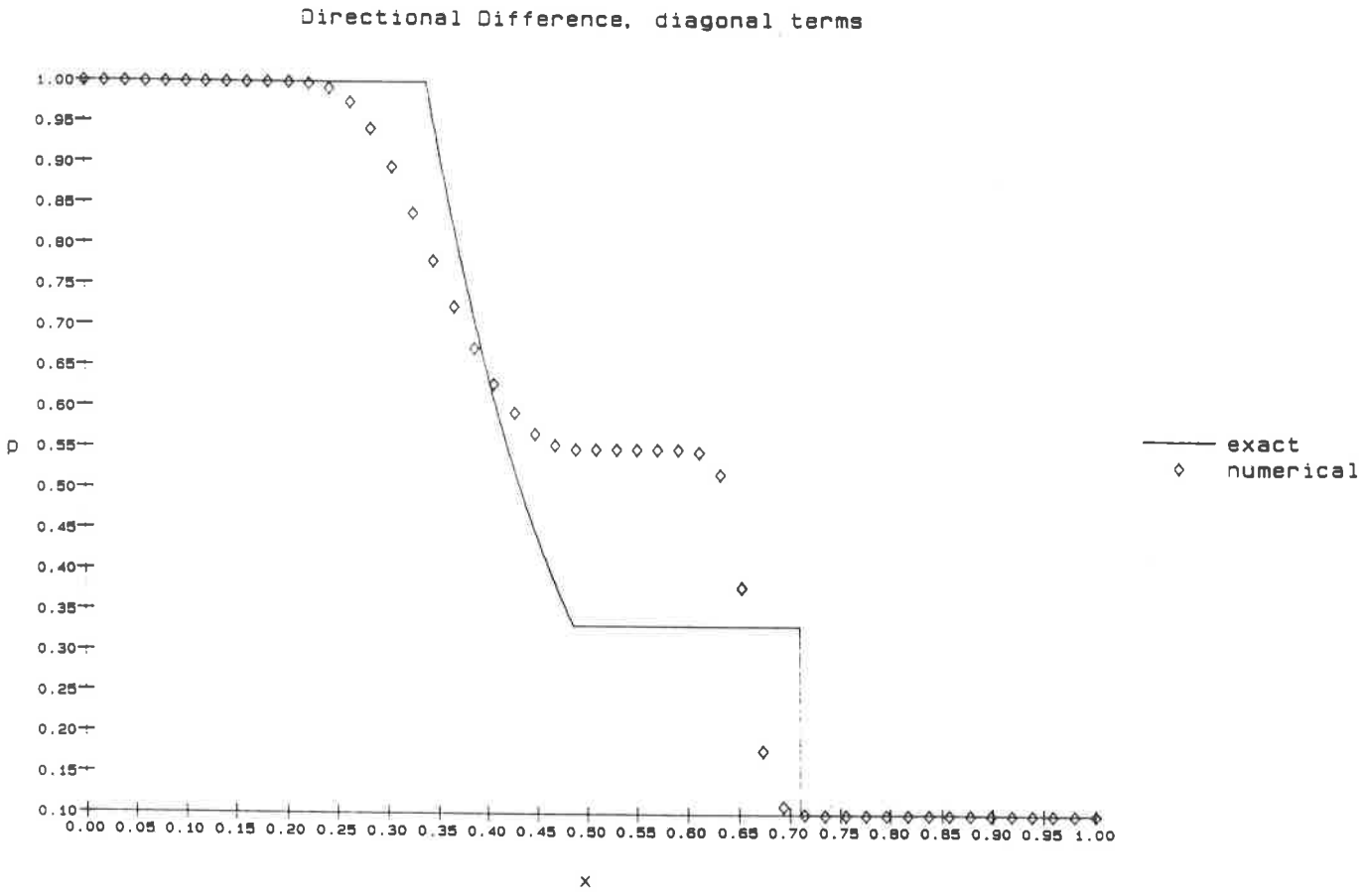

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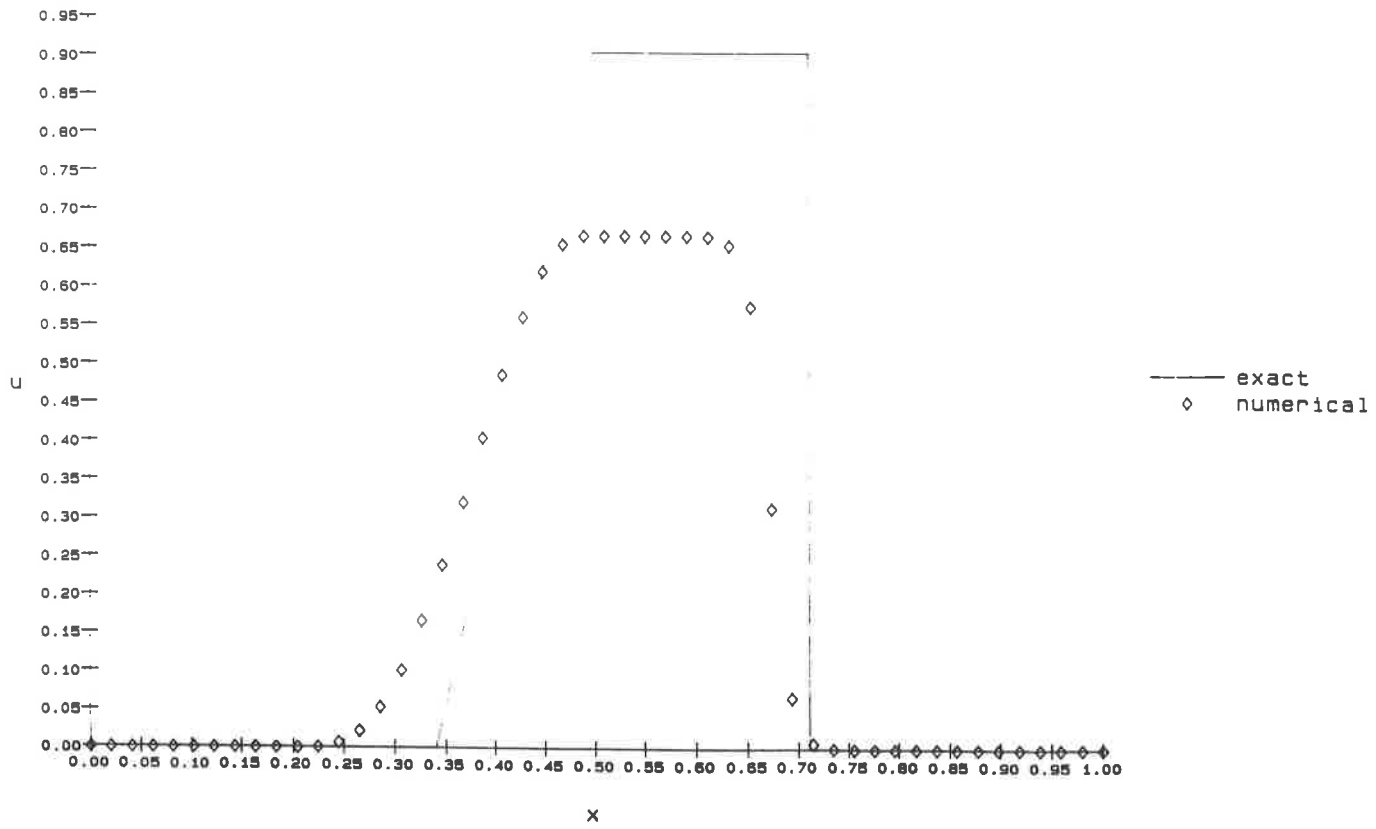
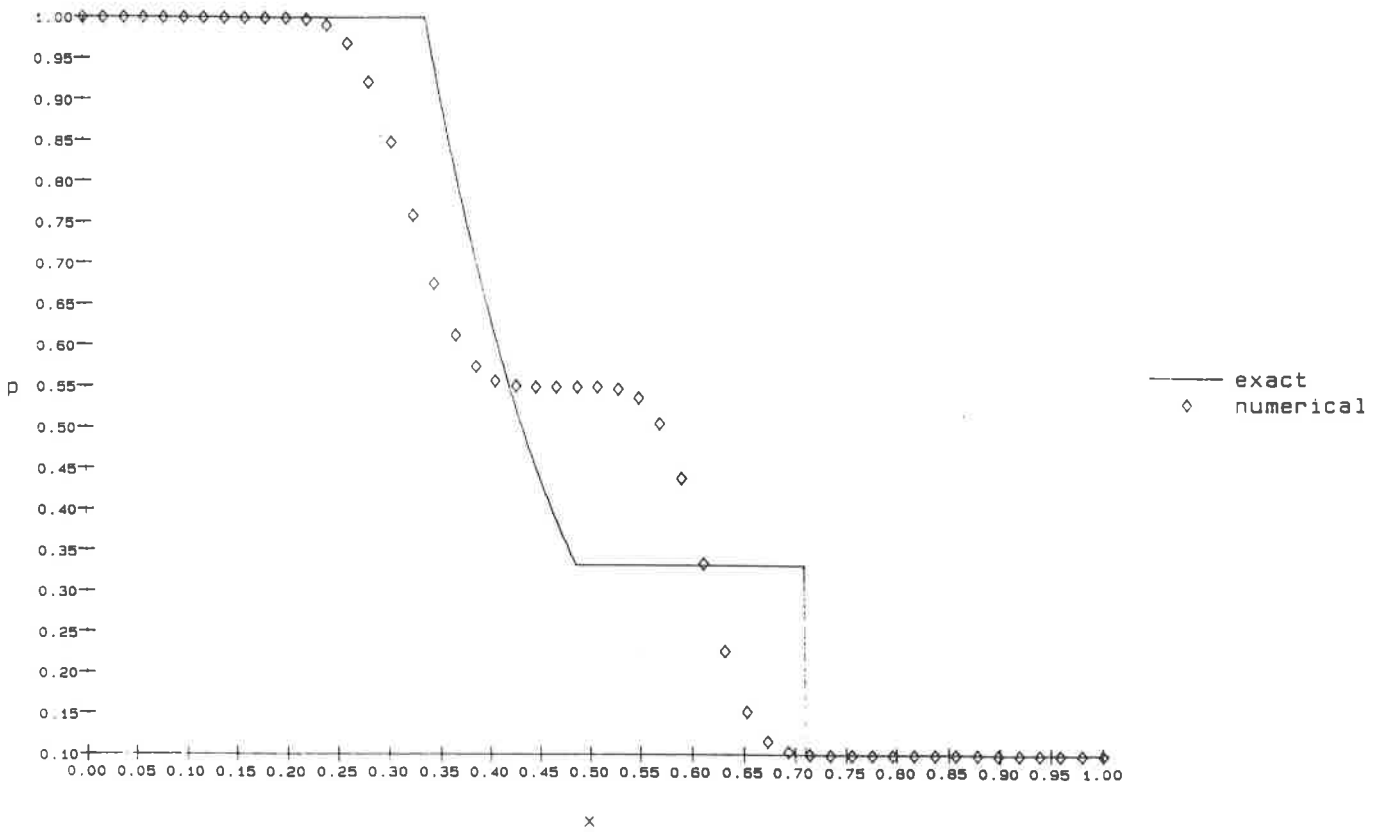
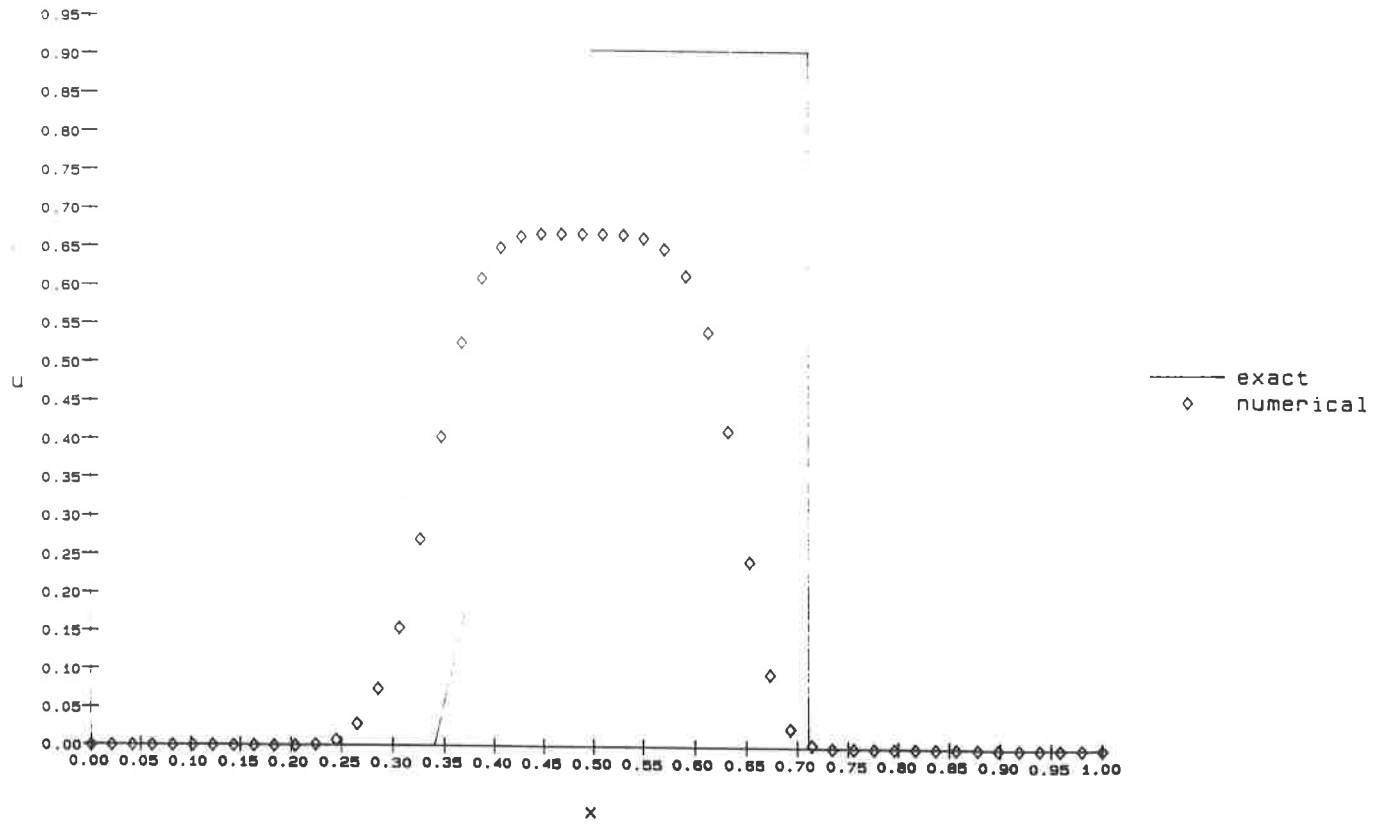


GRAPH_7A



GRAPH_7B



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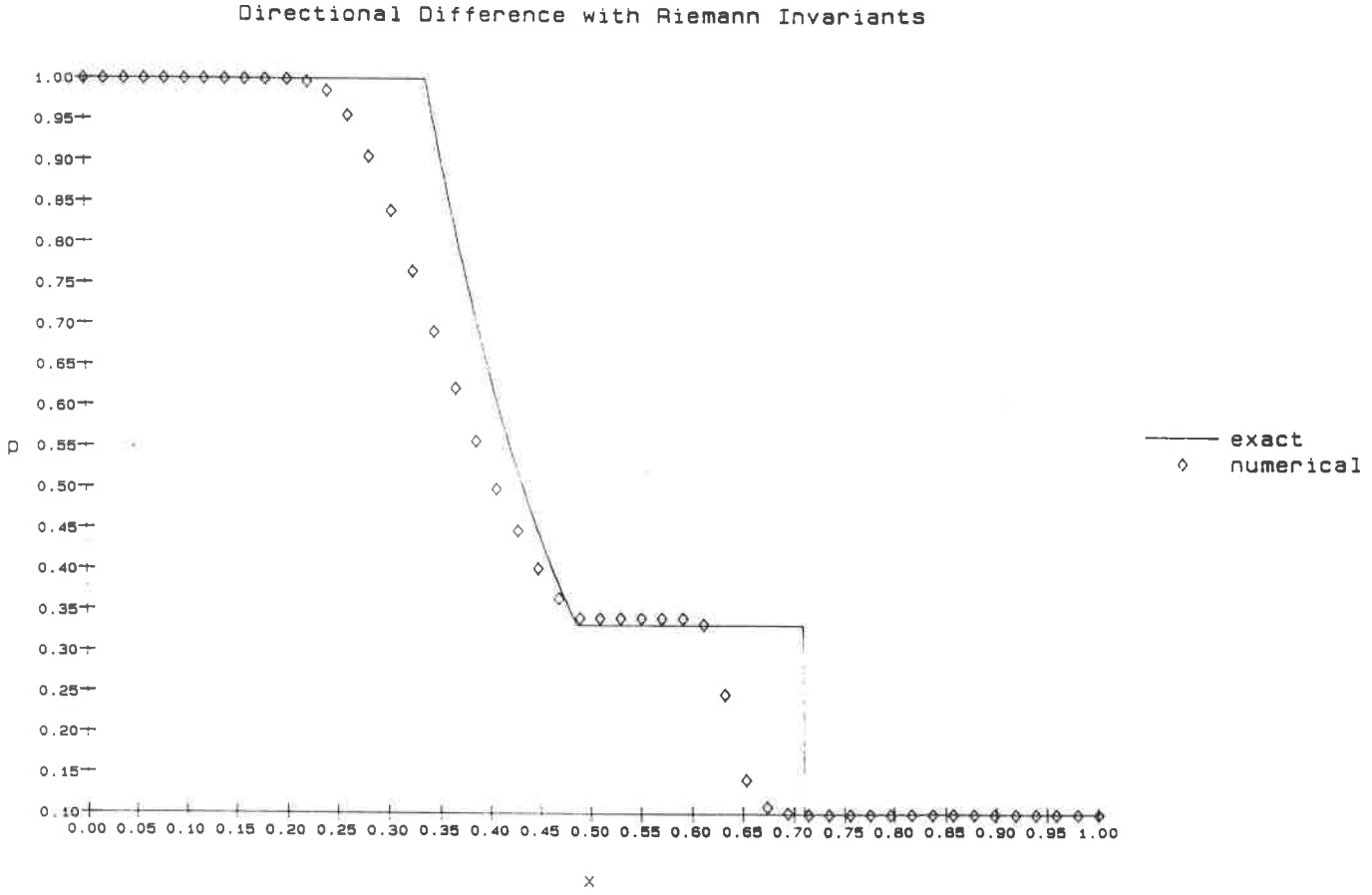
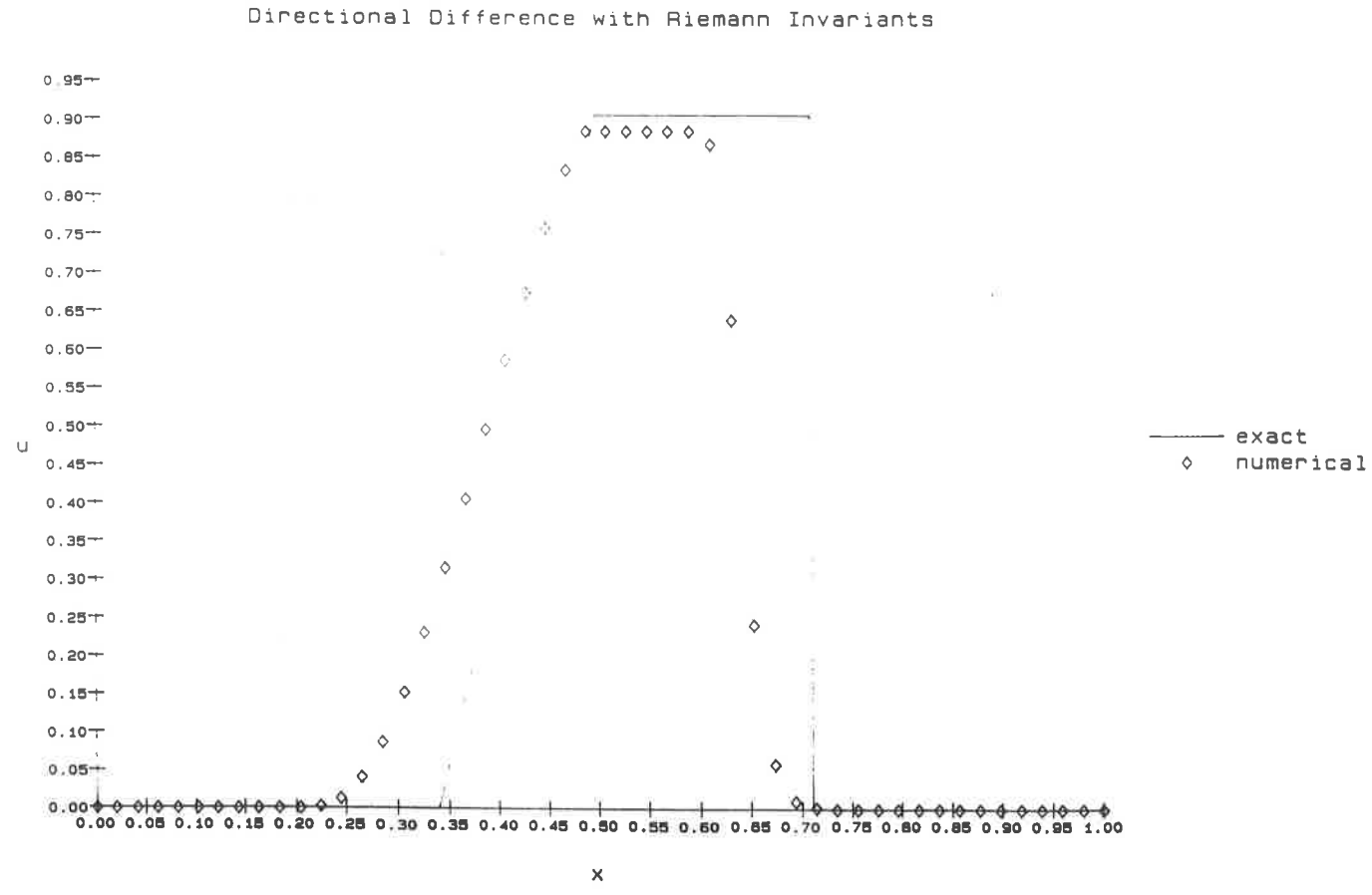


GRAPH_8B



TEST PROBLEM 2 - RESULTS

Graphs of pressure vs. time and velocity vs. time.

One set of each from an upstream and a downstream node.

Time step 0.01 (unless stated).

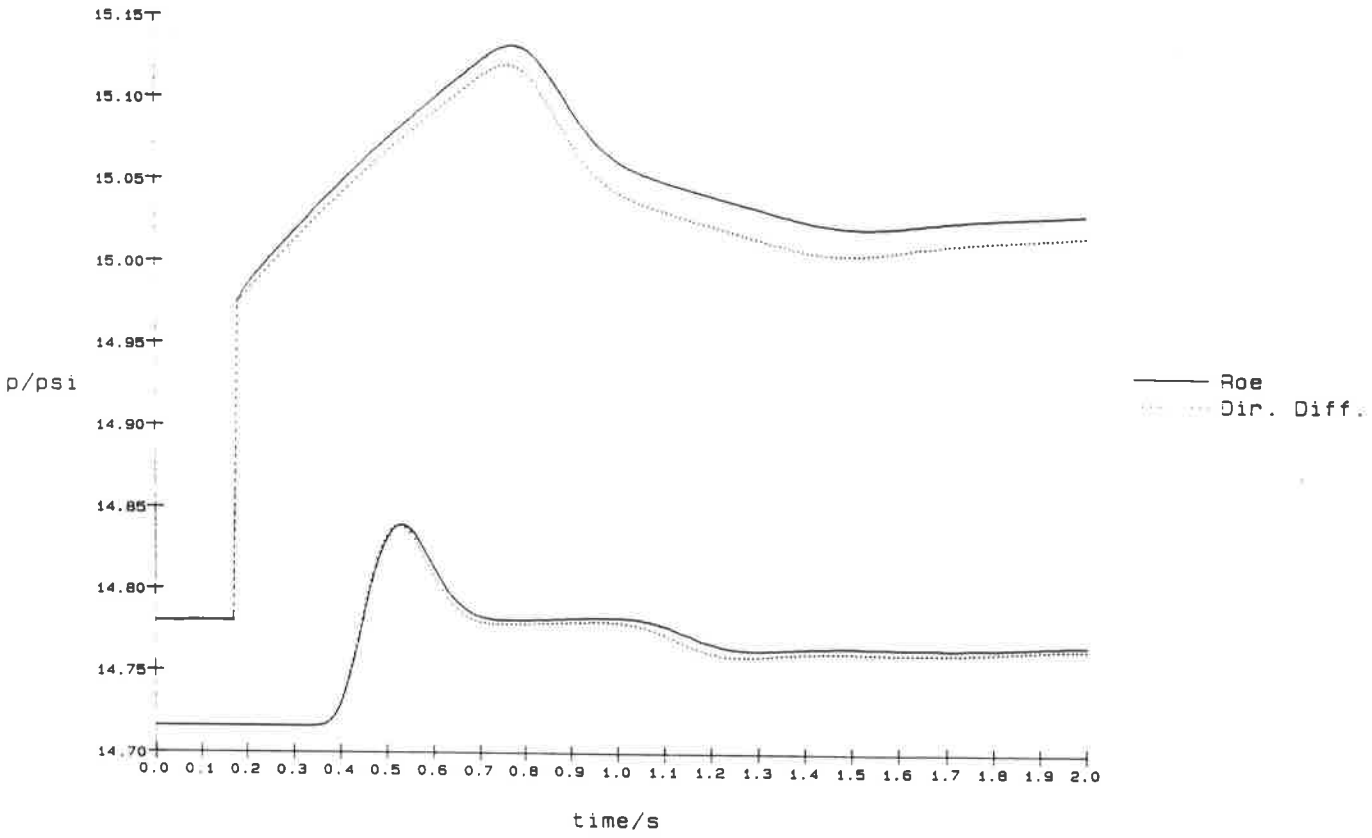
21 nodes used.

The pressure at nodes 1 and 17 is plotted.

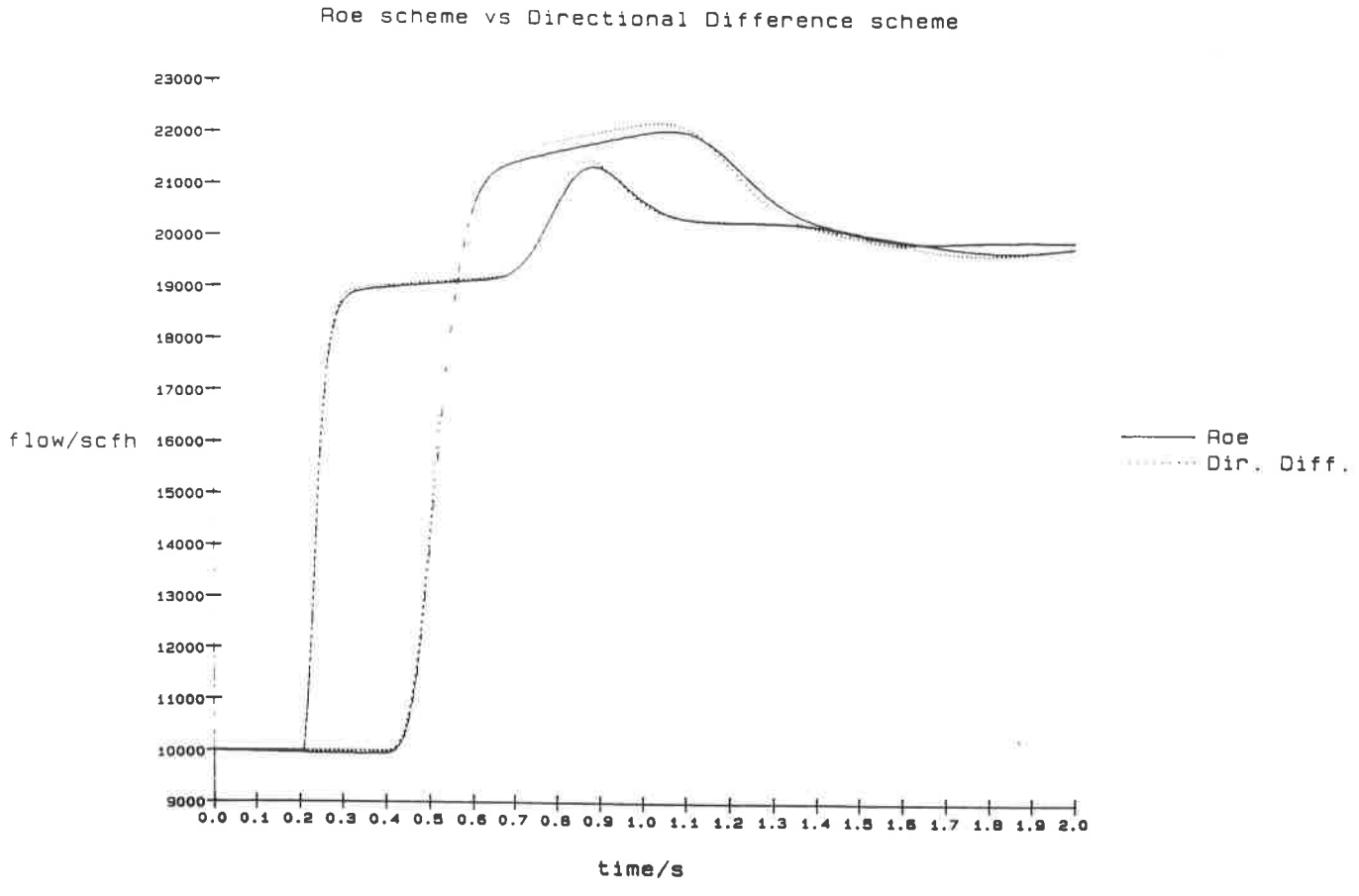
The flow at nodes 5 and 21 is plotted.

In each case, the upstream graph (low node number) responds to the flow increase before the downstream graph.

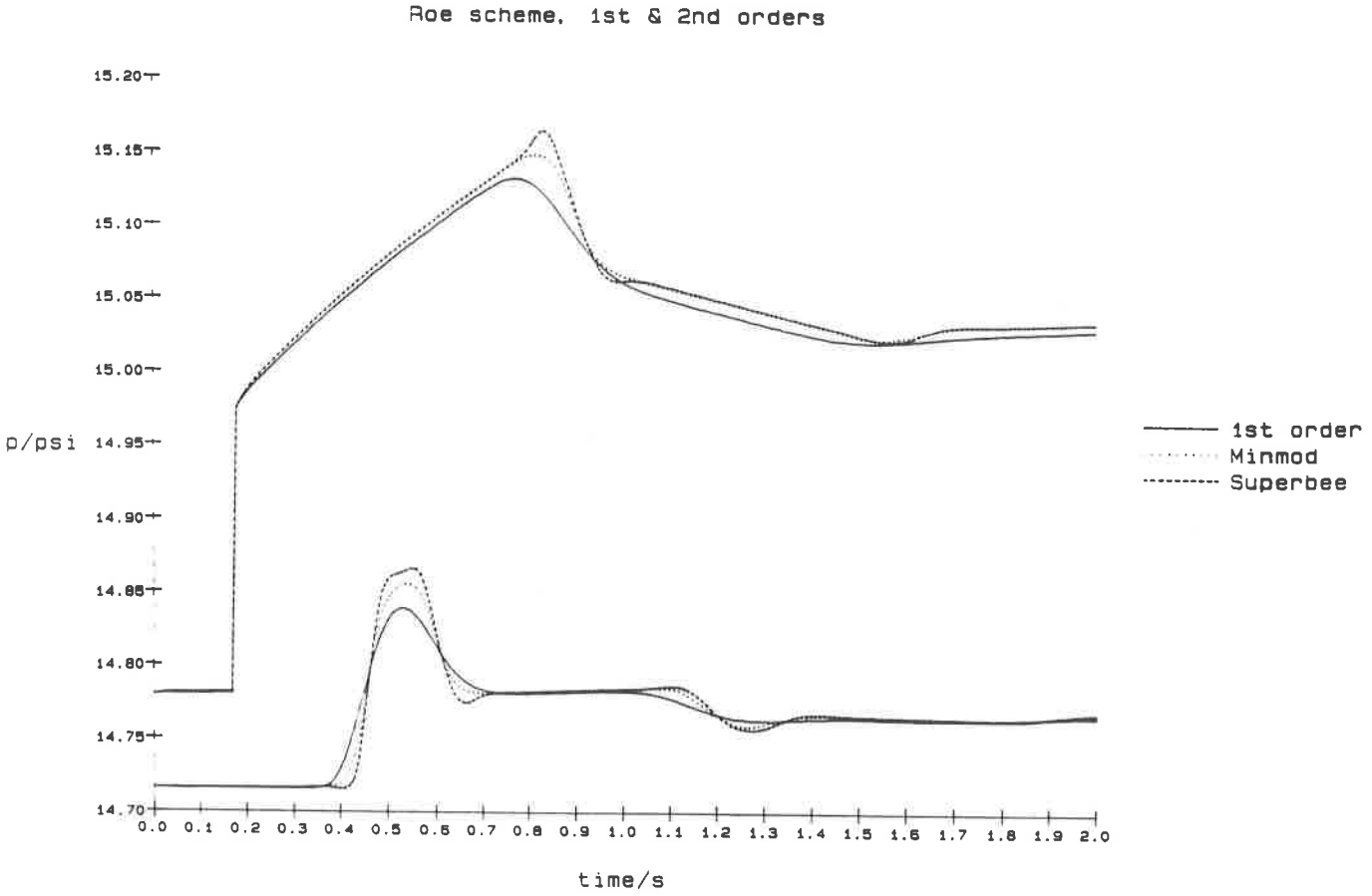
GRAPH_9A



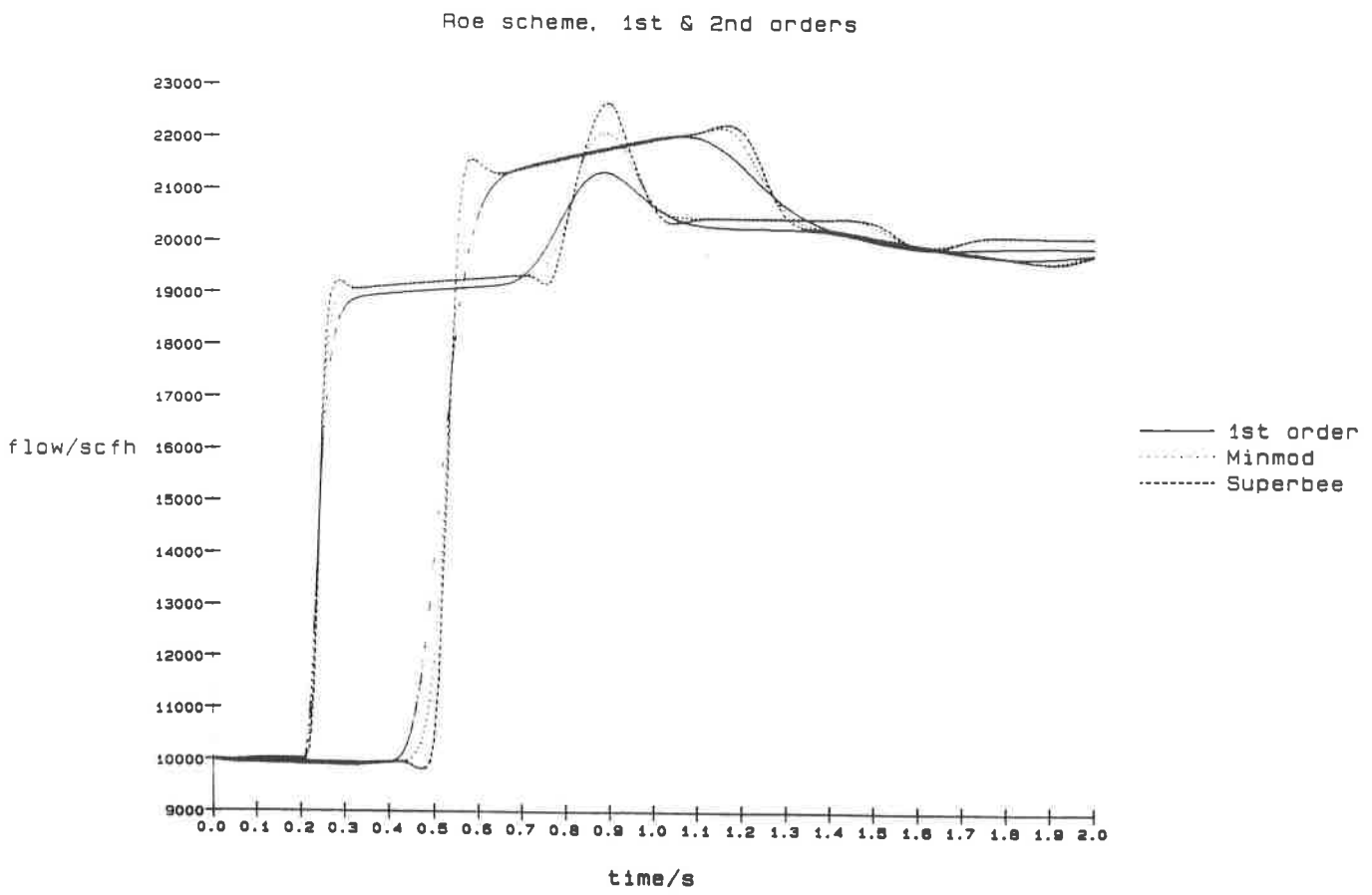
GRAPH_9B



GRAPH_10A



GRAPH_10B



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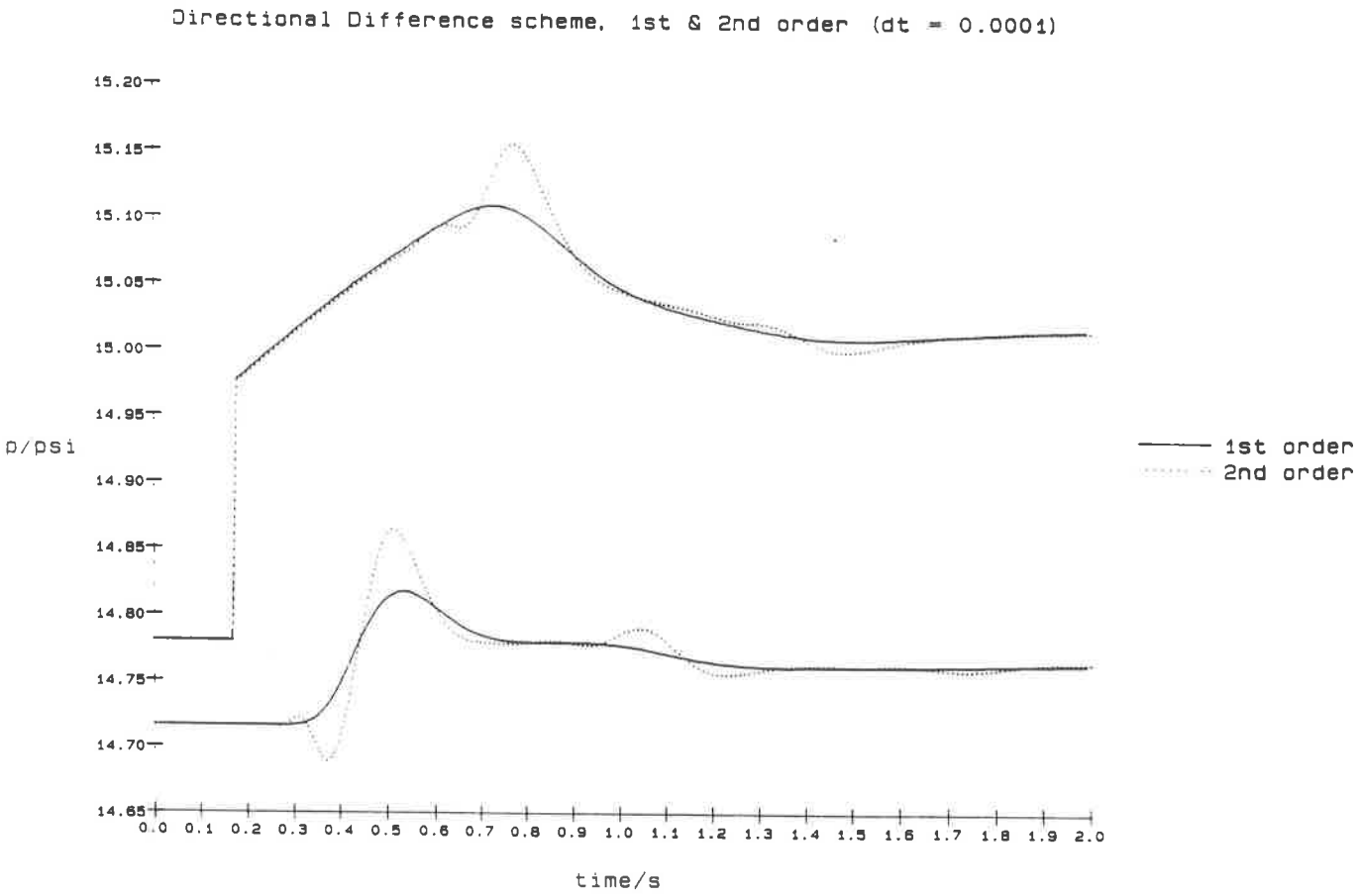

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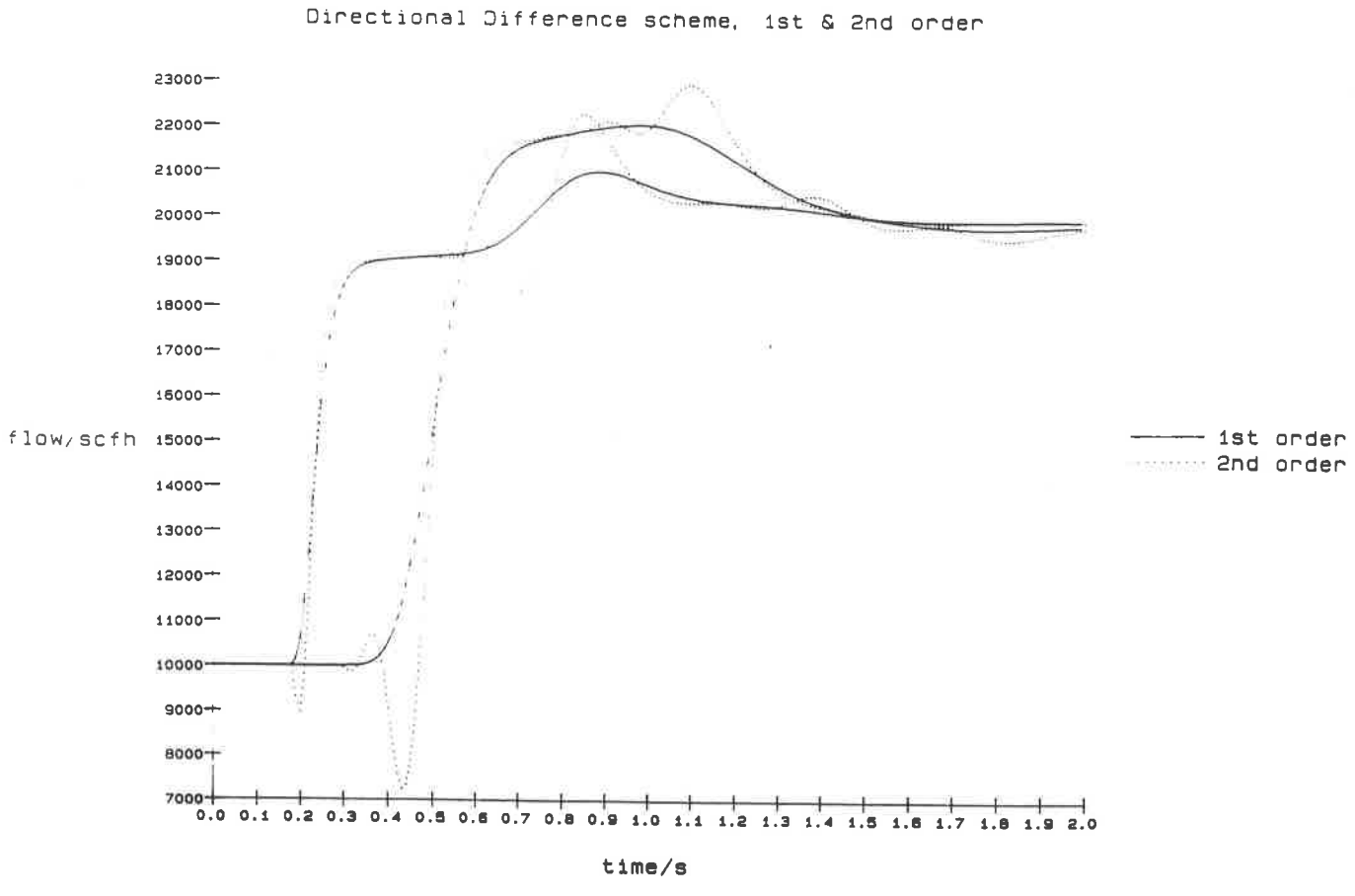
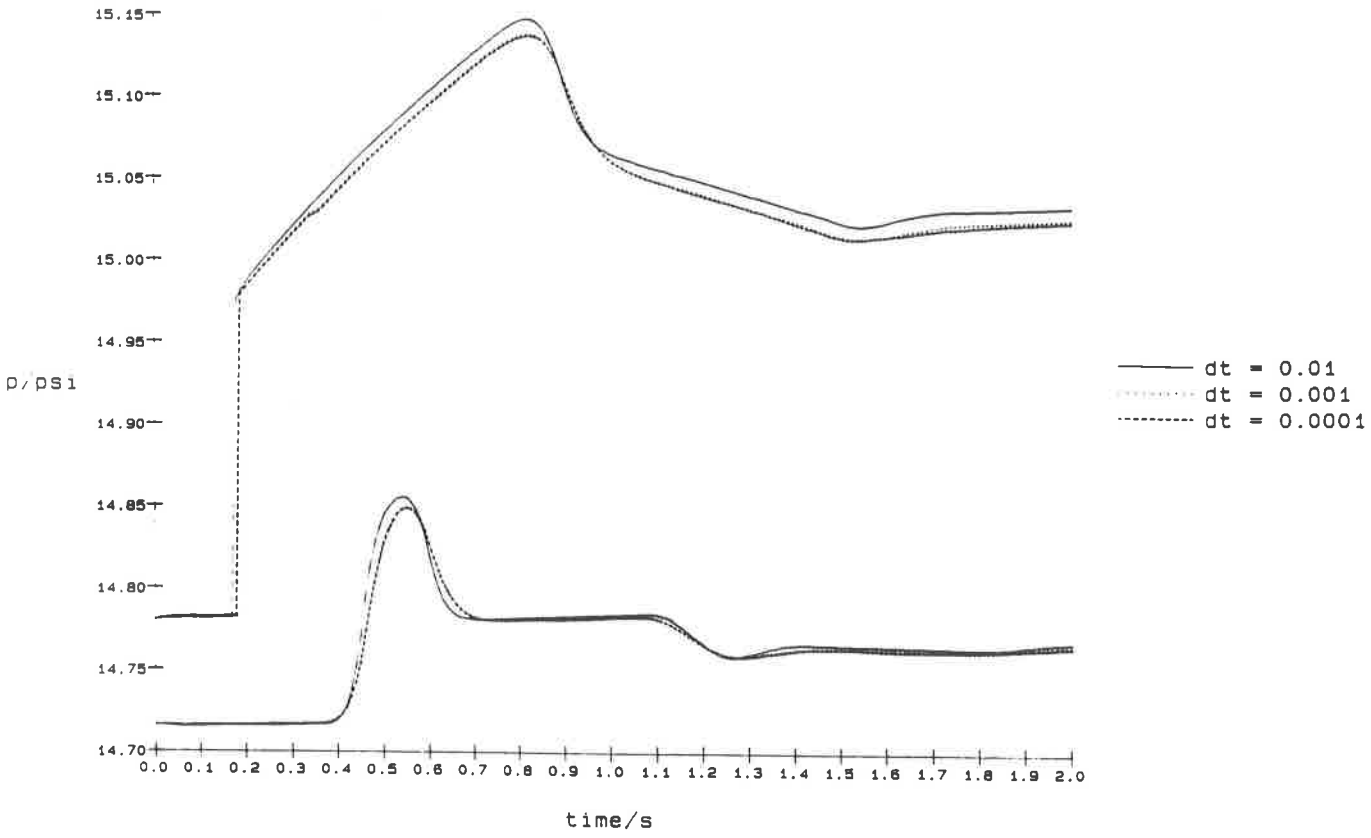


GRAPH_12



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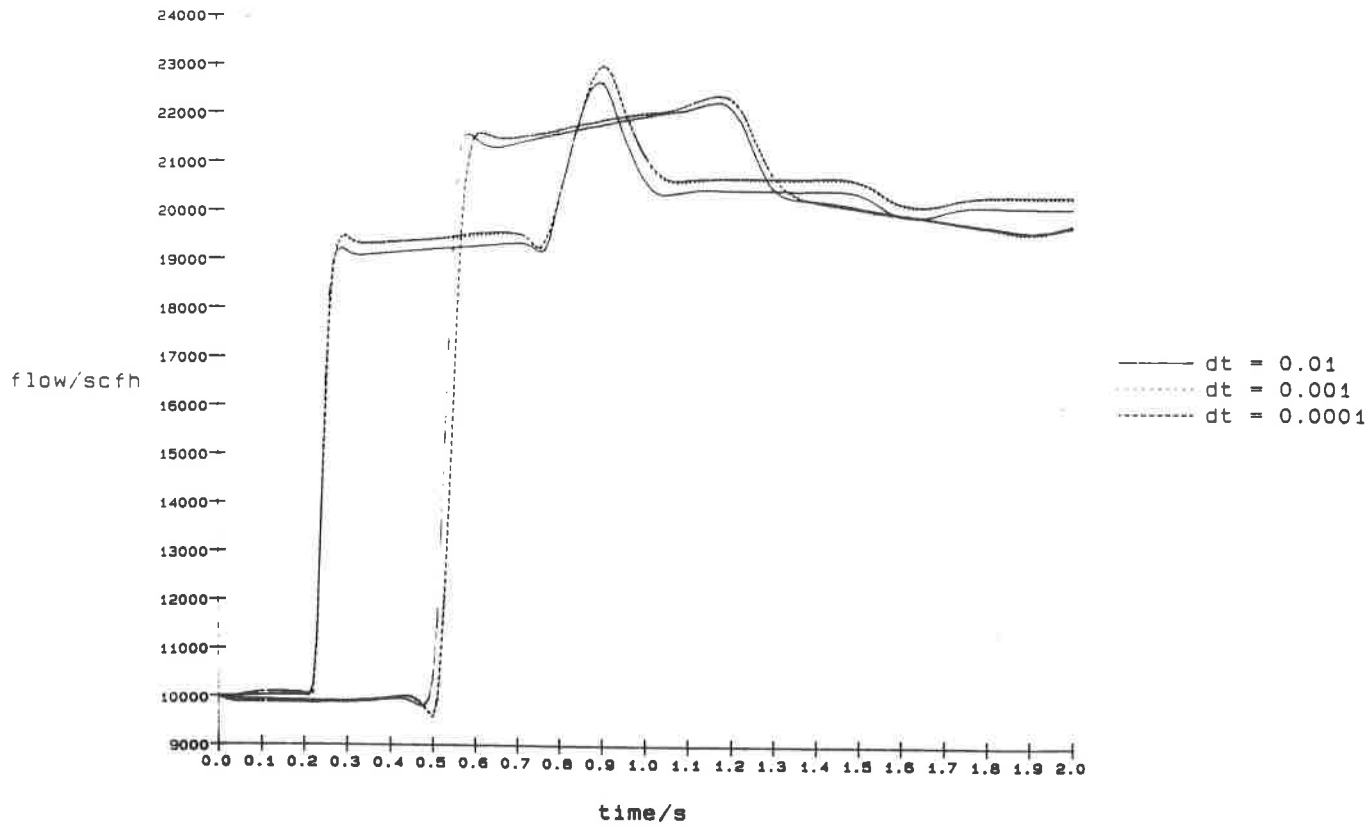


TEST PROBLEM 3 - RESULTS

Graphs of pressure vs. time, at inlet, and at outlet.

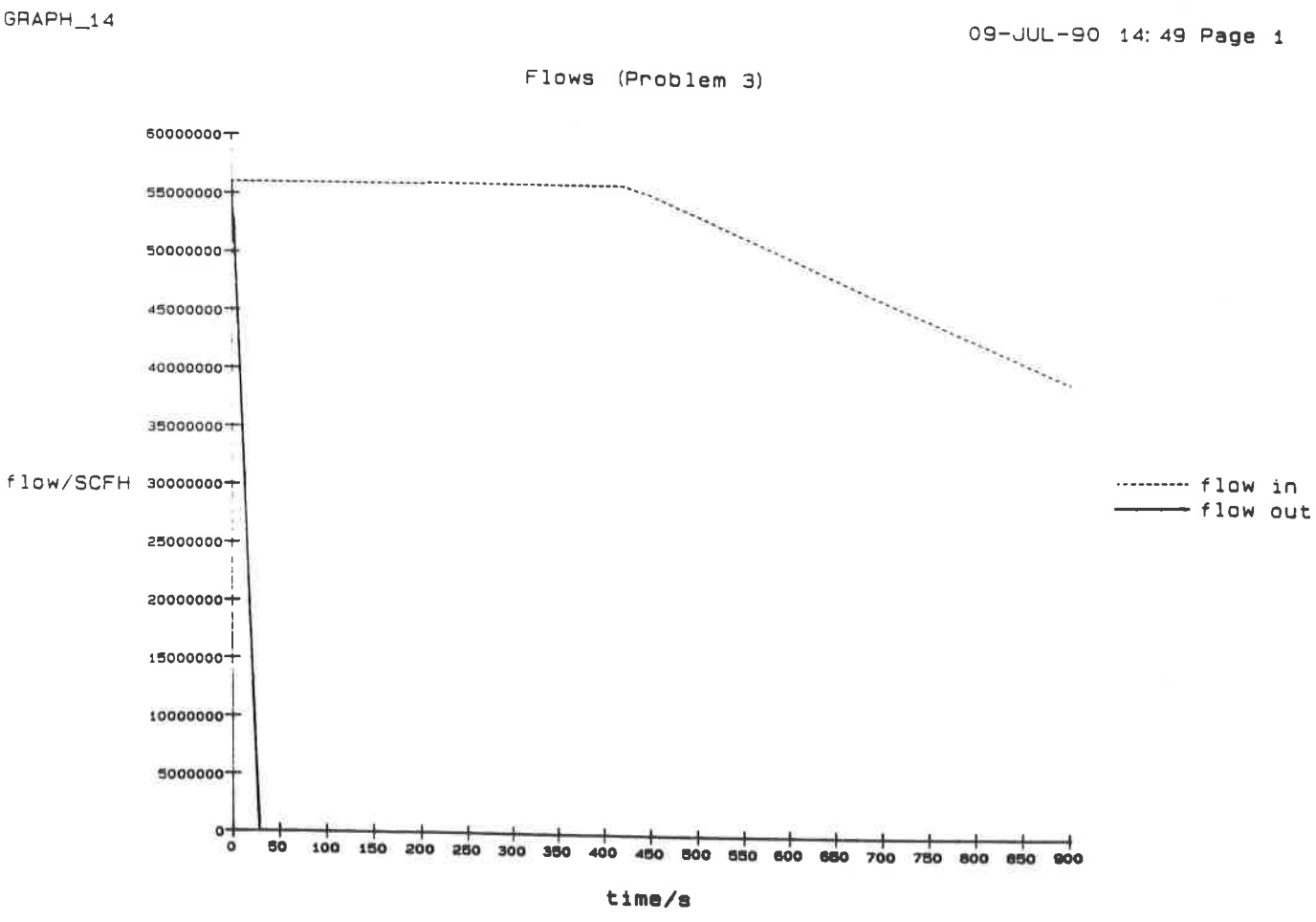
Time step 0.375s (unless stated).

161 nodes used.

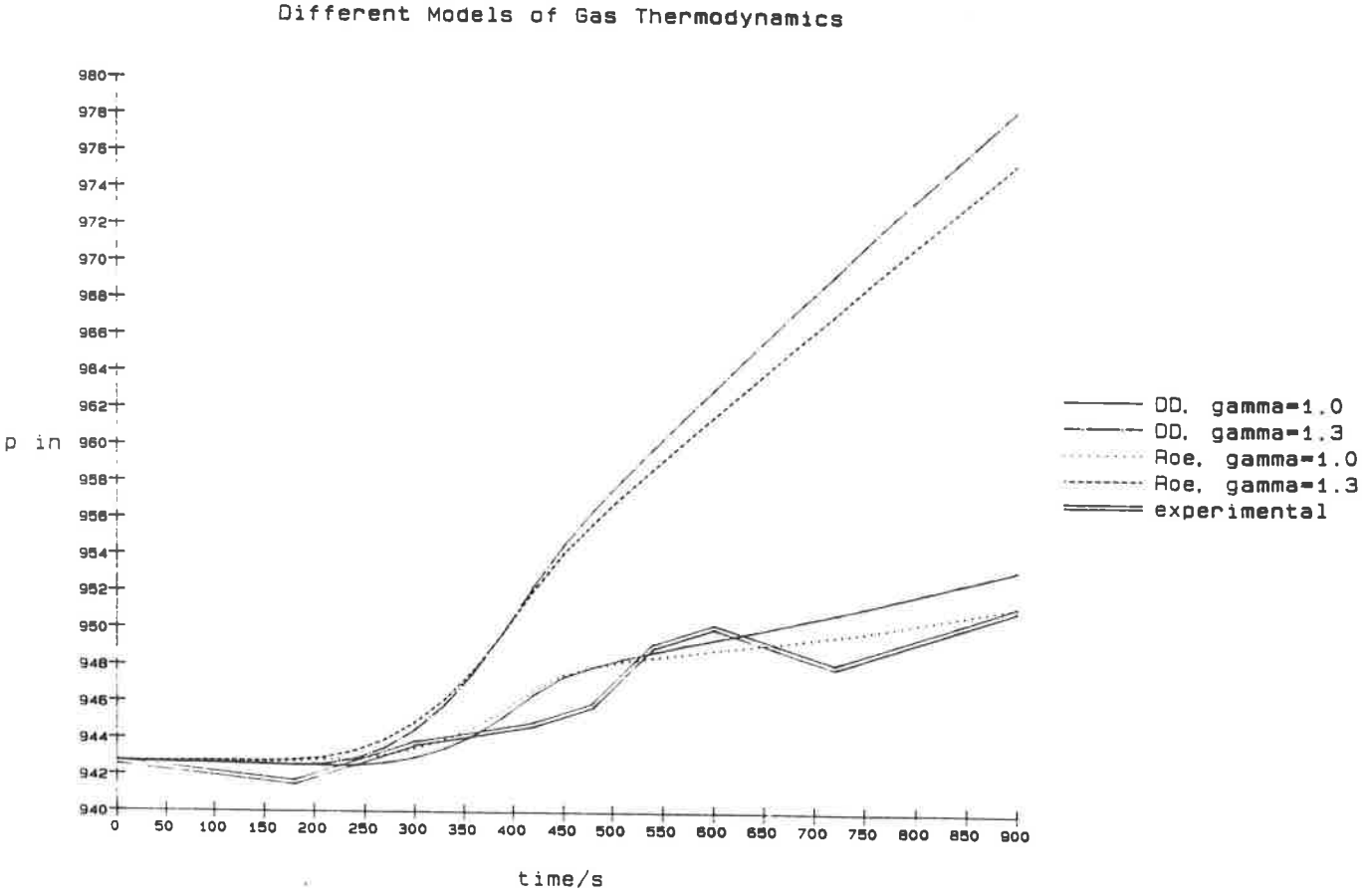
Where larger time steps are taken, fewer nodes are used so as to keep the ratio of time and space steps constant.

Experimental and numerical results.

The prescribed flows are below.



GRAPH_15A



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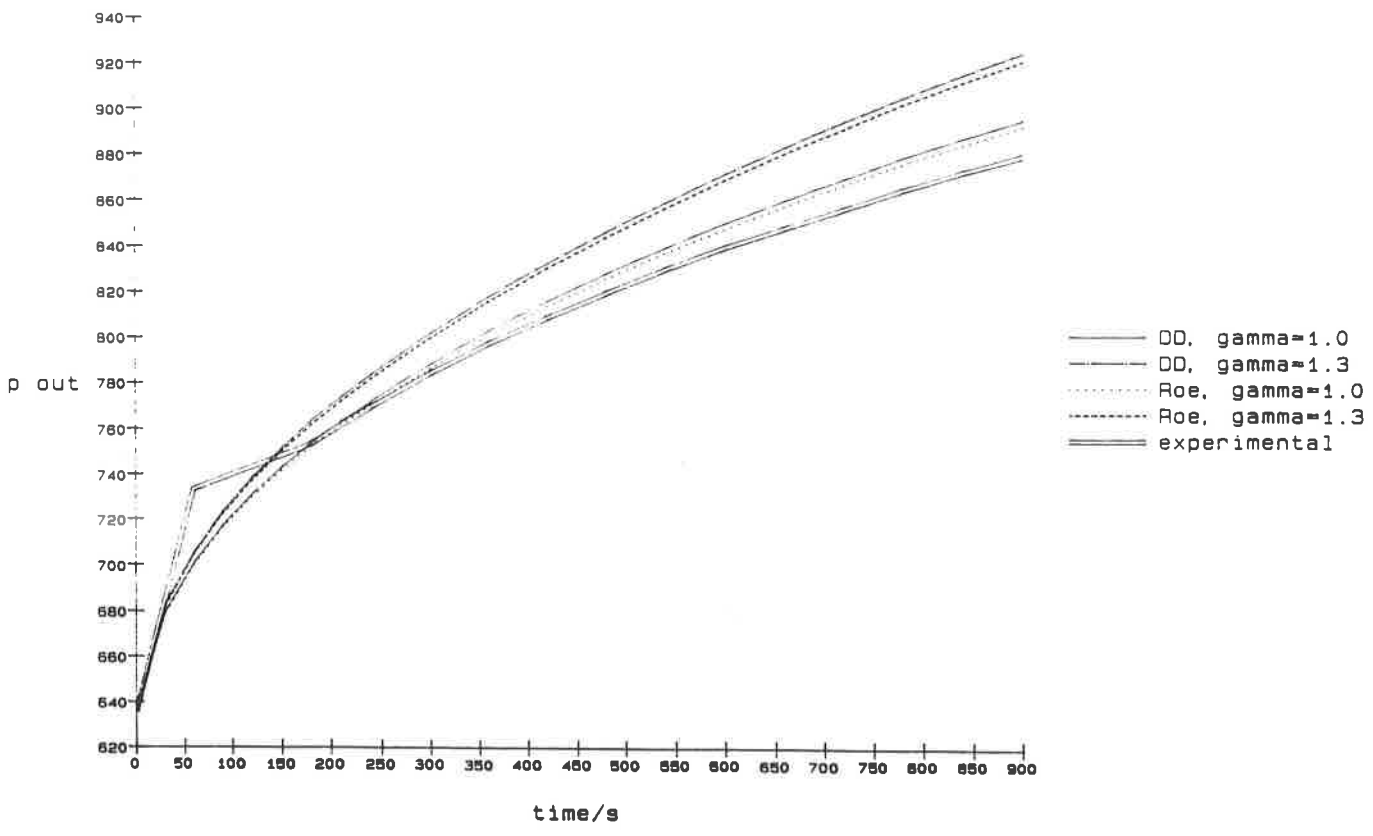

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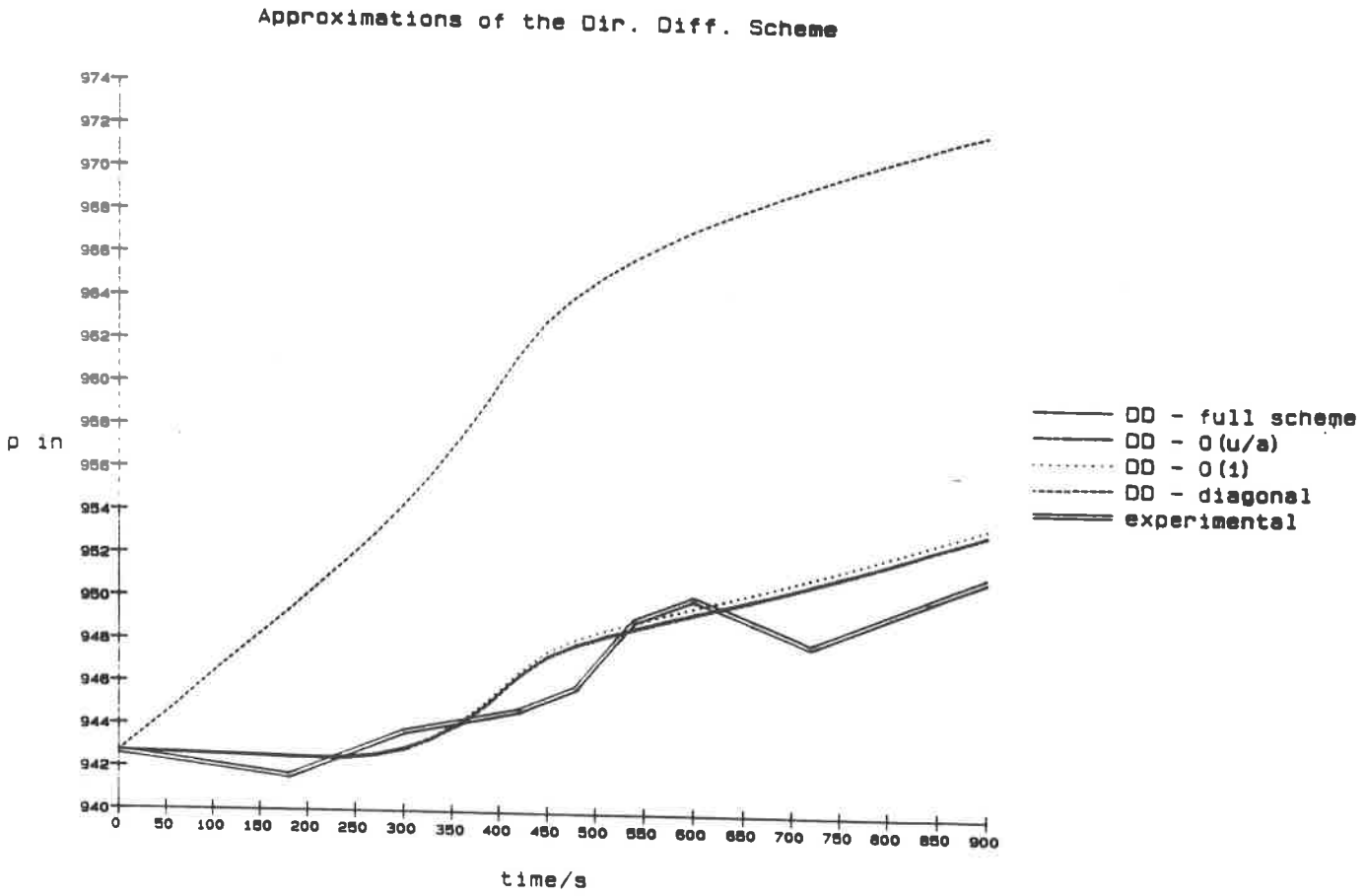

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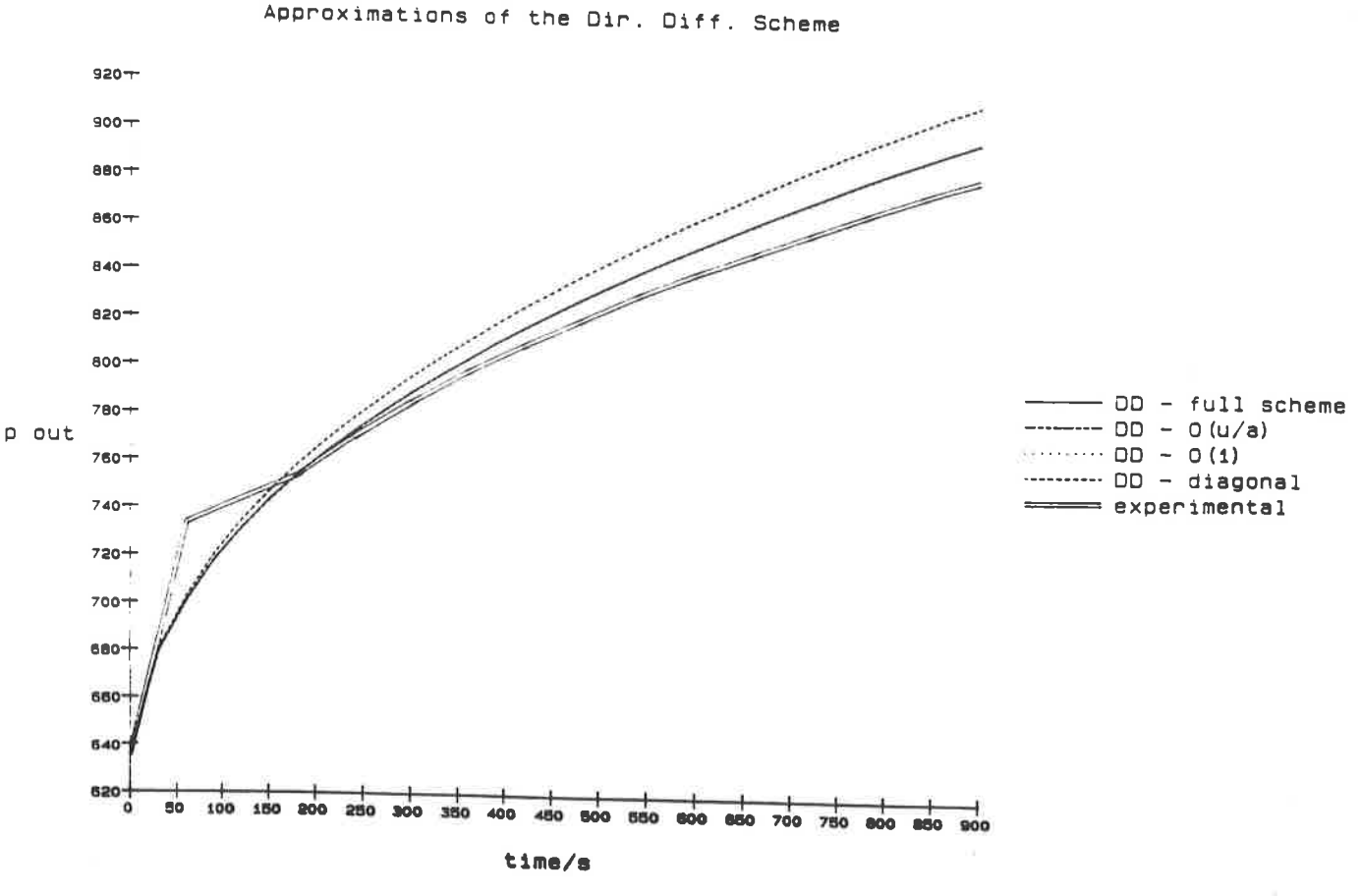

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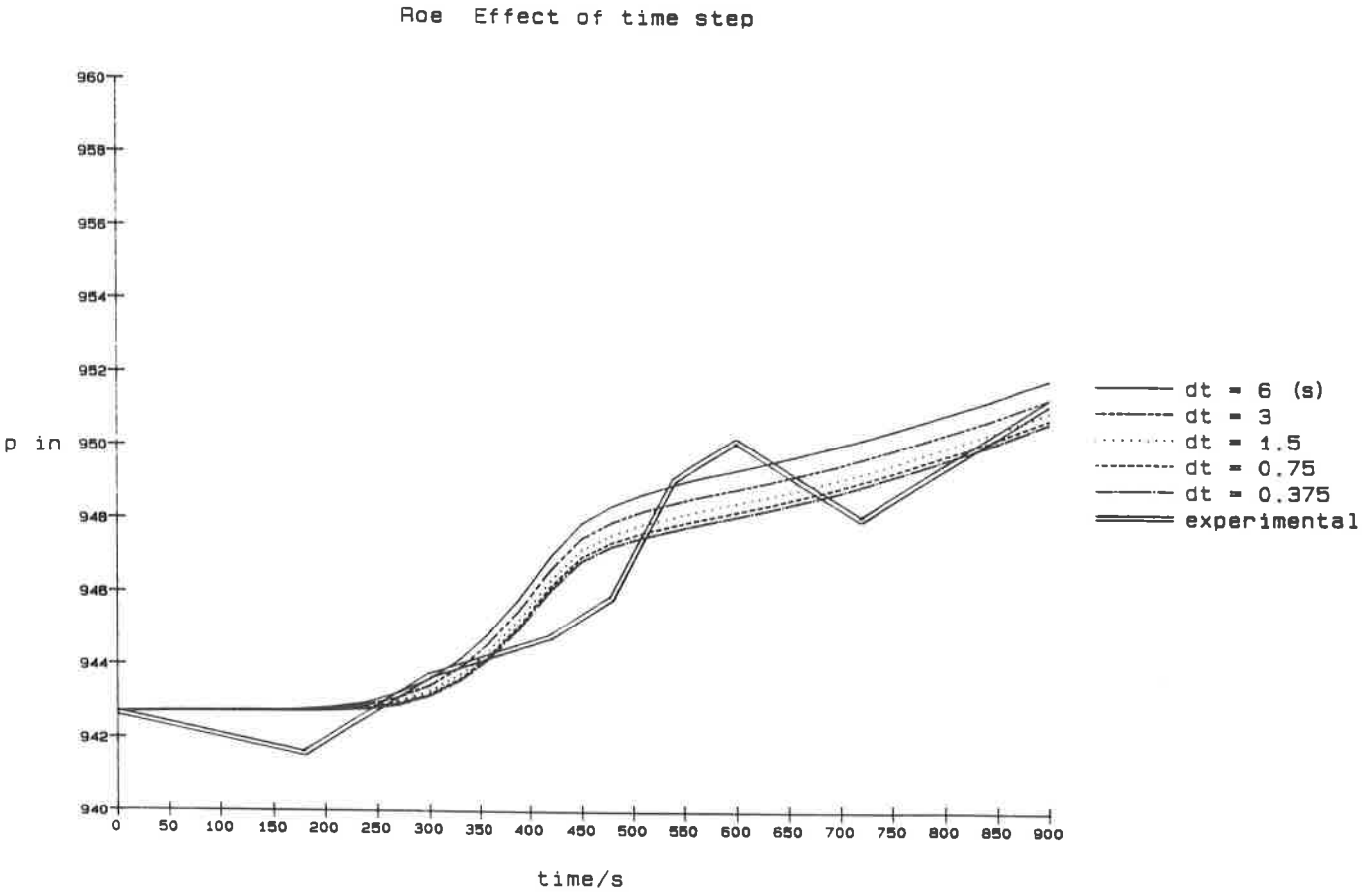

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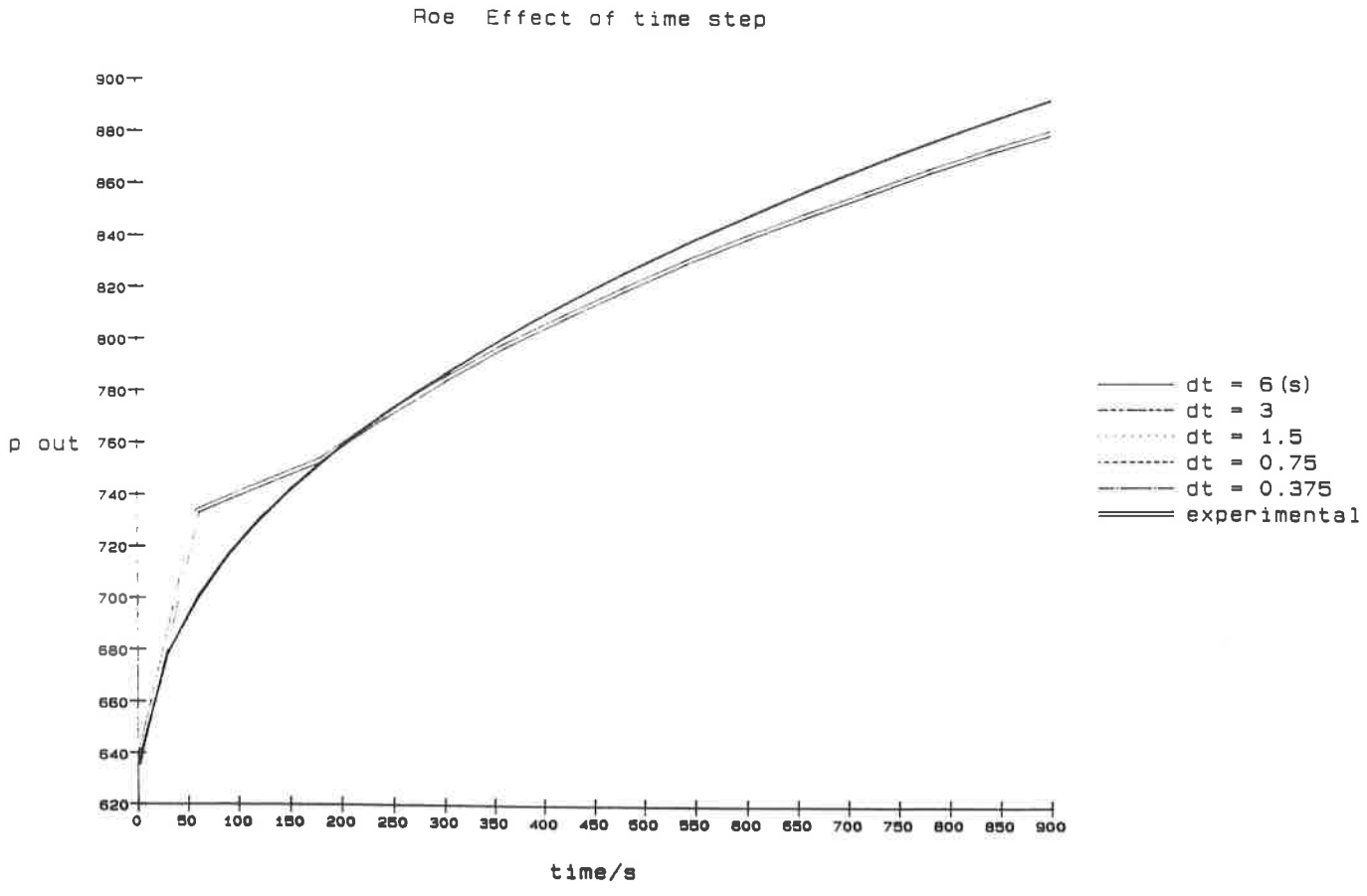
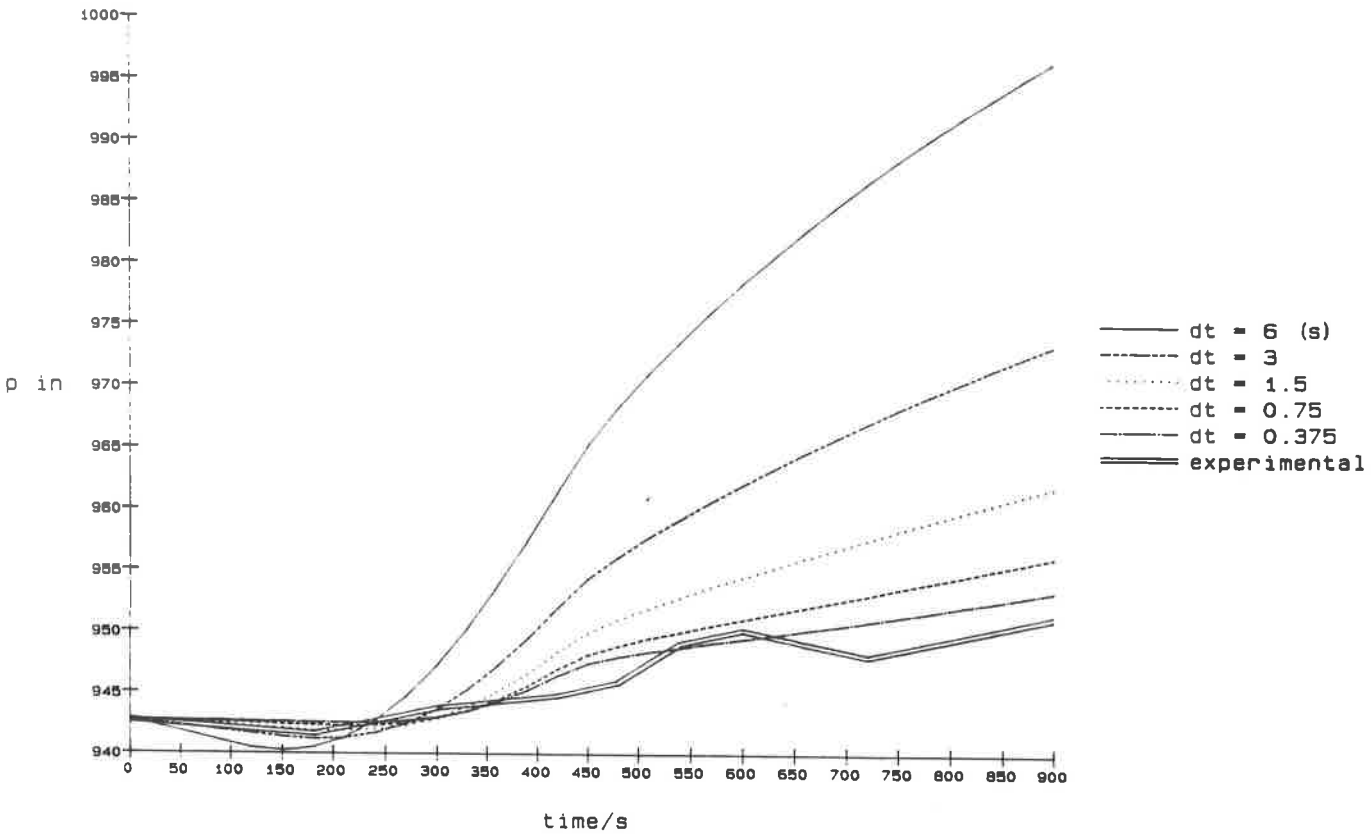


GRAPH_18A



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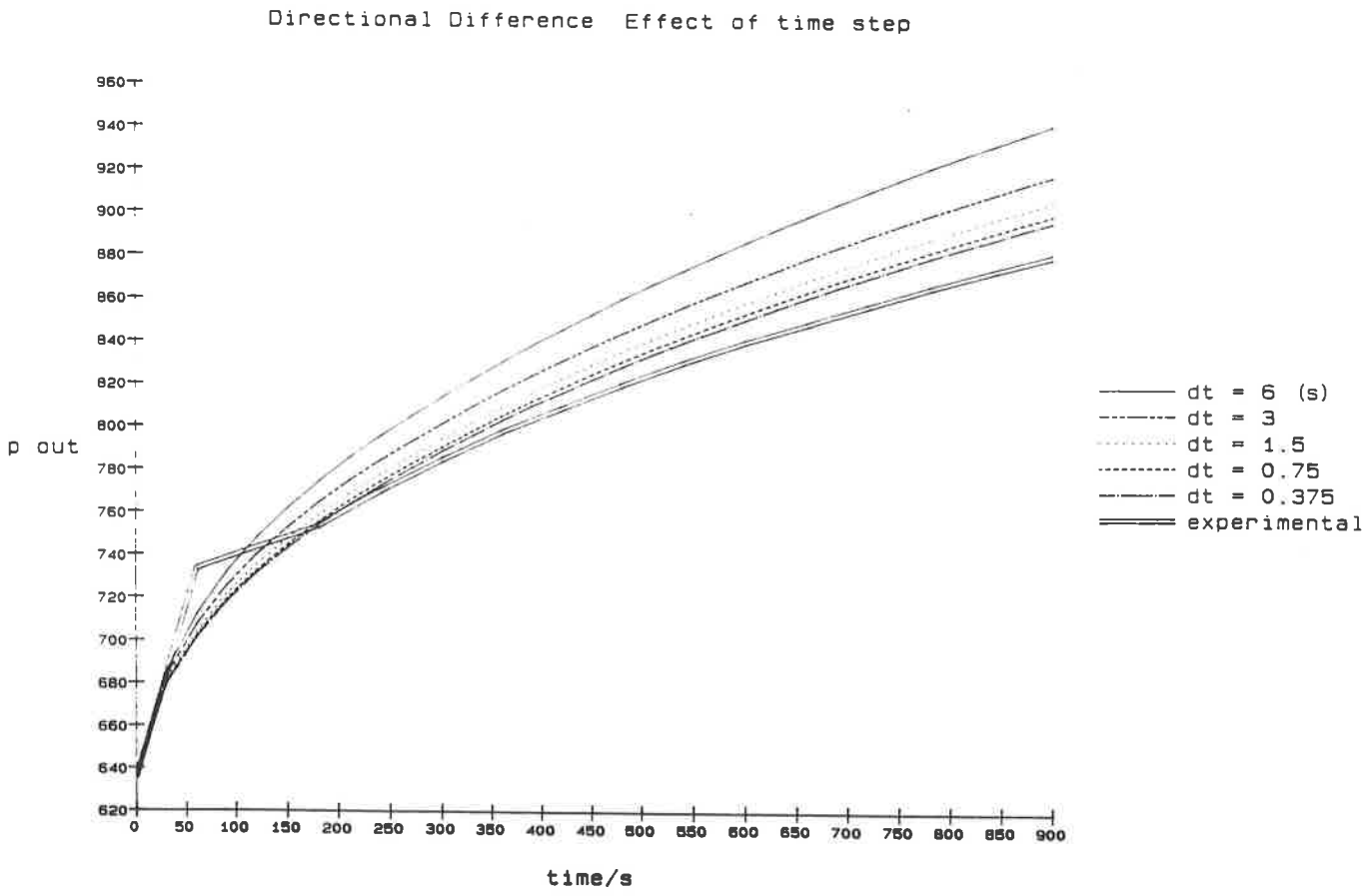
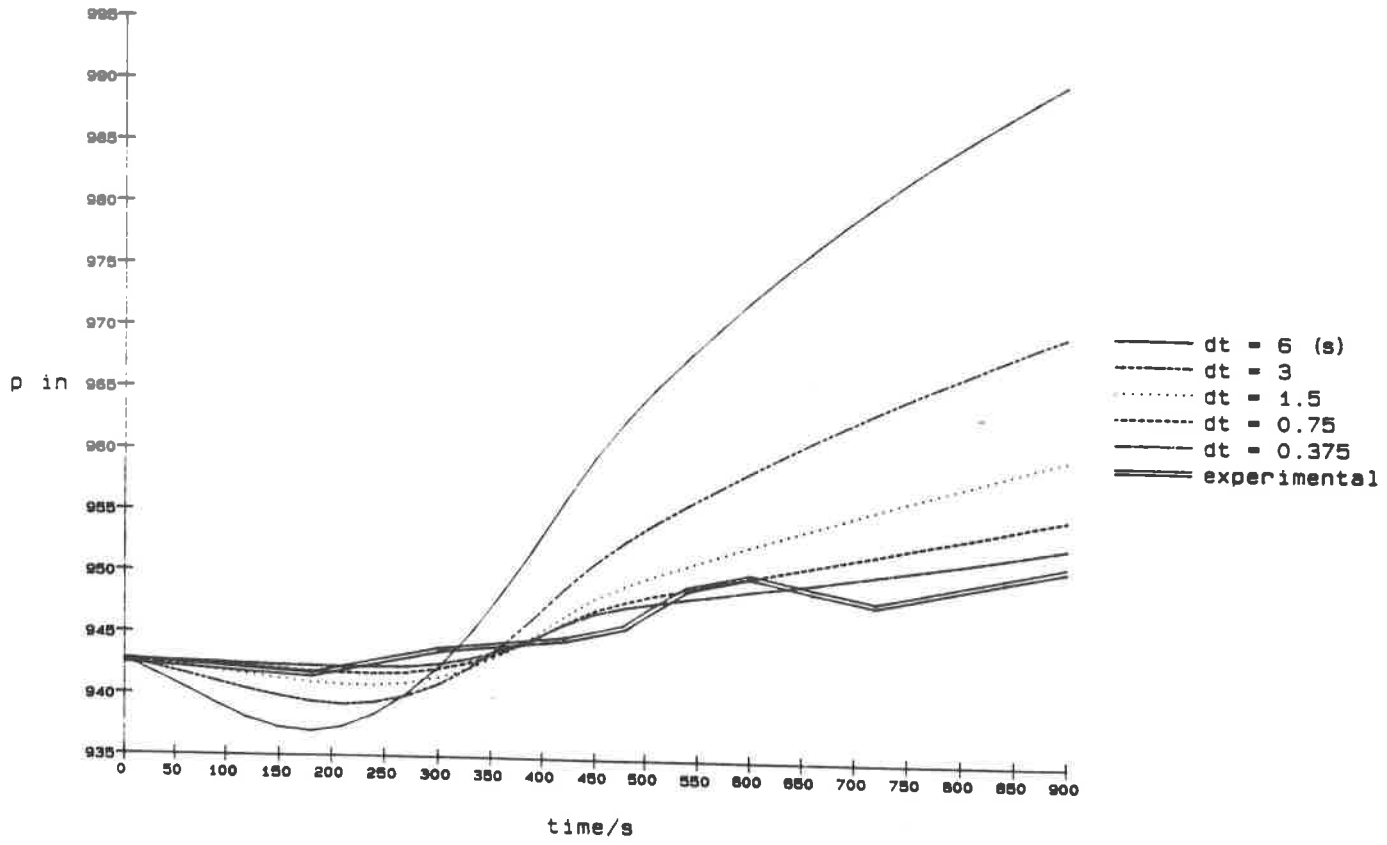
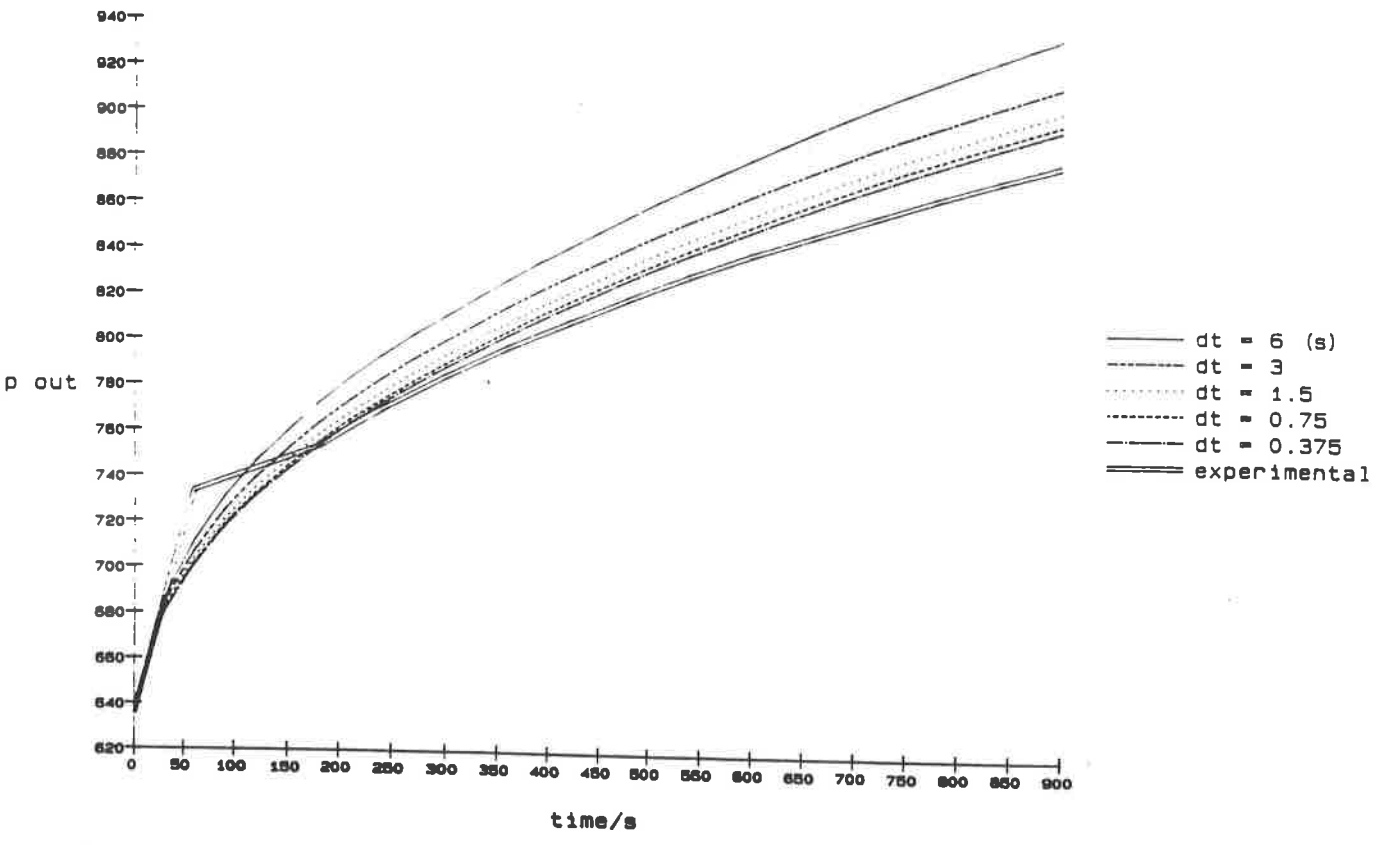


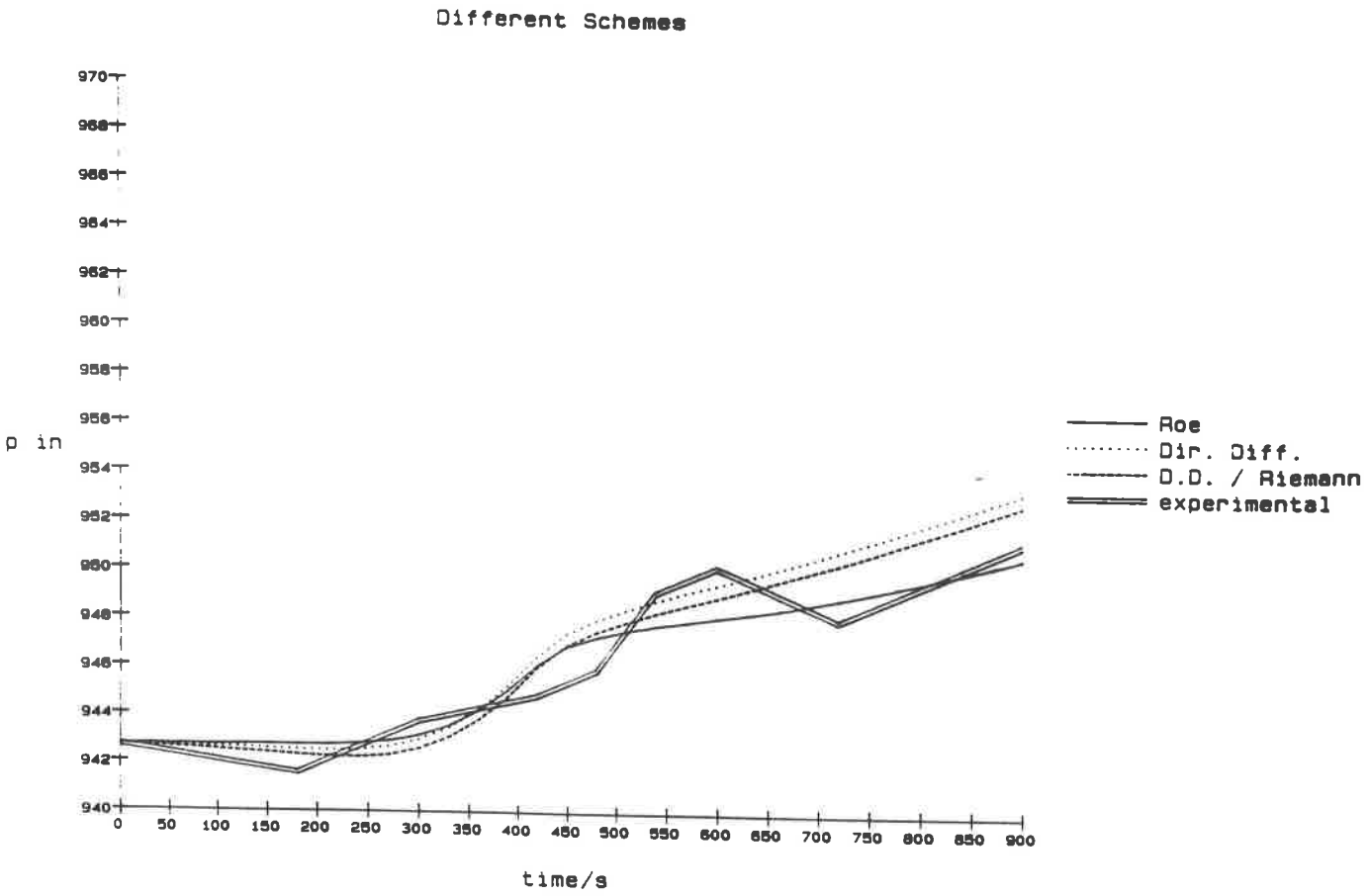
GRAPH_19A



GRAPH_19B



GRAPH_20A



GRAPH_20B