A HIGH ORDER NUMERICAL METHOD FOR THE SOLUTION OF THE ADVECTION EQUATION

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ABSTRACT

This report presents a numerical method which can be used to solve the advection equation

$$\frac{\partial\phi}{\partial t} + \frac{\partial[u(x,t)\phi]}{\partial x} = S(x,t)$$

where:

ϕ ≡ concentration field

$u(x,t)$ ≡ velocity field

$S(x,t)$ ≡ source term

Central to this method are the concept of particle path and the Eulerian interpretation of the time rate of change of the concentration field ϕ.

In actual comparison tests for particular cases with known solutions this method proved to be at least two orders of magnitude more accurate than the usual one sided upwind finite difference method.

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CHAPTER 1

INTRODUCTION

1.1 Definition of the Problem

This report presents a numerical method for integrating the advection equation

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u\phi)}{\partial x} = S(x,t) \tag{1.1.1}$$

where:

$\phi \equiv$ concentration field

$u \equiv$ velocity field

$S \equiv$ variable source term

The method employed here is similar to the 1D version of Leith's method[1], which was first presented by Noh and Protter[2] in 1963. Both of these methods use the concept of particle path and an Eulerian interpretation of the time rate of change of the variable $\phi(x,t)$ between two points connected by this path. However unlike Leith's method which can only be applied to cases of constant velocity field, the method presented here is quite general and can be used to solve the advection equation for the case of a velocity field that is a function of both x and t.

$$u = u(x,t)$$

Another advantage of this method is its accuracy. All approximations which are made here are of the order of:

$$O[\Delta x^{i} \Delta t^{j}]; \text{ where } (i+j) \geq 4 \qquad (1.1.2)$$

In comparison tests made for problems with known solutions this method consistently proved to be a least two orders of magnitude more accurate than the one sided upwind finite difference scheme which is commonly used for the solution of advective type differential equations.

1.2 Motivation for the Work

The containment and storage of radioactive substances is a topic of central importance in nuclear engineering today.

During operation, the radioactive material is mainly held in the fuel. In case of an accident its migration in the fuel, primary ciruit, containment and atmosphere is of interest. After removal of the fuel from the reactor it may be stored for some period in water filled pools after which it may be buried in stable and impervious geologic formations. While the fuel waste forms that are buried either before or after reprocessing, are expected to be highly resistant to leaching, still migration due to contact with ground water must be considered in the safety analysis of a nuclear wastes disposal site.

In general the fluid velocities transporting radionuclides are assumed to be known. Therefore their migration can be modelled by advection type equations that take diffusion and dispersion due to non uniform velocity fields into account. One way of modelling dispersion is by a diffusion type coefficient that may be a function of position in the media, as well as of the velocity field itself. Also decay of radionuclides must be taken into account. In its one dimensional form the advection-dispersion equation becomes:

$$\frac{\partial\phi}{\partial t} + \frac{\partial[u(x,t)\phi]}{\partial x} + \frac{\partial}{\partial x}[D(x,t)\frac{\partial\phi}{\partial x}] = k_1\phi + k_2 \tag{1.2.1}$$

There is no known analytical solution for the general equation described above and it must be solved by means of numerical techniques.

Our ultimate aim is to develop a very accurate numerical scheme which could be used to solve equation 1.2.1. In particular, numerical diffusion and dispersion effects are to be minimized.

The method we have developed can now be used to solve the advection equation

$$\frac{\partial\phi}{\partial t} + \frac{\partial(u\phi)}{\partial t} = S(x,t) \tag{1.2.2}$$

However it is written in such a manner that with little effort it can be generalized to solve equations of the type given by equation 1.2.1. Therefore it can become a useful tool in the analysis of advection-diffusion problems in nuclear engineering (and other fields) where high accuracy is needed.

The generalization of this method for the solution of multi-dimension advection dispersion equation is also possible by using the method of fractional time steps[3].

CHAPTER 2

METHOD OF SOLUTION

2.1 The Case of Constant Velocity Field

Consider the advection equation in conservation law form:

$$\frac{\partial\phi}{\partial t} + \frac{\partial(u\phi)}{\partial x} = 0 \qquad (2.1.1)$$

Expanding the spatial derivative and re-arranging we obtain:

$$\frac{\partial\phi}{\partial t} + u\frac{\partial\phi}{\partial x} = -\phi\,\frac{\partial u}{\partial x} \qquad (2.1.2)$$

If the velocity field is constant the right hand side of the above equation is zero and equation (2.1.2) reduces to:

$$\frac{\partial\phi}{\partial t} + u\,\frac{\partial\phi}{\partial x} = 0 \qquad (2.1.3)$$

where u is constant.

The solution of equation (2.1.3) is well known and is given by the general equation:

$$\phi(x,t) = F(x-ut) \qquad (2.1.4)$$

Which leads to the following relations:

$$\phi(x,t+\Delta t) = \phi(x-u\Delta t,t) \qquad (2.1.5)$$

$$\phi(x+u\Delta t,t) = \phi(x,t-\Delta t) \qquad (2.1.6)$$

Let us now construct a grid in the solution domain (the x-t plane). Let Δx be the increment in the x direction and let Δt be the time increment, so that each point on the discretized plane will be uniquely defined by an ordered pair of integers j and n

i.e. $\phi_j^n = \phi(j\Delta x,\ n\Delta t)$ (2.1.7)

Furthermore let the solution domain of interest be finite and have the following bounds:

$$0 \le j \le J \rightarrow 0 \le x \le J\Delta x$$

$$0 \le n \le N \rightarrow 0 \le t \le N\Delta t$$

Based on these conventions a graph can be drawn for the particle paths expressed by equations (2.1.5) and (2.1.6). Without loss of generality we assume that the velocity is positive. For convenience the courant number is introduced as:

$$\alpha = \frac{u\Delta t}{\Delta x} \qquad (2.1.8)$$

Referring to figure 2.1.1 equation 2.1.5 indicates that

$$\phi_j^{n+1} = \tilde{\phi}_j^{n+1}$$

and equation 2.1.6 indicates

$$\hat{\phi}_j^{n-1} = \phi_j^{n-1}$$

Again referring to figure 2.1.1 consider a value ϕ_o which is situated a distance $\xi\Delta x$ to the left of ϕ_j^n. $\phi(x,t)$ can be expanded in a Taylor series about the position of ϕ_o. In particular, in the spatial direction only, the expansion is:

$$\phi(x,t) = \phi_o + \sum_{i=1}^{\infty} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} [x - (j-\xi)\Delta x]^i \tag{2.1.9}$$

Equation 2.1.9 can be used to evaluate some of the neighbouring values of ϕ. The following expansions can be constructed:

$$\phi_\beta^n \simeq \phi_o + \sum_{i=1}^{(S-1)} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} [(\beta-j+\xi)\Delta x]^i \tag{2.1.10}$$

$$\hat{\phi}_\gamma^{n-1} \simeq \phi_o + \sum_{i=1}^{(S-1)} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} [(\gamma-j+\alpha+\xi)\Delta x]^i \tag{2.1.11}$$

$$\tilde{\phi}_j^{n+1} \simeq \phi_o + \sum_{i=1}^{(S-1)} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} [(\xi-\alpha)\Delta x]^i \tag{2.1.12}$$

The unknowns in the above equations are:

$$\tilde{\phi}_j^{n+1}, \ \phi_o \text{ and } \frac{\partial^i \phi}{\partial x^i} \ (i = 1, 2, \ldots, (S-1)) \tag{2.1.13}$$

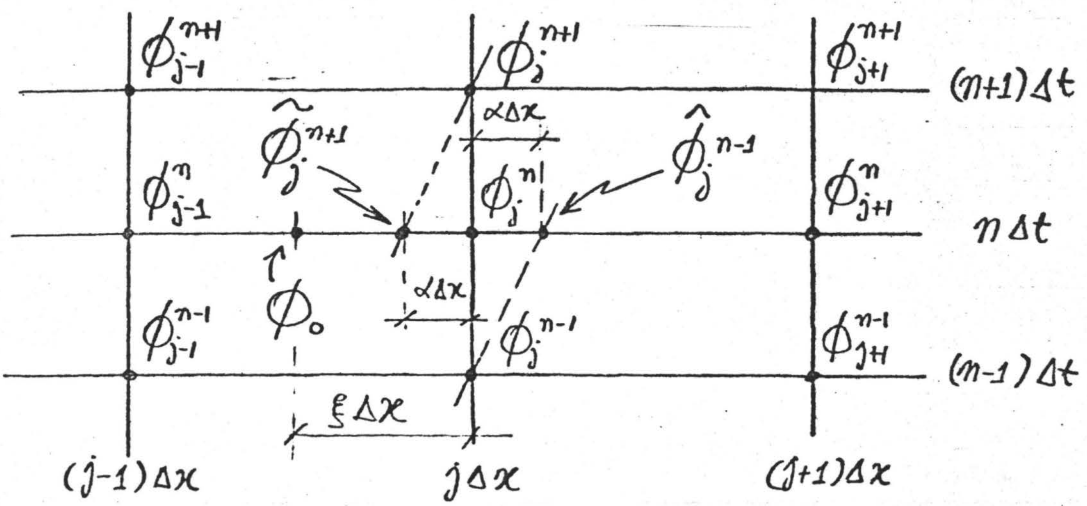


Figure 2.1.1: Particle paths for the case of constant velocity

$\therefore \rightarrow (S+1)$ unknowns

The highest number of values of β and γ that we can have is the total number of nodes in the grid. Thus it is possible to construct (2J+1) equations which are linear in the unknowns. In addition if

$$\alpha \neq \xi \text{ and } 0 < (\alpha,\xi) < 1$$

and
$$S + 1 = 2J + 1 \tag{2.1.14}$$

then the system of equations is linearly independent and it will have a unique solution. From equation 2.1.14 the value of S can be found:

$$(S+1) = 2J + 1$$

$$\therefore S = 2J \tag{2.1.15}$$

Thus by solving the system of equations as presented we can get a value for $\tilde{\phi}_J^{n+1}$. Referring to equations 2.1.10, 2.1.11 and 2.1.12 it can be seen that the largest distance from the origin is given by:

$$D_{MAX} = \{M\Delta X[(\beta-j+\xi);\ (\gamma-j+\alpha+\xi)]\}\ \Delta x \tag{2.1.16}$$

Thus the maximum error involved in these expansions can be calculated by

$$E_{MAX} = \left(\frac{1}{S!}\right) \left(\frac{\partial^S \phi}{\partial x^S}\right)_\xi [(D_{MAX})^S] \tag{2.1.17}$$

where $0 < \xi < (J\Delta x)$.

The maximum value that D_{MAX} can ever have have cannot exceed $(J+1)\Delta x$, this is an upper bound value, which happens when:

$j = 2$ and $\gamma = J$

$$\therefore D_{MAX} < (J+1)\Delta x \tag{2.1.18}$$

Substituting for D_{MAX} into equation 2.1.17

$$|E_{MAX}| \leq \left|\frac{(J+1)^S}{S!} \frac{\partial^S \phi}{\partial x^S} [\Delta x]^S\right| \tag{2.1.19}$$

But according to equation 2.1.15 $s = 2J$, thus the final expression for the maximum error becomes:

$$|E_{MAX}| \leq \left|\frac{(J+1)^{2J}}{(2J)!} \frac{\partial^{2J} \phi}{\partial x^{2J}} [\Delta x]^{2J}\right| \tag{2.1.20}$$

To get an idea of the magnitudes involves in the above equation, let us consider the case where

$J = 10$, $\Delta x = 0.1$

$$\rightarrow \qquad |E_{MAX}| \leq \left|\frac{(11)^{20}}{20!} \frac{\partial^{20} \phi}{\partial x^{20}} [0.1]^{20}\right| \simeq 2.76*10^{-18} \left|\left(\frac{\partial^{20} \phi}{\partial x^{20}}\right)\right|$$

And clearly this is an upper bound for the magnitude of the error.

Thus in theory we can solve for $\tilde{\phi}_j^{n+1}$ $(j = 1, 2, \ldots, J)$ with the accuracy just discussed. But according to the relation of equation (2.1.5), which is reproduced below

$$\phi(x,t+\Delta t) = \phi(x-u\Delta t,t)$$

$$\rightarrow \qquad \phi_j^{n+1} = \tilde{\phi}_j^{n+1}$$

Thus we have in fact solved for ϕ_j^{n+1} $(j = 1, 2, \ldots, J)$. So in theory at least it is possible to solve the advection equation very accurately by this method if the velocity field is constant. Our next step will be to try and generalize this idea for the case of variable velocity.

2.2 Generalization to Variable Velocity

Let us now try to generalize the concept developed in the last section for the case when the velocity field is a function of both time and space. Following the same convention as before we can again draw a graph of the particle path as in Figure 2.2.1, however unlike the previous section ϕ_j^{n+1} is not equal to $\tilde{\phi}_j^{n+j}$ in this case. Although the fluid particle originally situated at the location $\tilde{\phi}_j^{n+1}$ does move to the position of ϕ_j^{n+1} at the end of the time increment Δt, the right

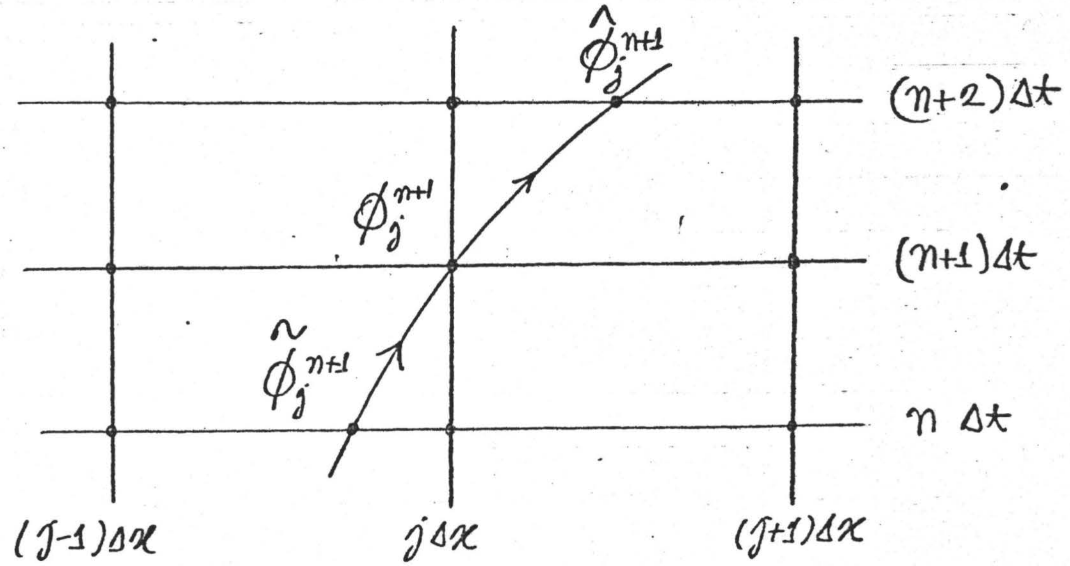


Figure 2.2.1: The particle path for the case of variable velocity.

hand side of the equation

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = -\phi \frac{\partial u}{\partial x} \tag{2.2.1}$$

has changed the value ϕ associated with this particle. The left hand side of equation 2.2.1 is the material derivative of the function ϕ. Equation 2.2.1 can be rewritten as:

$$\frac{D\phi}{Dt} = -\phi \frac{\partial u}{\partial x} \tag{2.2.2}$$

A Lagrangian interpretation can now be used in order to relate the value of ϕ_j^{n+1} to that of $\tilde{\phi}_j^{n+1}$. Integrating equation 2.2.2 with respect to time along the particle path

$$\int_{t=t_o}^{t} d\phi = - \int_{t=t_o}^{t} (\phi \frac{\partial u}{\partial x})dt \tag{2.2.3}$$

For $t_o = n\Delta t$ and $t = (n+1)\Delta t$

$$\phi_j^{n+1} - \tilde{\phi}_j^{n+1} = - \int_{n\Delta t}^{(n+1)\Delta t} (\phi \frac{\partial u}{\partial x})dt$$

$$\rightarrow \qquad \phi_j^{n+1} = \tilde{\phi}_j^{n+1} - \int_{n\Delta t}^{(n+1)\Delta t} (\phi \frac{\partial u}{\partial x})dt \tag{2.2.4}$$

The integral expression of equation 2.2.4 represents the amount by which $\tilde{\phi}_j^{n+1}$ changed before it got to the location of ϕ_j^{n+1}. This integral must be performed along the particle path which in general is not a straight line. If we could calculate the value of this integral we would then be able to generalize the idea developed in the previous section so that it could be applied for the solution of the advection equation in general.

Three pieces of information are needed to evaluate this integral:

(i) an equation for the particle path about the point $(j\Delta x,\ n\Delta t)$

(ii) A functional relationship for $\frac{\partial u}{\partial x}(t)$ along the particle path

(iii) A functional relationship for $\phi(t)$ along the particle path

In this section we will outline briefly how the above information can be obtained in general with high accuracy. In the next section we will go through the details for the case of a chosen order of accuracy.

In order to construct an equation for the particle path we must first have a functional relationship for the velocity as a function of x and t about the point $(j\Delta x,\ (n+1)\Delta t)$. Let U_z^w be the velocity near the point $(j\Delta x,\ n\Delta t)$ and let it be given by:

$$U_z^w \simeq \sum_{i=1}^{I} \sum_{m=1}^{M} \lambda_{im}[(z-j)\Delta x]^{(m-1)}[(w-n-1)\Delta t)]^{(i-1)} \qquad (2.2.5)$$

where z and w are not necessarily integer numbers and:

$|(z-j)|<1$ and $|(w-n)|<1$

The coefficients λ_{im} of equation 2.2.5 can be found by solving the linear system of equations:

$$U_k^{\ell} = \sum_{i=1}^{I} \sum_{m=1}^{M} \lambda_{im}[(k-j)\Delta x]^{(m-1)}[(\ell-n-1)\Delta t]^{(i-1)} \tag{2.2.6}$$

where $k = 1, 2, 3, \ldots, J$

$\ell = 1, 2, 3, \ldots, N$

For the above system of equation to have a unique solution set we must have the same number of linear indpendent equations as unknowns

$\therefore J*N = I*M$

$\therefore I = \frac{J*N}{M}$

and $M = \frac{J*N}{I}$

For the particular case when $I = M$

$$\therefore I = M \simeq \sqrt{J*N} \tag{2.2.7}$$

Thus if we know the velocity at every point on the grid we can in theory get an expression for the velocity field about the point $(j\Delta x, n\Delta t)$ which is

$$U_z^w \simeq \sum_{i=1}^{I} \sum_{m=1}^{I} \lambda_{im}[(z-j)\Delta x]^{(m-1)}[(w-n-1)\Delta t]^{(i-1)} \tag{2.2.8}$$

where I is given by equation (2.2.7).

Let us now try to construct an equation for the particle path about the point $(j\Delta x, (n+1)\Delta t)$. Consider figure 2.2.2 below. Along the particle path we have the following relation

$$\frac{dx(t)}{dt} = u(x,t) \tag{2.2.9}$$

Integrating the above equation along the particle path between $t = t_1$ and $t = t_k$ we get

$$\int_{t=t_1}^{t_k} dx(t) = \int_{t=t_1}^{t_k} u(x,t)dt \tag{2.2.10}$$

where $n\Delta t \leq t_1$ and $t_k \leq (n+2)\Delta t$. Let x_k denote $x(t=t_k)$. The above equation can be rewritten as:

$$x_k = x_1 + \int_{t=t_1}^{t_k} u(x,t)dt \tag{2.2.11}$$

Let us assume that the equation of the particle path is given by:

$$x(t) = \sum_{p=1}^{P} \alpha_p t^{(p-1)} \tag{2.2.12}$$

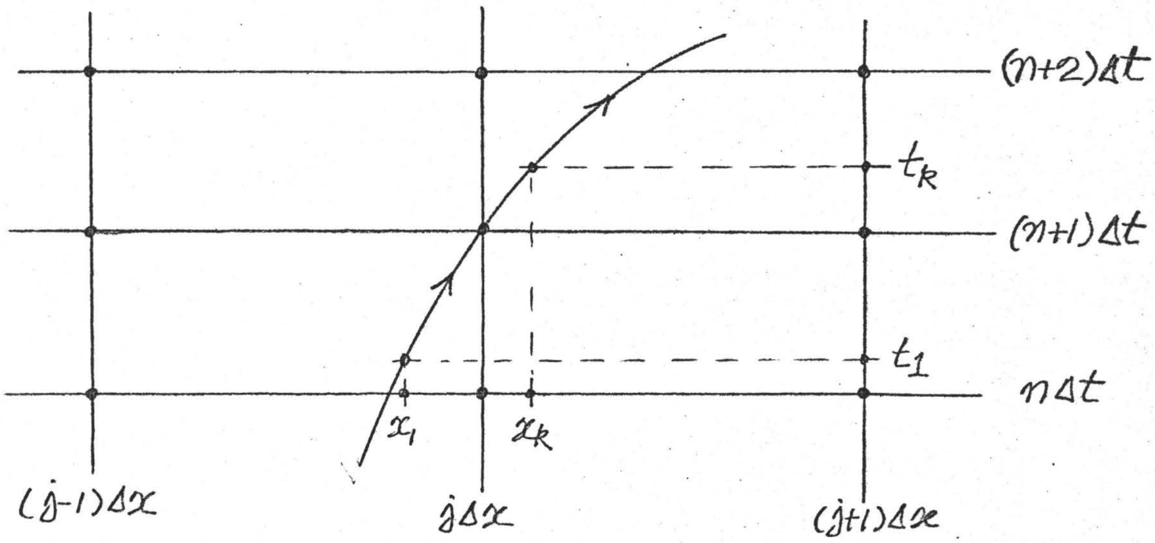


Figure 2.2.2: Limits of integration along the particle path.

Consider figure 2.2.3 below. The time interval is divided into K sub-intervals as shown. Each of these points on the particle path must be related by the particle path equation:

$$x_k = \sum_{p=1}^{P} \alpha_p t_k^{(p-1)}; \; k = 1, 2, \ldots, K \tag{2.2.13}$$

NOw if P = K then the coefficients α_p (p = 1, 2, ..., K) can be uniquely defined as a linear function of x_k (k = 1, 2 ..., K).

$$\alpha_p = \alpha_p(x_1, x_2, \ldots, x_K), \; p = 1, 2, \ldots k \tag{2.2.14}$$

We thus have the coefficients that we needed in equation 2.2.12. For P = K

$$x(t) = \sum_{p=1}^{K} \alpha_p(x_1, x_2 \ldots, x_K) t^{(p-1)} \tag{2.2.15}$$

We have an expression for the velocity which is given by:

$$u_z^w \simeq \sum_{i=1}^{I} \sum_{m=1}^{I} \lambda_{im}[(z-j)\Delta x]^{(m-1)}[(w-n-1)\Delta t]^{(i-1)} \tag{2.2.16}$$

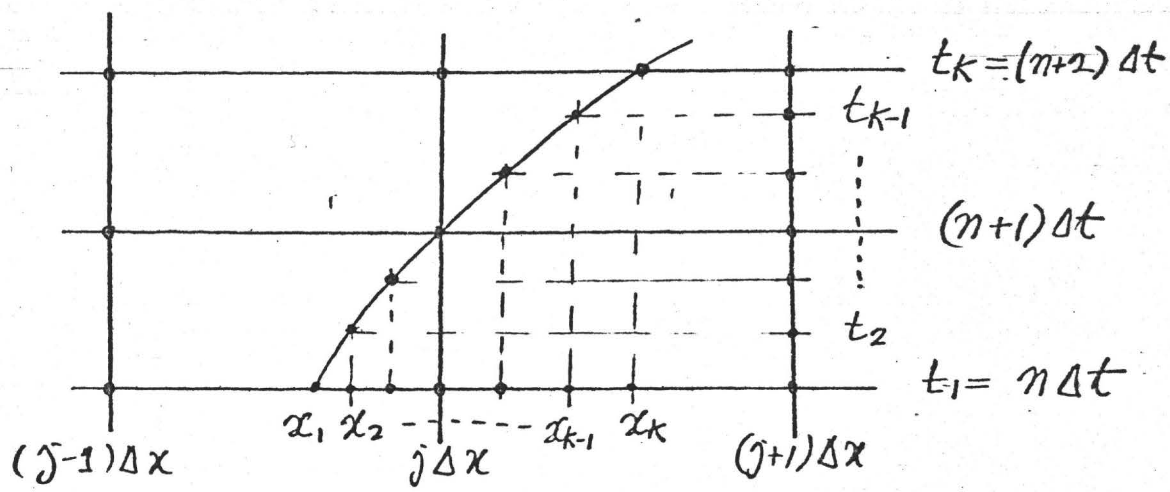


Figure 2.2.3: Subdivision of the particle path into k segments.

Along the particle path the above equation can be represented as a function of t only. Let:

$$(w-n-1)\Delta t = t \text{ and } (z-j)\Delta x = x(t)$$

$$\rightarrow \quad u(t) \simeq \sum_{i=1}^{I} \sum_{m=1}^{I} \lambda_{im}[x(t)]^{(m-1)}[t]^{(i-1)} \tag{2.2.17}$$

Substituting for x(t) from equation 2.2.15 we get

$$u(t) \simeq \sum_{i=1}^{I} \sum_{m=1}^{I} \lambda_{im}[\sum_{p=1}^{K} \alpha_p(x_1,x_2,\ldots,x_K)t^{(p-1)}]^{(m-1)} * [t]^{(i-1)} \tag{2.2.18}$$

where u(t) is now a polynomial in t only, thus it can be rewritten as:

$$u(t) = \sum_{s=1}^{S} \gamma_s(x_1,x_2,\ldots,x_K)t^{(s-1)} \tag{2.2.19}$$

where $S = K(I-1)$ and γ_s is no longer linear in the x_k, $k = 1,2,\ldots,K$. Substituting for u(t) from equation 2.2.18 into equation 2.2.11

$$x_k = x_1 + \int_{t=t_1}^{t_k}[\sum^{S} \gamma_s(x_1,x_2,\ldots,x_k)t^{(s-1)}]dt \tag{2.2.20}$$

Evaluating the integral on the right

$$x_k = x_1 + \sum_{s=1}^{S}\left(\frac{\gamma_s(x_1,x_2,\ldots,x_k)}{s}\right)[t_k^s-t_1^s] \tag{2.2.21}$$

where $k = 1,2,3,\ldots,K$. The only unknowns in equation 2.2.20 are x_1, $x_2,\ldots,x_K$ and thus it can be solved for. This can be done by solving a system of K equations which are non-linear in the unknowns. The magnitude of K has no theoretical limitation and in principle can be as high as desirable. After solving for x_k $(k = 1,2,3,\ldots,K)$ we can go back and calculate the value of the coefficients α_p (p=1, 2,...,K)

$$\alpha_p = \alpha_p(x_1, x_2, \ldots, x_K) \tag{2.2.22}$$

Thus we now have an equation for the particle path about the point ($j\Delta x$, $n\Delta t$) which is:

$$x(t) = \sum_{p=1}^{K} \alpha_p t^{(p-1)} \tag{2.2.23}$$

A functional relationship for $\frac{\partial u}{\partial x}(t)$ can now be easily constructed. Along the particle path the velocity field is given by equation 2.2.17 which is reproduced below:

$$U(t) \simeq \sum_{i=1}^{I} \sum_{m=1}^{I} \lambda_{im}[x(t)]^{(m-1)}[t]^{(i-1)}$$

$$\therefore \frac{\partial u}{\partial x}(t) = \sum_{i=1}^{I} \sum_{m=1}^{I} (m-1)\lambda_{im}[x(t)]^{(m-2)}[t]^{(i-1)} \tag{2.2.24}$$

Substituting for x(t) from equation 2.2.23 and simplifying

$$\frac{\partial u}{\partial x}(t) = \sum_{i=1}^{R} \beta_i t^{(i-1)} \tag{2.2.25}$$

where $R = (I-1)(1+K)-K$

The last piece of information that we need is an expression for $\phi(t)$ along the particle path. Consider figure 2.2.4 below. Let ϕ_k be the value associated with the point $t = t_k$ on the particle path. Furthermore let $\phi(t)$ along the particle path be given by:

$$\phi(t) \simeq \sum_{i=1}^{K} \xi_i t^{(i-1)} \tag{2.2.26}$$

We can thus construct K equations

$$\phi_k \simeq \sum_{i=1}^{K} \xi_i t_k^{(i-1)} \quad (k = 1,2,\ldots,K) \tag{2.2.27}$$

and solve for the coefficients ξ_i as linear functions of the values of ϕ along the particle path:

$$\xi_i = \xi_i(\phi_1, \phi_2, \phi_3, \ldots, \phi_K) \tag{2.2.28}$$

where i = 1,2,3,...,K. Substituting for the above expression into equation 2.2.26

$$\phi(t) \simeq \sum_{i=1}^{K} \xi_i(\phi_1, \phi_2, \ldots, \phi_K) t^{(i-1)} \tag{2.2.29}$$

Multiplying the above equation by equation 2.2.25

$$\phi(t)[\frac{\partial u}{\partial x}(t)] = [\sum_{i=1}^{K} \xi_i(\phi_1, \phi_2, \ldots, \phi_K) t^{i-1}]$$

$$*[\sum_{i=1}^{R} \beta_i t^{(i-1)}]$$

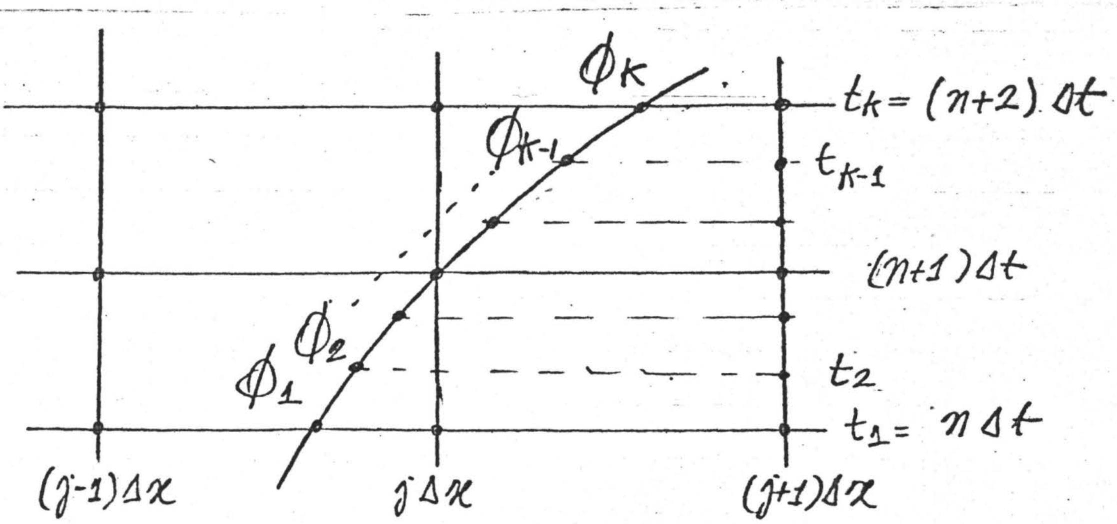


Figure 2.2.4: Values of ϕ along the particle path.

which can be simplified to:

$$\phi(t)[\frac{\partial u}{\partial x}(t)] = \sum_{i=1}^{Q} \eta_i(\phi_1, \phi_2, \ldots, \phi_K)t^{(i-1)} \tag{2.2.30}$$

where $Q = K + R - 2$ and the η_i are linear functions of ϕ_k $(k = 1,2,\ldots,K)$. Consider equation 2.2.4 which is reproduced below:

$$\phi_j^{n+1} = \tilde{\phi}_j^{n+1} - \int_{t=n\Delta t}^{(n+1)\Delta t} (\phi \frac{\partial u}{\partial x})dt$$

If we change the upper bound of the definite integral to $t = t_k$ we then have:

$$\phi_k = \tilde{\phi}_j^{n+1} - \int_{t=n\Delta t}^{t_k} (\phi \frac{\partial u}{\partial x})dt$$

substituting for the integrand from equation 2.2.30 we get

$$\phi_k = \tilde{\phi}_j^{n+1} - \int_{t=t_1=n\Delta t}^{t_k} [\sum_{i=1}^{Q} \eta_i(\phi_1,\phi_2,\ldots,\phi_K)t^{(i-1)}]dt$$

Performing the definite integration

$$\phi_k = \tilde{\phi}_j^{n+1} - \sum_{i=1}^{Q} \{\frac{\eta_i(\phi_1,\phi_2,\ldots,\phi_K)}{i} [t_k^i - t_1^i]\} \tag{2.2.31}$$

where $k = 1,2,3,\ldots,K$. The above equation prepresents a system of equations which are linear in the unknowns ϕ_k $(k=1,2,3,\ldots,K)$. Since the number of equations is equal to the number of unknowns then a unique solution set can be obtained.

Referring to figure 2.2.5 below it can be seen that the solution of the system of equations represented by equation 2.2.31 will give ϕ_j^{n+1} and $\hat{\phi}_j^{n+1}$.

$$\phi_j^{n+1} = \phi_{j=\ell} \text{ where } t_\ell = (n+1)\Delta t$$

$$\hat{\phi}_j^{n+1} = \phi_{j=k} = \phi_k \text{ where } t_k = (n+2)\Delta t$$

We have thus shown that the method introduced here can at least in theory be generalized to solve the advection equation for the general case of variable velocity field. In the next section we will describe in detail a working version of this method.

2.3. A Functional Scheme

The method described in the previous section is theoretically valid and great accuracy can be achieved in the solution of the advection equation for any given velocity field.

However from a practical point of view the scheme may be too cumbersome to develop and economically prohibitive to use.

We tried to strike a balance between the accuracy achieved and the complexity involved. A functional scheme was developed which can solve the general advection equation with good accuracy and at the same time it is not extremely expensive to use, we will come

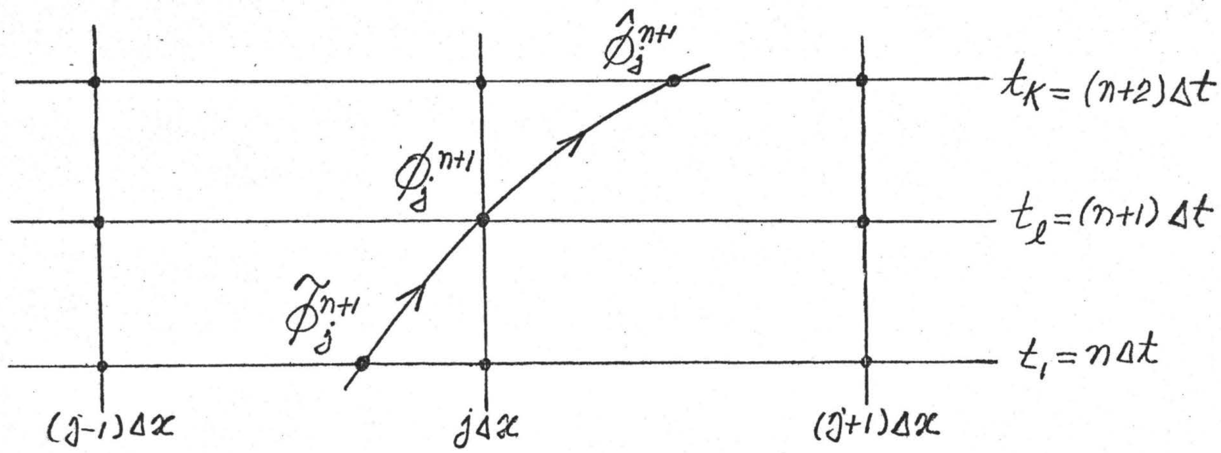


Figure 2.2.5: Selected values of ϕ along the particle path.

back to this point in chapter 5.

Let the velocity field near the point $(j\Delta x, (n+1)\Delta t)$ be given by the double power series expansion:

$$u(x,t) = \sum_{i=1}^{3} \sum_{j=1}^{3} \lambda_{ij} x^{(j-1)} t^{(i-1)} \tag{2.3.1}$$

The reason for choosing the above expansion is purely economical. A third degree expansion for each variable would imply solving a 16 x 16 matrix at each node for each time step, thus it would not be in accordance with the balance we are trying to achieve. Let u_j^n represent $u(x=j\Delta x, n\Delta t)$. By choosing the point $(j\Delta x, (n+1)\Delta t)$ as the origin of the expansion and using the convention above we can then rewrite equation 2.3.1 as:

$$u_\ell^m = \sum_{i=1}^{3} \sum_{k=1}^{3} \lambda_{ik} [(\ell-j)\Delta x]^{(k-1)} [(m-n-1)\Delta t]^{(i-1)} \tag{2.3.2}$$

where
$$\ell = (j-1),\ j,\ j+1$$
$$m = n,\ (n+1),\ (n+2)$$

We then have nine equations and nine unknowns. Since the equations are linearly independent a unique solution for the coefficients λ_{ik} $(i, k = 1,2,3)$ can be obtained. This is accomplished by solving a 9 x 9 matrix at each node. The points surrounded by a circle in Figure 2.3.1 represent the points of known velocity which are used to determine these coefficients.

Let's assume that the particle path which goes through the point $(j\Delta x, (n+1)\Delta t)$ can be described by the function:

$$x(t) = \sum_{i=1}^{5} \alpha_i t^{(i-1)} \tag{2.3.3}$$

We can subdivide the time interval into five equal segments as shown in Figure 2.3.2. The reason for choosing five subdivisions here is again in accordance to our intention of striking a balance between the accuracy attainable and the complexity involved, six subdivisions would add considerably to the complexity of the solution. Let x_k represent $x(t=t_k)$ we can then construct five equations:

$$x_k = \sum_{i=1}^{5} \alpha_i t_k^{(i-1)} \tag{2.3.4}$$

which can be solved for the coefficients α_i $(i = 1,2,...,5)$ as a linear function of the position $x_k (k = 1,2,...,5)$. The functional relationship in this case turns out to be:

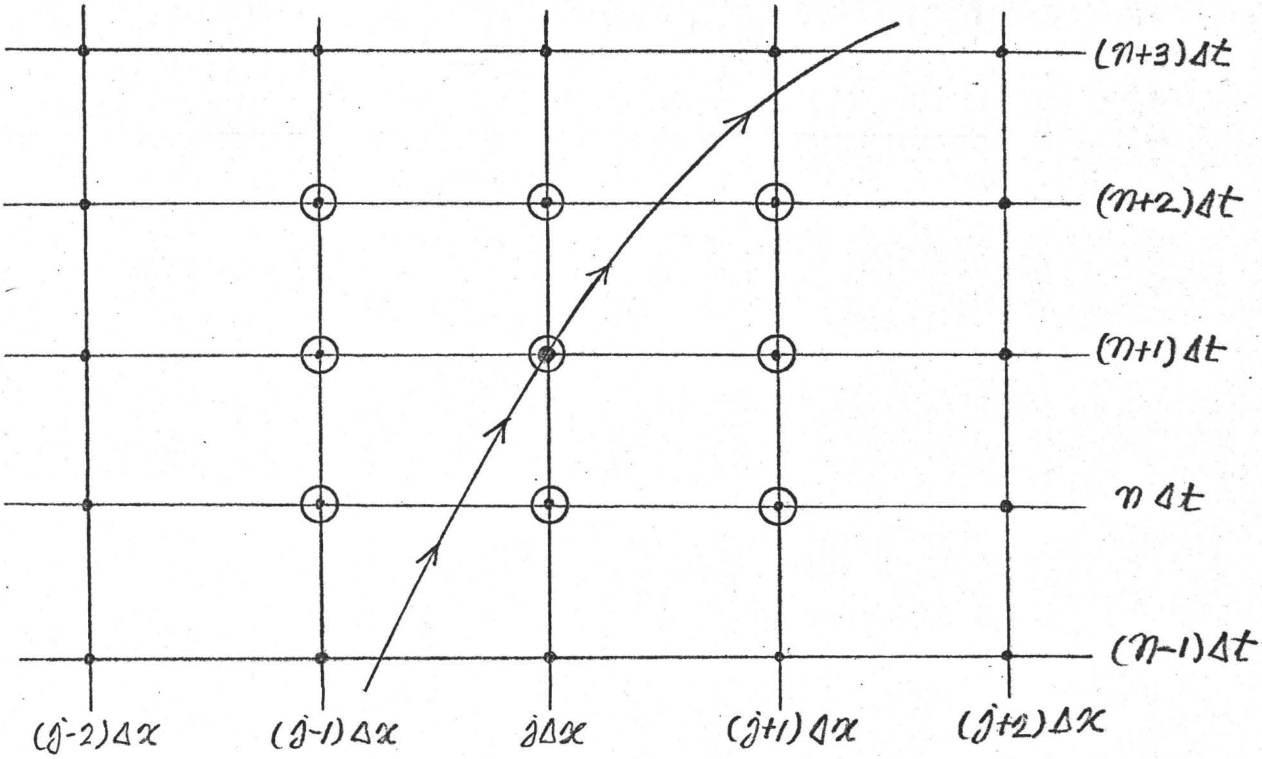


Figure 2.3.1: The chosen points of known velocity about the point $(j\Delta x, (n+1)\Delta t)$.

$$\alpha_1 = 0$$

$$\alpha_2 = \left(\frac{1}{6\Delta t}\right) [-x_5 + 8x_4 - 8x_2 + x_1]$$

$$\alpha_3 = \left(\frac{1}{6\Delta t^2}\right) [-x_5 + 16x_4 + 16x_2 - x_1] \tag{2.3.5}$$

$$\alpha_4 = \left(\frac{2}{3\Delta t^3}\right) [x_5 - 2x_4 + 2x_2 - x_1]$$

$$\alpha_5 = \left(\frac{2}{3\Delta t^4}\right) [x_5 - 4x_4 - 4x_2 + x_1]$$

The details of the missing algebra can be found in Appendix 1.

Substituting for x(t) into equation 2.3.1

$$u[x(t),t] = u(t) = \sum_{i=1}^{3} \sum_{j=1}^{3} \lambda_{ij}[x(t)]^{(j-1)}[t]^{(i-1)}$$

which can be written as:

$$u(t) = \sum_{i=1}^{11} e_i t^{(i-1)} \tag{2.3.6}$$

where the coefficients are:

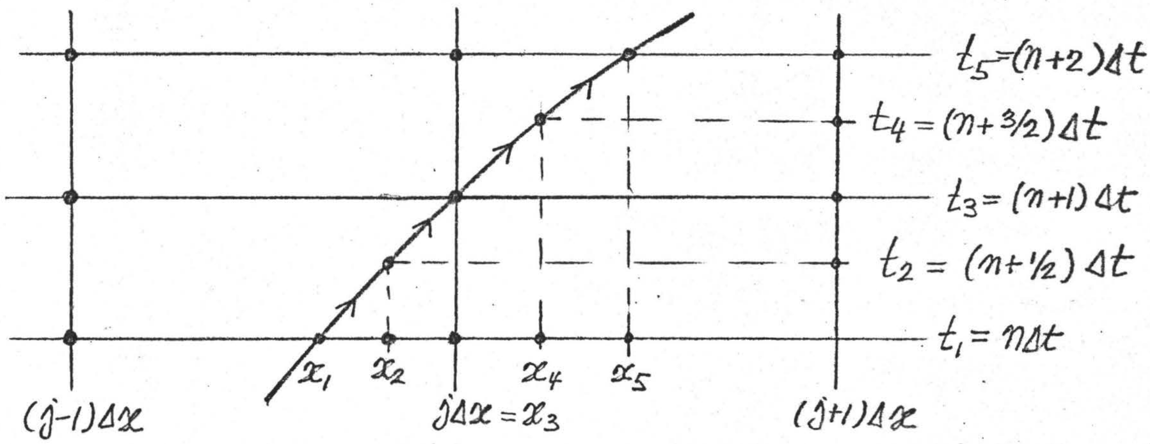


Figure 2.3.2: Subdivision of the particle path into five equal time segments.

$$e_1 = \lambda_{11}$$

$$e_2 = \lambda_{21} + \lambda_{12}\alpha_2$$

$$e_3 = \lambda_{31} + \lambda_{12}\alpha_3 + \lambda_{22}\alpha_2 + \lambda_{13}\alpha_2^2$$

$$e_4 = \lambda_{12}\alpha_4 + \lambda_{22}\alpha_3 + \lambda_{32}\alpha_2 + 2\lambda_{13}\alpha_2\alpha_3 + \lambda_{23}\alpha_2^2$$

$$e_5 = \lambda_{12}\alpha_5 + \lambda_{22}\alpha_4 + \lambda_{32}\alpha_3 + \lambda_{13}(2\alpha_2\alpha_4 + \alpha_3^2) + 2\lambda_{33}\alpha_2\alpha_3$$

$$e_6 = \lambda_{12}\alpha_5 + \lambda_{22}\alpha_4 + \lambda_{32}\alpha_3 + \lambda_{13}(2\alpha_2\alpha_4 + \alpha_3^2) + 2\lambda_{23}\alpha_2\alpha_3 + \lambda_{33}\alpha_2^2$$

$$e_7 = \lambda_{22}\alpha_5 + \lambda_{32}\alpha_4 + 2\lambda_{13}(\alpha_2\alpha_5 + \alpha_3\alpha_4) + \lambda_{23}(2\alpha_2\alpha_4 + \alpha_3^2) + 2\lambda_{33}\alpha_2\alpha_4$$

$$e_8 = \lambda_{32}\alpha_5 + \lambda_{13}(2\alpha_3\alpha_5 + \alpha_4^2) + 2\lambda_{23}(\alpha_2\alpha_5 + \alpha_3\alpha_4) + \lambda_{33}(2\alpha_2\alpha_4+\alpha_3^2$$

$$e_9 = 2\lambda_{13}\alpha_4\alpha_5 + \lambda_{23}(2\alpha_3\alpha_5 + \alpha_4^2) + 2\lambda_{33}(\alpha_2\alpha_5 + \alpha_3\alpha_4)$$

$$e_{10} = \lambda_{13}\alpha_5^2 + 2\lambda_{23}\alpha_4\alpha_5 + \lambda_{33}(2\alpha_3\alpha_5 + \alpha_4^2)$$

$$e_{11} = \lambda_{33}\alpha_5^2$$

Please refer to Appendix 2 for the details of the algebra.

Substituting for equation 2.3.6 into the integrand of equation 2.2.11 we get:

$$x_k = x_1 + \int_{t=t_1}^{t_k} [\sum_{i=1}^{11} e_i \, t^{(i-1)}]dt$$

Evaluating the definite integral

$$x_k = x_1 + \sum_{i=1}^{11} [\frac{e_i}{i} (t_k^i - t_1^i)] \tag{2.3.7}$$

For $k = 2,3,4,5$ equation 2.3.7 represents a system of four equations in which the only unknowns are x_1, x_2, x_4, x_5, since $x_3 = 0$.

However these equations are non-linear in the unknowns, we can construct a homogeneous function H_k:

$$H_k = x_k - x_1 - \sum_{i=1}^{11} [\frac{e_k(x_1,x_2,x_4,x_5)}{i} (t_k^i - t_1^i)] = 0 \qquad (2.3.8)$$

The problem then reduces to finding the values of x_1, x_2, x_4 and x_5 which will make H_k equal to zero. We can use the Newton-Raphson technique to solve it. The value of x_k given by the pth iteration is given by:

$$x_{k_{p+1}} = x_{k_p} - \frac{H_{k_p}}{\left[\frac{\partial H_k}{\partial x_\ell}\right]_p} \qquad (2.3.9)$$

where ℓ = 1, 2, 4, 5. The above system can be rearranged into the following format:

$$\left[\frac{\partial H_k}{\partial x_\ell}\right] (\Delta x_{k_p}) = -H_{k_p} \qquad (2.3.10)$$

where $\Delta x_{k_p} = x_{k_{p+1}} - x_{k_p}$

Thus the value of x_k after the pth iteration is given by

$$x_{k_{p+1}} = x_{k_p} + \Delta x_{k_p} \qquad (2.3.11)$$

Where Δx_{k_p} is the solution of the linear system of equation (2.3.10), the matrix on the left is the Jacobian matrix and its elements are:

$$\frac{\partial H_k}{\partial x_\ell} = \begin{bmatrix} \frac{\partial H_2}{\partial x_1} & \frac{\partial H_2}{\partial x_2} & \frac{\partial H_2}{\partial x_4} & \frac{\partial H_2}{\partial x_5} \\ \frac{\partial H_3}{\partial x_1} & \frac{\partial H_3}{\partial x_2} & \frac{\partial H_3}{\partial x_4} & \frac{\partial H_3}{\partial x_5} \\ \frac{\partial H_4}{\partial x_1} & \frac{\partial H_4}{\partial x_2} & \frac{\partial H_4}{\partial x_4} & \frac{\partial H_4}{\partial x_5} \\ \frac{\partial H_5}{\partial x_1} & \frac{\partial H_5}{\partial x_2} & \frac{\partial H_5}{\partial x_4} & \frac{\partial H_5}{\partial x_5} \end{bmatrix} \tag{2.3.12}$$

The expression for each element can be found in Appendix 3.

The convergence criterium adopted here is to iterate until

$$\frac{|\Delta x_{k_p}|}{|x_{k_{p+1}}|} < 10^{-12}$$

In the runs done to date the above condition is usually met with only a few iterations. The program prints an error message if more than ten iterations are required.

Once the values of x_1, x_2, x_4 and x_5 are found then the coefficients of the particle path function can be calculated since their functional relationship to x_k is already known (Equation 2.3.5).

Now that the particle path equation of interest has been established it becomes a simple matter to find the point on the line $t = n\Delta t$ which the particle path crosses, as shown on Figure 2.3.3. The value of ϕ at this point is $\tilde{\phi}_j^{n+1}$ and will be needed for our calculation.

The value of $\tilde{\phi}_j^{n+1}$ can be found by interpolation. By expanding

$\tilde{\phi}_j^{n+1}$ and other known values of ϕ in a Taylor series the following equations can be constructed:

$$\tilde{\phi}_j^{n+1} = \phi_o + \sum_{i=1}^{4} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} \left[\frac{\Delta x}{2} - x_1\right]^i \tag{2.3.13}$$

$$\phi_{j-2}^{n} = \phi_o + \sum_{i=1}^{4} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} \left[\frac{-3\Delta x}{2}\right]^i \tag{2.3.14}$$

$$\phi_{j-1}^{n} = \phi_o + \sum_{i=1}^{4} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} \left[\frac{-\Delta x}{2}\right]^i \tag{2.3.15}$$

$$\phi_{j}^{n} = \phi_o + \sum_{i=1}^{4} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} \left[\frac{\Delta x}{2}\right]^i \tag{2.3.16}$$

$$\hat{\phi}_{j-2}^{n-1} = \phi_o + \sum_{i=1}^{4} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} \left[\frac{-3\Delta x}{2} + d2_{j-2}\right]^i \tag{2.3.17}$$

$$\hat{\phi}_{j-1}^{n-1} = \phi_o + \sum_{i=1}^{4} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial x^i} \left[- \frac{\Delta x}{2} + d2_{j-1}\right]^i \tag{2.3.18}$$

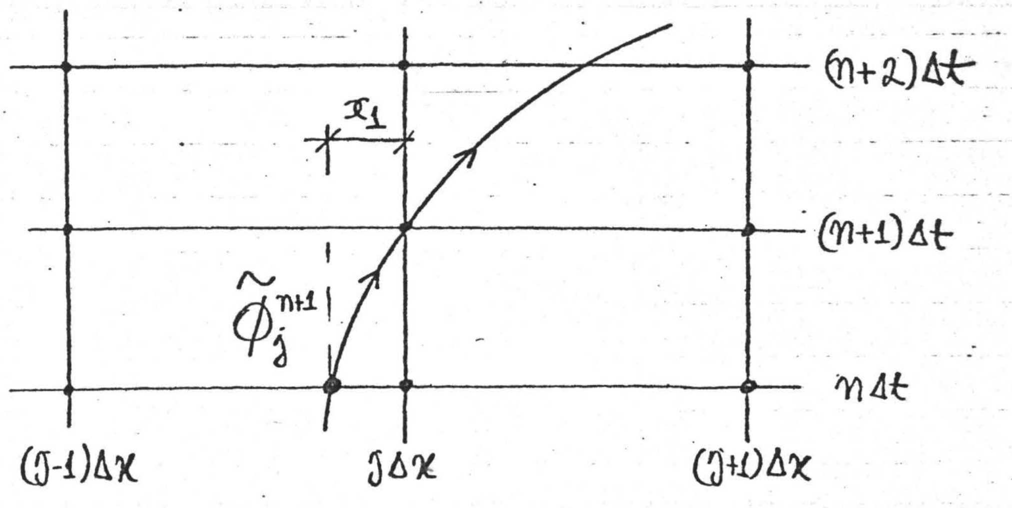


Figure 2.3.3: The intersection of the particle path with the line $t = n\Delta t$.

Where the centre of expansion is taken to be $\Delta x/2$ to the left of the point $(j\Delta x,\ n\Delta t)$ as shown on Figure 2.3.4.

There are six unknowns in equations 2.3.13 to 2.3.18, namely,

$$\tilde{\phi}_j^{n+1}\ ;\ \phi_o \text{ and } \frac{\partial^i\phi}{\partial x^i}\quad i = 1,\ 2,\ 3,\ 4$$

and since we have the same number of independent equations the solution set will be unique. These equations can be written in matrix notations as:

$$\begin{bmatrix} -1 & 1 & (\frac{\Delta x}{2} - x_1) + \ldots\ldots + (\frac{\Delta x}{2} - x_1)^4 \\ 0 & 1 & (\frac{-3\Delta x}{2}) + \ldots\ldots\ldots + (\frac{-3\Delta x}{2})^4 \\ 0 & 1 & (\frac{-\Delta x}{2}) + \ldots\ldots\ldots\ldots + (\frac{-\Delta x}{2})^4 \\ 0 & 1 & (\frac{\Delta x}{2}) + \ldots\ldots\ldots\ldots\ldots + (\frac{\Delta x}{2})^4 \\ 0 & 1 & (\frac{-3\Delta x}{2} + d2_{j-2}) + \ldots + (\frac{-3\Delta x}{2} + d2_{j-2})^4 \\ 0 & 1 & (\frac{-\Delta x}{2} + d2_{j-1}) + \ldots + (\frac{-\Delta x}{2} + d2_{j-1})^4 \end{bmatrix} \begin{bmatrix} \tilde{\phi}_j^{n+1} \\ \phi_o \\ \frac{\partial\phi}{\partial x} \\ \frac{1}{2!}\frac{\partial^2\phi}{\partial x^2} \\ \frac{1}{3!}\frac{\partial^3\phi}{\partial x^3} \\ \frac{1}{4!}\frac{\partial^4\phi}{\partial x^4} \end{bmatrix} = \begin{bmatrix} 0 \\ \phi_{j-2}^n \\ \phi_{j-1}^n \\ \phi_j^n \\ \hat{\phi}_{j-2}^{n-1} \\ \hat{\phi}_{j-1}^{n-1} \end{bmatrix}$$

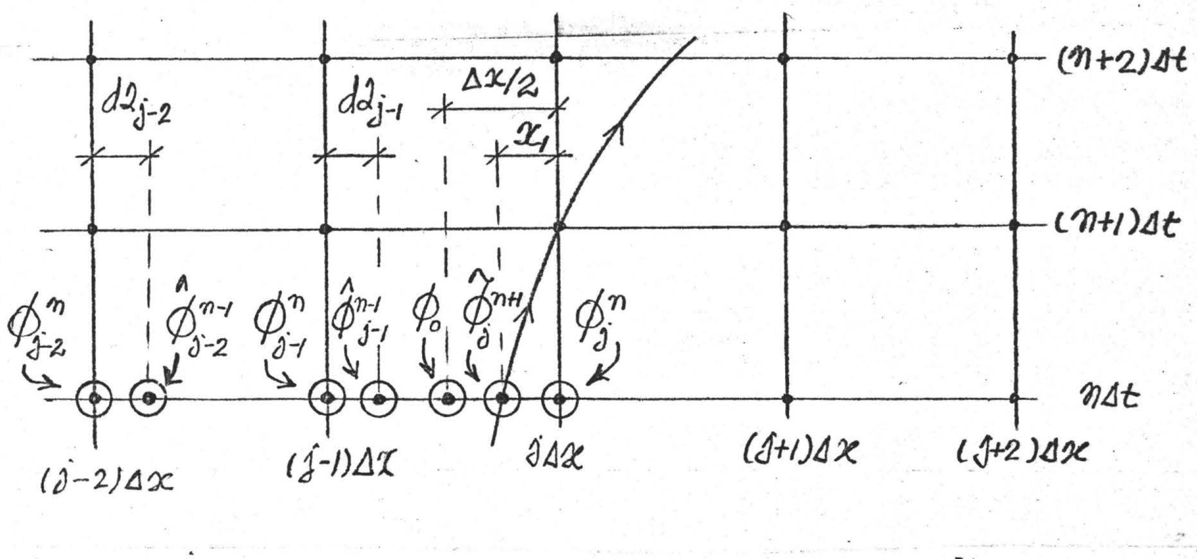


Figure 2.3.4: Values of ϕ used for the calculation of $\tilde{\phi}_j^{n+1}$.

A matrix solution routine is used to solve the above system. If we do this for every value of j $(1 \leq j \leq J)$ we will then have all the values of $\tilde{\phi}_j^{n+1}$ along the line $t = n\Delta t$.

A functional relationship for $\frac{\partial u}{\partial x}(t)$ along the particle path can now be constructed. The spatial derivative of equation 2.3.1 gives:

$$\frac{\partial u(x,t)}{\partial x} = \sum_{i=1}^{3} \sum_{j=1}^{3} (j-1)\ \lambda_{ij}\ x^{(j-2)} t^{(i-1)}$$

Substituting for the particle path equation for x above

$$\frac{\partial u}{\partial x}(t) = \sum_{i=1}^{3} \sum_{j=1}^{3} (j-1)\ \lambda_{ij}[x(t)]^{(j-2)}[t]^{(i-1)}$$

$$= \sum_{i=1}^{3} \sum_{j=1}^{3} \{(j-1)\ \lambda_{ij}\ [\sum_{p=2}^{5} \alpha_p t^{(p-1)}]^{(j-2)}[t]^{i-1}\}$$

which reduces to:

$$\frac{\partial u}{\partial t}(t) = \sum_{i=1}^{7} D_i t^{(i-1)} \tag{2.3.13}$$

where the coefficients are given by:

$$\begin{aligned}
D_1 &= \lambda_{12} \\
D_2 &= 2\lambda_{13}\alpha_2 + \lambda_{22} \\
D_3 &= 2\lambda_{13}\alpha_3 + 2\lambda_{23}\alpha_2 + \lambda_{32} \\
D_4 &= 2\lambda_{13}\alpha_4 + 2\lambda_{23}\alpha_3 + 2\lambda_{33}\alpha_2 \\
D_5 &= 2\lambda_{13}\alpha_5 + 2\lambda_{23}\alpha_4 + 2\lambda_{33}\alpha_3 \\
D_6 &= 2\lambda_{23}\alpha_5 + 2\lambda_{33}\alpha_4 \\
D_7 &= 2\lambda_{33}\alpha_5
\end{aligned} \tag{2.3.14}$$

The missing algebra can be found in Appendix 2.

Now let's assume that $\phi(x)$ along the particle path can be represented by:

$$\phi(x) = \sum_{i=1}^{5} \beta_i x^{(i-1)} \tag{2.3.15}$$

Let ϕ_K be the value of ϕ at the point $x_k = x(t_k)$ on the particle path. We can construct 5 equations represented by:

$$\phi_k = \sum_{i=1}^{5} \beta_i x_k^{(i-1)}, \; k = 1, 2, \ldots, 5 \tag{2.3.16}$$

We can again solve for the coefficients $\beta_i (i=1,2,\ldots,5)$ as linear functions of ϕ_k $(k = 1,2,\ldots,5)$. The details of the solution and the final format of these functions are given in Appendix 1.

So now we have an expression for $\phi(x)$ along the particle path which is a linear function of ϕ_k $(k = 1,2,\ldots,5)$.

$$\phi(x) = \sum_{i=1}^{5} \beta_i(\phi_1, \phi_2, \ldots \phi_5) x^{(i-1)} \tag{2.3.22}$$

Substituting for the particle path equation into equation 2.3.22 we then have $\phi(t)$ along the particle path:

$$\begin{aligned} \phi[x(t)] = \phi(t) &= \sum_{i=1}^{5} \beta_i(\phi_1, \phi_2, \ldots, \phi_5)\,[x(t)]^{(i-1)} \\ &= \sum_{i=1}^{5} \{\beta_i(\phi_1, \phi_2, \ldots, \phi_5)[\sum_{p=1}^{5} \alpha_p t^{(p-1)}]^{(i-1)}\} \end{aligned}$$

which can be written as:

$$\phi(t) = \sum_{i=1}^{17} \xi_i(\phi_1, \phi_2, \ldots, \phi_5) t^{(i-1)} \tag{2.3.23}$$

The coefficients ξ_i ($i = 1, 2, \ldots, 17$) are given in Appendix 2.

We can now find an expression for the function

$$F(t) = \phi(t) * \frac{\partial u}{\partial x}(t)$$

along the particle path. This can be accomplished by multiplying equation 2.3.23 by equation 2.3.13

$$F(t) = \left[\sum_{i=1}^{17} \xi_i(\phi_1, \phi_2, \ldots, \phi_5) t^{(i-1)}\right]\left[\sum_{i=1}^{7} D_i t^{(i-1)}\right]$$

which can be written as:

$$F(t) = \sum_{i=1}^{23} R_i(\phi_1, \phi_2, \ldots, \phi_5) t^{(i-1)} \qquad (2.3.24)$$

The coefficients R_i ($i = 1, 2, \ldots, 23$) are also given in Appendix 2.

We can now go back to the line integral developed in section 2 (equation 2.2.3):

$$\int_{t=t_o}^{t} d\phi = - \int_{t=t_o}^{t} \left(\phi \frac{\partial u}{\partial x}\right) dt$$

Replacing the lower bound of the definite integral by $t = t_1$ as shown on Figure 2.3.5 and the upper bound by $t = t_k$ and substituting

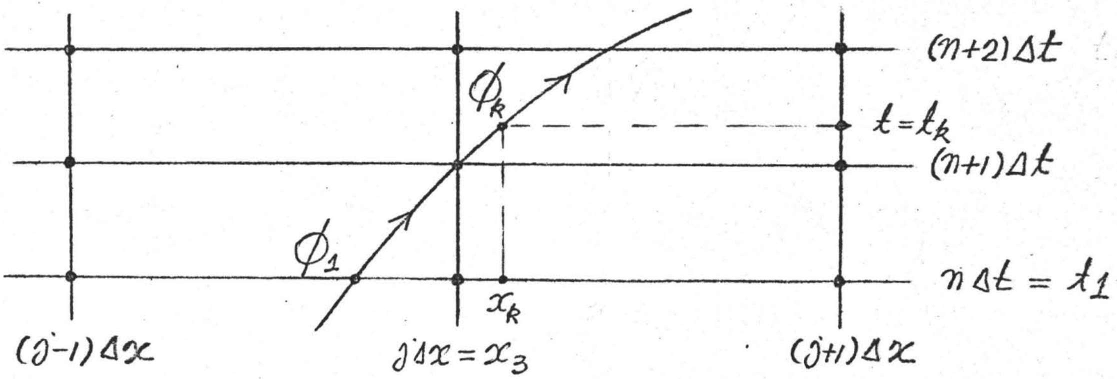


Figure 2.3.5: The bounds of integration along the particle path.

for F(t) from equation 2.3.24 for the integrand

$$\int_{t_1}^{t_k} d\phi = -\int_{t_1}^{t_k} [\sum_{i=1}^{23} R_i(\phi_1, \phi_2, \ldots, \phi_5)t^{(i-1)}]dt$$

$$\rightarrow \qquad \phi_k = \phi_1 - \int_{t_1}^{t_k} [\sum_{i=1}^{23} R_i(\phi_1, \phi_2, \ldots, \phi_5)t^{(i-1)}]dt$$

After evaluating the definite integral on the right we get:

$$\phi_k = \phi_1 - \sum_{i=1}^{23} \{[\frac{R_i(\phi_1, \phi_2, \ldots, \phi_5)}{i}]*[t_k^i - t_1^i]\} \tag{2.3.25}$$

The above expression represents a system of linear equations in four unknowns, namely ϕ_2, ϕ_3, ϕ_4 and ϕ_5. If we take k = 2, 3, 4 and 5 we can construct four linear independent equations with respect to the unknowns, thus a unique solution set can be obtained. To simplify the algebra involved we construct a homogeneous function S_k by transferring all the elements of equation 2.3.25 to one side:

$$S_k = \phi_k - \phi_1 + \sum \{[\frac{R_1(\phi_1, \phi_2, \ldots, \phi_5)}{i}]*[t_k^i - t_1^i]\} = 0 \tag{2.3.26}$$

where k = 2, 3, 4, 5. Now since S_k is linear in ϕ_j it can be seen that

$$S_k = \sum_{j=1}^{5} \{[\frac{\partial S_k}{\partial \phi_j}] \phi_j\} = 0$$

Using this concept the matrix representation of the system can now be written as:

$$\begin{pmatrix} \frac{\partial S_2}{\partial \phi_2} & \frac{\partial S_2}{\partial \phi_3} & \frac{\partial S_2}{\partial \phi_4} & \frac{\partial S_2}{\partial \phi_5} \\ \frac{\partial S_3}{\partial \phi_2} & \frac{\partial S_3}{\partial \phi_3} & \frac{\partial S_3}{\partial \phi_4} & \frac{\partial S_3}{\partial \phi_5} \\ \frac{\partial S_4}{\partial \phi_2} & \frac{\partial S_4}{\partial \phi_3} & \frac{\partial S_4}{\partial \phi_4} & \frac{\partial S_4}{\partial \phi_5} \\ \frac{\partial S_5}{\partial \phi_2} & \frac{\partial S_5}{\partial \phi_3} & \frac{\partial S_5}{\partial \phi_4} & \frac{\partial S_5}{\partial \phi_5} \end{pmatrix} \begin{pmatrix} \phi_3 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{pmatrix} = \begin{pmatrix} -\frac{\partial S_2}{\partial \phi_1}\phi_1 \\ -\frac{\partial S_3}{\partial \phi_1}\phi_1 \\ -\frac{\partial S_4}{\partial \phi_1}\phi_1 \\ -\frac{\partial S_5}{\partial \phi_1}\phi_1 \end{pmatrix} \tag{2.3.27}$$

Where the partial derivatives used above are given by:

$$\frac{\partial S_k}{\partial \phi_j} = \frac{\partial \phi_k}{\partial \phi_j} - \frac{\partial \phi_1}{\partial \phi_j} + \sum_{i=1}^{23} \{\frac{1}{i} * \frac{\partial R_i}{\partial \phi_j} * [t_k^i - t_1^i]\} \tag{2.3.28}$$

More details of the derivation above can be found in Appendix 3.

The solution of the linear system of equation 2.3.27 will give the value of ϕ_j^{n+1} and also $\hat{\phi}_j^{n+1}$ since:

$$\phi_j^{n+1} = \phi_3$$

$$\hat{\phi}_j^{n+1} = \phi_5$$

as can be seen in figure 2.3.6.

By going through this procedure for all values of j $(1 \leq j \leq J)$ the solution to the advection equation will be advanced by one time step. We will then have:

$$\phi(x,t+\Delta t) = \phi_j^{n+1} \qquad j = 1, 2, \ldots, J$$

and the value of $\hat{\phi}_j^{n+1}$ which will be used for the interpolation of $\tilde{\phi}_j^{n+2}$ at the next time step.

This procedure can be repeated for as many time steps as necessary, such that at the end we have:

$$\phi(x=j\Delta x,\ t=n\Delta t) \qquad \text{for} \qquad \begin{array}{l} j = 1, 2, 3, \ldots J \\ n = 1, 2, 3, \ldots N \end{array}$$

which is the solution to the general advection equation for the finite domain of interest which was estipulated at the beginning.

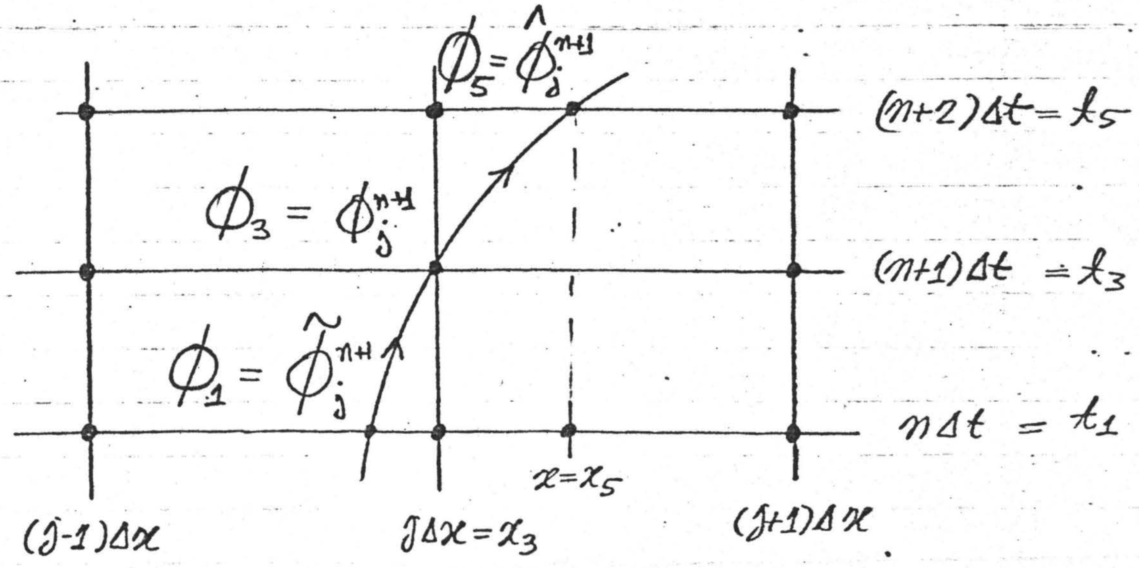


Figure 2.3.6: The position of ϕ_j^{n+1} and $\hat{\phi}_j^{n+1}$ on the particle path.

2.4 Description of the Computer Program

A listing of the computer program is attached at the end of this report. The identification of the variables used, the function of each subroutine and a block diagram are presented in this section.

Variable Identification

PHI (J,N) ≡ ϕ_j^n

PHIBAR (J,N) ≡ $\tilde{\phi}_j^n$

PHIHAT (J,N) ≡ $\hat{\phi}_j^n$

PHIUSED (J,N) ≡ The concentration as given by the one-sided F.D. method

PHITRUE (J,N) ≡ The true analytical solution

RU (J,N) ≡ The velocity field

D1 (J,N) ≡ x_1

D2 (J,N) ≡ x_5

DUDX (J,N) ≡ Spatial derivative of the velocity field

S (J,N) ≡ Source term

RL ≡ Pipe length

JJ ≡ Total number of nodes

DT ≡ Time step

DX ≡ Node length

TIME ≡ Real time

TIMEF ≡ Total real time

NTS ≡ Total number of time steps

UCOEF (3,3,J) ≡ Coefficients of the local velocity field expansion

PCOEF (5,3) ≡ Coefficients of the local particle path function

SCOEF (3,3,J) ≡ Coefficients of the local source function

PHIPLOT (*,*,*) ≡ Array containing selected points to be plotted

Description of Subroutines

UPDATE:

It supplies initial and boundary conditions and updates all other variables in the three time level scheme.

FIT:

It finds a functional representation for the local velocity field and source term by means of double Taylor series expansion.

PPATH:

It finds an equation for the local particle path by the method of Pickard and the method of Newton-Raphson for the solution of the non-linear system.

PHIBARS:

It finds the value of $\tilde{\phi}_j^{n+1}$ by a 5th order interpolation.

SOLVE:

It solves the final equation and gives numerical values for ϕ_j^{n+1} and $\hat{\phi}_j^{n+1}$.

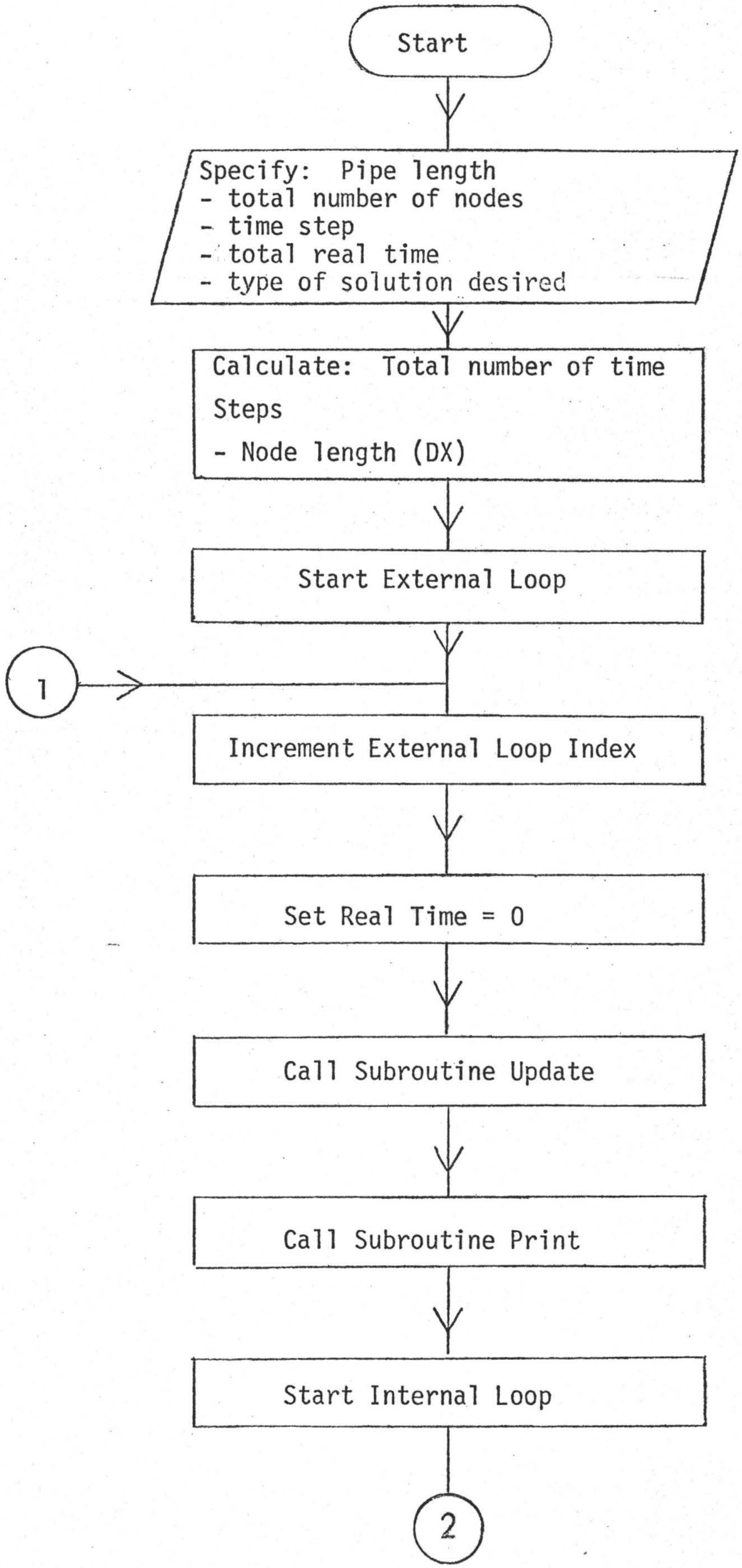
PRINT:

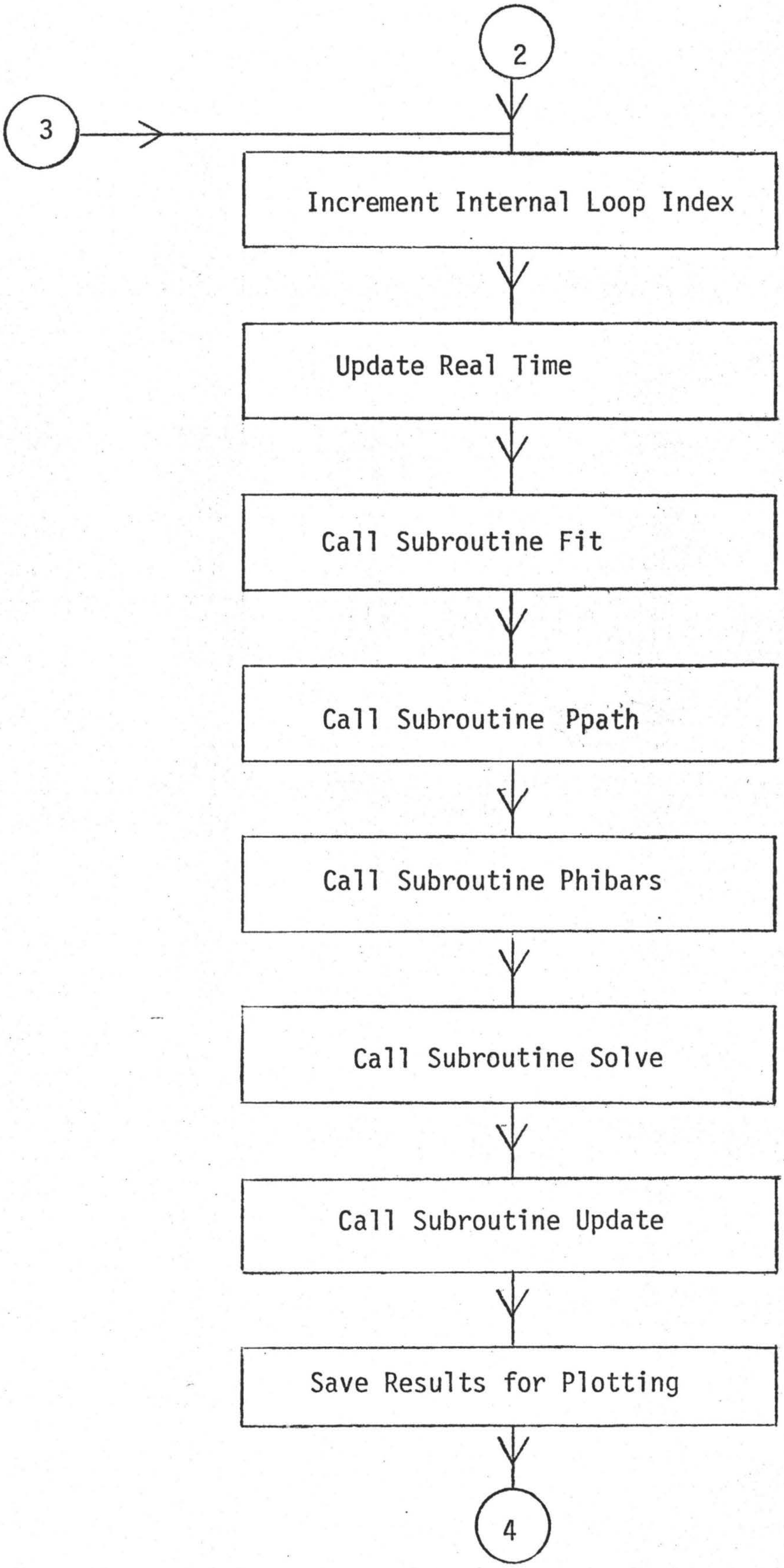
This subroutine simply prints the results in a prespecified format.

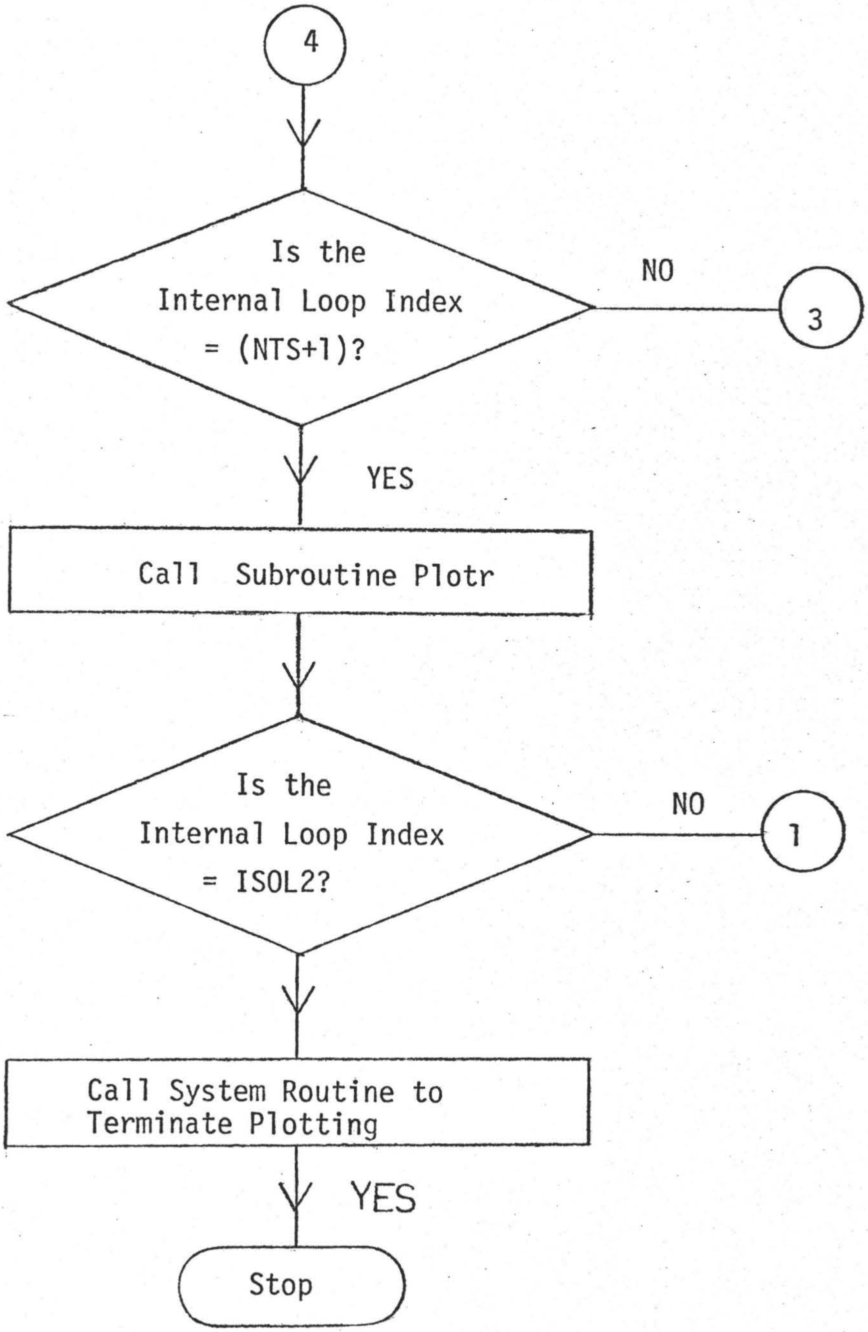
PLOTR:

Plots select results.

BLOCK DIAGRAM




2
3
Increment Internal Loop Index
Update Real Time
Call Subroutine Fit
Call Subroutine Ppath
Call Subroutine Phibars
Call Subroutine Solve
Call Subroutine Update
Save Results for Plotting
4


4
Is the
Internal Loop Index
= (NTS+1)?
NO
3
YES
Call Subroutine Plotr
Is the
Internal Loop Index
= ISOL2?
NO
1
Call System Routine to
Terminate Plotting
YES
Stop

CHAPTER 3

ERROR PROPAGATION ANALYSIS

In the functional scheme outlined in section 2.3 power series expansions were used to approximate the value of several functions within some prescribed domain. All of these approximations carry with them an inherent error due to the finite number of terms used in their power series representation. In this chapter we will try to identify each error in particular and look at the total compound effect that they all have in the final solution.

3.1 The Velocity Field Approximation

Let f(x,t) be a continuous and differentiable function of x and t. Consider an arbitrary point (Δx, Δt) near the origin. If Δx and Δt lie within the radius of convergence of the Taylor series expansion of f(x,t) then the value of f at the point (Δx, Δt) can be obtained by the relation:

$$f(\Delta x,\ \Delta t) = f_o + \sum_{p=1}^{\infty} \{(\frac{1}{p!}) \sum_{r=0}^{p} [\binom{p}{r} \frac{\partial^p f}{\partial x^r \partial y^{(p-r)}} \Delta x^r \Delta t^{(p-r)} \tag{3.1.1}$$

where f_o = f(x=0, t = 0) and the partial derivatives of f are evaluated at the origin. Expanding the first four terms in the above equation

$$f(\Delta x,\ \Delta t) = f(0,0) + [\frac{\partial f}{\partial x} \Delta x + \frac{\partial f}{\partial t} \Delta t]$$

$$+ \frac{1}{2!} [\frac{\partial^2 f}{\partial x^2} \Delta x^2 + 2 \frac{\partial^2 f}{\partial x \partial t} \Delta x \Delta t + \frac{\partial^2 f}{\partial t^2} \Delta t^2]$$

$$+ \frac{1}{3!}\left[\frac{\partial^3 f}{\partial x^3}\Delta x^3 + 3\frac{\partial^3 f}{\partial x^2 \partial t}\Delta x^2 \Delta t + 3\frac{\partial^3 f}{\partial x \partial t^2}\Delta x \Delta t^2 + \frac{\partial^3 f}{\partial t^3}\Delta t^3\right]$$

$$+ \frac{1}{4!}\left[\frac{\partial^4 f}{\partial x^4}\Delta x^4 + 4\frac{\partial^4 f}{\partial x^3 \partial t}\Delta x^3 \Delta t + 6\frac{\partial^4 f}{\partial x^2 \partial t^2}\Delta x^2 \Delta t^2 + 4\frac{\partial^4 f}{\partial x \partial t^3}\Delta x \Delta t^3\right.$$

$$\left. + \frac{\partial^4 f}{\partial t^4}\Delta t^4\right] + R_4(\Delta x, \Delta t) \tag{3.1.2}$$

Where $R_4(\Delta x, \Delta t)$ stands for the remainder terms and is given by

$$R_4(\Delta x, \Delta t) = \frac{1}{5!}\left(\Delta x \frac{\partial}{\partial x} + \Delta t \frac{\partial}{\partial t}\right)^5 f(\theta\Delta x, \theta\Delta t) \tag{3.1.3}$$

and $0 \leq \theta \leq 1$.

Let $U_A(x,t)$ stand for the approximate local velocity field about the point $(j\Delta x, (n+1)\Delta t)$ as given by equation 2.3.1 which is reproduced below:

$$U(x,t) = \sum_{i=1}^{3}\sum_{j=1}^{3} \lambda_{ij} x^{(j-1)} t^{(i-1)} \tag{3.1.4}$$

Expanding the above equation for $x = \Delta x$ and $t = \Delta t$

$$U_A(\Delta x, \Delta t) = \lambda_{11} + [\lambda_{12}\Delta x + \lambda_{21}\Delta t]$$

$$+ [\lambda_{13}\Delta x^2 + \lambda_{22}\Delta x\Delta t + \lambda_{31}\Delta t^2]$$

$$+ [0\Delta x^3 + \lambda_{23}\Delta x^2\Delta t + \lambda_{32}\Delta x\Delta t^2 + 0\Delta t^3]$$

$$+ [0\Delta x^4 + 0\Delta x^3\Delta t + \lambda_{33}\Delta x^2\Delta t^2 + 0\Delta x\Delta t^3 + 0\Delta t^4] \tag{3.1.5}$$

If $f(x,t)$ is replaced by $u(x,t)$ in equation 3.1.2 then it becomes the true velocity at $(x = \Delta x, t = \Delta t)$, let it be denoted by

$u_T(\Delta x, \Delta t)$. The error introduced in the approximation of equation 3.1.5 can then be obtained by the equation:

$$E_U(\Delta x, \Delta t) = u_T(\Delta x, \Delta t) - u_A(\Delta x, \Delta t)$$

$$= R_4(\Delta x, \Delta t) + \frac{1}{3!}\left[\frac{\partial^3 u}{\partial x^3}\Delta x^3 + \frac{\partial^3 u}{\partial t^3}\Delta t^3\right]$$

$$+ \frac{1}{4!}\left[\frac{\partial^4 u}{\partial x^4}\Delta x^4 + 4\frac{\partial^4 u}{\partial x^3 \partial t}\Delta x^3 \Delta t + 4\frac{\partial^4 u}{\partial x \partial t^3}\Delta x \Delta t^3 + \frac{\partial^4 u}{\partial t^4}\Delta t^4\right] \quad (3.1.6)$$

Equation 3.1.6 represents the amount by which the approximation to the velocity field about the point $(j\Delta x, (n+1)\Delta t)$ differs from the true value.

Thus the approximate velocity field can be written in terms of the true velocity field by:

$$u_A(\Delta x, \Delta t) = u_T(\Delta x, \Delta t) - E_u(\Delta x, \Delta t) \quad (3.1.7)$$

Where $E_u(\Delta x, \Delta t)$ is given by equation 3.1.6.

3.2 The Particle Path Approximation

Let $x(t)$ be a continuous and differentiable function of time. For some values of $t = \Delta t$ which lie within the radius of convergence of its Taylor series expansion about the origin $(x=0)$ we may write:

$$\Delta x = x(\Delta t) = \sum_{i=1}^{n} \left(\frac{1}{i!}\right)\left(\frac{\partial^i x}{\partial t^i}\right)_o \Delta t^i + R_n(\Delta t) \quad (3.2.1)$$

where the remainder R_n can be written as:

$$R_n(\Delta t) = \frac{1}{(n+1)!}\left(\frac{\partial^{n+1} x}{\partial t^{n+1}}\right)_{\xi \Delta t} \Delta t^{n+1} \quad (3.2.2)$$

and $0 \le \xi \le \Delta t$.

Let the true particle path equation about the point $(j\Delta x, (n+1)\Delta t)$ be given by equation 3.2.1. In section 2.3 we made an approximation for x(t) which was:

$$x_A(t) = \sum_{p=1}^{5} \alpha_p t^{(p-1)} \tag{3.2.3}$$

The error in this approximation for $t = \Delta t$ is given by

$$E_x(\Delta t) = x_T(\Delta t) - x_A(\Delta t)$$

$$= \frac{1}{5!} \left(\frac{\partial^5 x}{\partial t^5}\right)_{\xi\Delta t} \Delta t^5$$

where $0 \lesssim \xi \lesssim 1$.

$$\Delta x_A = x_A(\Delta t) = x_T(\Delta t) - E_x(\Delta t) \tag{3.2.5}$$

If we now substitute for Δx_A into $u_A(\Delta x, \Delta t)$ we will have an expression for the approximate velocity field about the origin point $(j\Delta x, (n+1)\Delta t)$ as a function of Δt only. This can be accomplished by substituting for Δx_A from equation 3.2.5 into equation 3.1.7.

$$u_A(t) = u_A(\Delta x_A, \Delta t) = u_T(\Delta x_A, \Delta t) - E_u(\Delta x_A, \Delta t) \tag{3.2.6}$$

The expression for $u_T(\Delta x_A, \Delta t)$ can be obtained by substituting for Δx_A into the true expansion for $u(\Delta x, \Delta t)$:

$$u_T(\Delta x_A, \Delta t) = u(0, 0) + [\frac{\partial u}{\partial x} \Delta x_A + \frac{\partial u}{\partial t} \Delta t]$$

$$+ \frac{1}{2!} [\frac{\partial^2 u}{\partial x^2} \Delta x_A^2 + 2 \frac{\partial^2 u}{\partial x \partial t} \Delta x_A \Delta t + \frac{\partial^2 u}{\partial t^2} \Delta t^2]$$

$$+ \frac{1}{3!}\left[\frac{\partial^3 u}{\partial x^3}\Delta x_A^3 + 3\frac{\partial^3 u}{\partial x \partial t^2}\Delta x_A \Delta t^2 + 3\frac{\partial^3 u}{\partial x \partial t^2}\Delta x_A \Delta t^2 + \frac{\partial^3 u}{\partial t^3}\Delta t^3\right]$$

$$+ \frac{1}{4!}\left[\frac{\partial^4 u}{\partial x^4}\Delta x_A^4 + 4\frac{\partial^4 u}{\partial x \partial t^3}\Delta x_A \Delta t^3 + 6\frac{\partial^4 u}{\partial x^2 \partial t^2}\Delta x_s^2 \Delta t^2 + 4\frac{\partial^4 u}{\partial x \partial t^3}\Delta x \Delta t^3\right.$$

$$\left. + \frac{\partial^4 u}{\partial t^4}\Delta t^4\right] + R_4(\Delta x_A, \Delta t) \qquad (3.2.7)$$

If we now substitute for Δx_A from equation 3.2.5 into the above equation and re-arranging we get:

$$u_T(\Delta x_A, \Delta t) = u_T(\Delta x_T, \Delta t) + Su(\Delta x_A, \Delta t) \qquad (3.2.8)$$

where Su is given by:

$$Su(\Delta x_A, \Delta t) = \sum_{p=1}^{\infty} \left(\frac{1}{p!}\right)\left\{\sum_{r=0}^{p}\left[\binom{p}{r}\frac{\partial^p u}{\partial x^r \partial t^{(p-r)}} D^r[\Delta x]\Delta t^{(p-r)}\right]\right.$$

$$\left. - \frac{\partial^p U}{\partial t^p}\Delta t^p\right\} \qquad (3.2.9)$$

and the operator $D^r[\Delta x]$ is defined as:

$$D^r[\Delta x] = \begin{cases} [\Delta x_A^r - \Delta x_T^r] & \text{For } r \neq 0 \\ 1 & \text{For } r = 0 \end{cases}$$

Substituting for $u_T(\Delta x_A, \Delta t)$ from equation (3.2.8) into equation 3.2.6 we have:

$$u_A(t) = u_T(\Delta x_T, \Delta t) + Su(\Delta x_A, \Delta t) - E_u(\Delta x_A, \Delta t)$$

The first term on the right hand side of the above equation is in fact the true velocity along the particle path as a function of time only; thus the error in $_A(t)$ can now be expressed by:

$$Eu_A = u_A(t) - u_T(t)$$

$$Eu_A = Su(\Delta x_A, \Delta t) - E_u(\Delta x_A, \Delta t) \tag{3.2.10}$$

Where $Su(\Delta x_A, \Delta t)$ and $E_u(\Delta x_A, \Delta t)$ are given by equation 3.2.9 and 3.1.6 respectively.

Equation 3.2.10 expresses the total error of the approximation used for u(t) along the particle path about the point $(j\Delta x, (n+1)\Delta t)$. The approximate expression for u(t) can thus be written as:

$$u_A(\Delta t) = u_T(\Delta t) + Eu_A \tag{3.2.11}$$

where EU_A is given by equation 3.2.10.

The particle path calculation arises from the solution of the integral equation:

$$\int_{x=x_1}^{x_R} dX_A = \int_{t=t_1}^{t_k} u_A(t)dt$$

$$\therefore x_{A_k} = x_{A_1} + \int_{t=t_1}^{t_k} u_A(t)dt \tag{3.2.12}$$

Now since Δt and Δx were assumed to be arbitrary values we can replace them by t and x respectively in equation 3.2.11. We can then substitute for $U_A(t)$ into equation 3.2.12.

$$x_{A_k} = x_{A_1} + \int_{t=t_1}^{t_k} [u_T(t) + Eu_A]dt \tag{3.2.13}$$

We know that by definition the true value of x_k is given by

$$x_{T_k} = x_{T_1} + \int_{t=t_1}^{t_k} [u_T(t)]dt \qquad (3.2.14)$$

Subtracting equation 3.2.13 from equation 3.2.14 we get:

$$(x_{T_k} - x_{A_k}) = (x_{T_1} - x_{A_1}) - \int_{t=t_1}^{t_k} [Eu_A]dt \qquad (3.2.15)$$

which can be written as:

$$Sx_k = Sx_1 - \int_{t=t_1}^{t_k} [Eu_A]dt \qquad (3.2.16)$$

where: $Sx_k = x_{T_k} - x_{A_k}$

$Sx_1 = x_{T_1} - x_{A_1}$

and Eu_A is given by equation 3.2.10.

Equation 3.2.16 is an expression for the discrepancy between the true value of x_k and its approximate value. If $k = 3$ then the left hand side of equation 3.2.16 is identically zero since:

$$x_{T_3} = x_{A_3} = 0$$

Thus the value of Sx_1 can be obtained directly

$$Sx_1 = \int_{t=t_1}^{t_3} [Eu_A]dt \qquad (3.2.17)$$

Substituting for the above equation into equation 3.2.16 we have:

$$Sx_k = \int_{t=t_1}^{t_3} [Eu_A]dt - \int_{t=t_1}^{t_k} [Eu_A]dt \tag{3.2.18}$$

but:

$$\int_{t=t_1}^{t_k} [Eu_A]dt = \int_{t=t_1}^{t_3} [Eu_A]dt + \int_{t=t_3}^{t_k} [Eu_A]dt$$

$$\therefore \quad Sx_k = - \int_{t=t_3}^{t_k} [Eu_A]dt \tag{3.2.19}$$

Now since $t_3 = 0$

$$\rightarrow \quad Sx_k = - \int_0^{t_k} [Eu_A]dt \tag{3.2.20}$$

Substituting for E_A from equation 3.2.10

$$\rightarrow \quad Sx_k = -\int_0^{t_k} [Su(x_A,t) - E_u(x_A,t)]dt$$

Substituting for $Su(x_A,t)$ and $Eu(x_A,t)$ from equations 3.2.9 and 3.1.6 respectively into the above equation and performing the integration

$$Sx_k = - \sum_{p=1}^{\infty} \left(\frac{1}{p!}\right) \{\sum_{r=0}^{p} \binom{p}{r} \frac{\partial^p u}{\partial x^r \partial t^{(p-r)}} D^r[x] \left(\frac{t_k}{(p+1-r)}\right.$$

$$\left. - \frac{\partial^p u}{\partial t^p} \left(\frac{t_k^{p+1}}{p+1}\right)\} + \frac{1}{3!} \{\frac{\partial^3 u}{\partial x^3} x^3 t_k + \frac{1}{4} \frac{\partial^3 u}{\partial t^3} t_k^4\}\right.$$

$$+ \frac{1}{4!} \{\frac{\partial^4 u}{\partial x^4} x^4 t_k + 2 \frac{\partial^4 u}{\partial x^3 \partial t} x^3 t_k^2 + \frac{\partial^4 u}{\partial x \partial t^3} x \; t_k^4$$

$$+ \frac{1}{5} \frac{\partial^4 u}{\partial t^4} t_k^5\} \tag{3.2.21}$$

where

$$D^r[x] = \begin{cases} (x_A^r - x_T^r) & \text{for } r \neq 0 \\ 1 & \text{for } r = 0 \end{cases}$$

$$|t_k| \leq \Delta t$$

$$|x| \leq \Delta x$$

Equation 3.2.21 expresses the total error in the position x_k found by this method. The operator $D^r[x]$ is fifth order in x thus the second term in the above equation becomes the dominant one in the limit of small x and t.

$$\therefore\ Sx_k = O[\Delta x^i \Delta t^j] \qquad (3.2.22)$$

where $(i+j) \geq 4$

3.3 Error Due to Interpolation

The value of $\tilde{\phi}_j^{n+1}$ is found by solving the linear system given by equations 2.3.13 to 2.3.18 which are reproduced below:

$$\phi_k = \phi_o + \sum_{i=1}^{4} \left(\frac{1}{i!}\right) \frac{\partial^i \phi}{\partial z^i} z_k^i + R_k^5 \qquad (3.3.1)$$

where:

$$\phi_1 = \tilde{\phi}_j^{n+1} \quad ; \quad z_1 = [\tfrac{\Delta x}{2} - x_1]$$

$$\phi_2 = \phi_{j-2}^n \quad ; \quad z_2 = [- \tfrac{3\Delta x}{2}]$$

$$\phi_3 = \phi_{j-1}^n \quad ; \quad z_3 = [\tfrac{-\Delta x}{2}]$$

$$\phi_4 = \phi_j^n \quad ; \quad z_4 = [\tfrac{\Delta x}{2}]$$

$$\phi_5 = \hat{\phi}_{j-2}^{n-1} \quad ; \quad z_5 = [\tfrac{-3\Delta x}{2} + d2_{j-2}]$$

$$\phi_6 = \hat{\phi}_{j-1}^{n-1} \quad ; \quad z_6 = [- \tfrac{\Delta x}{2} + d2_{j-1}]$$

The remainder term R_k is made up of two terms. The first one is the normal Taylor series remainder, the second one is the error introduced by the wrong values of x_1, $d2_{j-2}$ and $d2_{j-1}$. Let:

$$z_k = z_{T_k} + Sx_k \qquad k = 1, 5, 6 \tag{3.3.2}$$

where z_{T_k} stands for the true value of z_k and sx_k stands for the discrepancy in x_k as given by equation 3.2.21. The general remainder term of equation 3.3.1 can then be written

$$R_k^5 = \frac{1}{5!}\frac{\partial^5\phi}{\partial z^5}[\theta z_{T_k}]^5 + S_k \tag{3.3.3}$$

where $0 \leq \theta \leq 1$ and

$$S_k = \begin{cases} \sum\limits_{i=1}^{4} \left(\frac{1}{i!}\right) \frac{\partial^i\phi}{\partial z^i} D^i[z_k] & k = 1, 5, 6 \\ 0 & k = 2, 3, 4 \end{cases} \tag{3.3.4}$$

$$D^i[z_k] = O[z_{T_k}^k \; Sx_k^\ell] \quad \text{where } k + \ell = i$$

Equation 3.2.22 gives:

$$Sx_k = O[\Delta x^m \Delta t^n] \quad \text{where } (m+n) \geq 4$$

$$\therefore \quad D^i[zk] = O[z_{T_k}^k (\Delta x^m \Delta t^n)^\ell] \tag{3.3.6}$$

where: $(m+n) \geq 4$ and $k + \ell = i$

In the limit of small x and t the lower powers become the dominant terms. For i = 1 the expression in equation 3.3.4 becomes

$$S_k = \begin{cases} \dfrac{\partial\phi}{\partial z} Sx_k & \text{for } k = 1, 5, 6 \\ \\ 0 & \text{for } k = 2, 3, 4 \end{cases} \tag{3.3.7}$$

where $Sx_k = O[\Delta x^m \Delta t^n]$, $(m+n) \geq 4$

For Courant numbers smaller than unity

$(x_1, d2_{j-2}, d2_{j-2}) < \Delta x$

$\rightarrow \quad |z_k| < \frac{3\Delta x}{2}$

Thus the total error in the approximations of the selected values of ϕ can be written:

$$|R_{total}| \leq \left|\frac{1}{5!} \frac{\partial^5\phi}{\partial x^5} \left[\frac{3\theta\Delta x}{2}\right]^5 \right| + |S_k| \tag{3.3.8}$$

where S_k is given by equation 3.3.7.

The value of $\tilde{\phi}_j^{n+1}$ will be given by the solution of the linear system of equation 3.3.1. Thus the total error in $\tilde{\phi}_j^{n+1}$ will be a linear combination of the error for each equation which are bounded by the expression of equation 3.3.8.

The approximate value of $\tilde{\phi}_j^{n+1}$ can then be written

$$\tilde{\phi}_{A_j}^{n+1} = \tilde{\phi}_{T_j}^{n+1} + KR_{total} \tag{3.3.9}$$

Where the subscripts A and T refer to the approximate and true values respectively and K is a constant which arises from the solution of the linear system.

3.4 The Calculation of the Line Integral

The value of ϕ_j^{n+1} is found by solving equation 2.2.4 which is reproduced below:

$$\phi_j^{n+1} = \tilde{\phi}_j^{n+1} - \int_{n\Delta t}^{(n+1)\Delta t} \phi \frac{\partial u}{\partial x}]dt \qquad (3.4.1)$$

Each term in the above equation contains an error. The error in the first term is given by equation 3.3.9

$$\tilde{\phi}_{A_j}^{n+1} = \tilde{\phi}_{T_j}^{n+1} + K\, R_{total} \qquad (3.4.2)$$

The integrand of equation 3.4.1 is made up of two terms. The first one is obtained by assuming that on the particle path:

$$\phi_A(x) = \sum_{i=1}^{5} \beta_i x^{(i-1)}$$

when in general

$$\phi_T(x) = \sum_{i=1}^{5} \beta_i\, x^{(i-1)} + R_5^{(x)} \qquad (3.4.3)$$

Thus the approximate value of ϕ can be represented in terms of its true value

$$\phi_A(x) = \phi_T(x) - R_5(x) \qquad (3.4.4)$$

where $R_5(x)$ is the usual Taylor series remainder and is given by:

$$R_5(x) = \frac{1}{5!} \left(\frac{\partial^5 \phi}{\partial x^5}\right)_{\theta x} x^5 \qquad (3.4.5)$$

where $0 \lesssim \theta \lesssim 1$.

The approximate particle path function which is given by equation 3.2.5 is

$$x_A(t) = x_T(t) - \frac{1}{5}\left(\frac{\partial^5 x}{\partial t^5}\right)_{\xi t} t^5 \tag{3.4.6}$$

where $0 \leq \xi \leq 1$. The approximate value of ϕ along the approximate particle path can be obtained by substituting for $x_A(t)$ from equation 3.4.6 into equation 3.4.4:

$$\phi_A(t) = \phi[x_A(t)] = \phi_T[x_A(t)] - R_5[x_A(t)] \tag{3.4.7}$$

$$\phi_T[x_A(t)] = \sum_{i=1}^{\infty} \beta_i\{x_T(t)]^{(i-1)} + D^{(i-1)}[x_A(t)]\} \tag{3.4.8}$$

where $D^i[x_A(t)] = [x_A(t)]^i - [x_T(t)]^i$

Equation 3.4.8 can be separated into two distinct parts:

$$\phi_T[x_A(t)] = \sum_{i=1}^{\infty} \beta_i[x_T(t)]^{(i-1)} + \sum_{i=1}^{\infty} \beta_i D^{(i-1)}[x_A(t)]$$

The first term in the equation above is in fact the true value of ϕ along the true particle path, substituting for this equation into equation 3.4.7 and rearranging

$$\rightarrow \qquad \phi_A(t) = \phi_T(t) + R^+_{total} \tag{3.4.9}$$

where $$R^+_{total} = \sum_{i=0}^{\infty} \frac{1}{i!}\left(\frac{\partial^i \phi}{\partial x^i}\right)[(x_A(t))^i - (x_T(t))^i]$$

$$- \frac{1}{5!}\left(\frac{\partial^5 \phi}{\partial x^5}\right)_{\theta x} x^5 \tag{3.4.10}$$

where $0 \leq \theta,\eta \leq 1$.

These approximations are used only in the domain

$-\Delta x \leq x \leq \Delta x$ and $-\Delta t \leq t \leq \Delta t$

Thus the order of the remainder of equation 3.4.10 can be written as:

$$R^{+}_{total} = O[\Delta t^5 \Delta x] + O[\Delta x^5] \tag{3.4.11}$$

The spatial derivative of the velocity was approximated by:

$$\left(\frac{\partial u}{\partial x}\right)_A = \sum_{i=1}^{3} \sum_{j=2}^{3} (j-1)\, \lambda_{ij}\, z^{(j-2)}\, t^{(i-1)}$$

$$\rightarrow \qquad \left(\frac{\partial u}{\partial x}\right)_A = \lambda_{12}$$

$$+ [2\lambda_{13}x + \lambda_{22}t]$$

$$+ [2\lambda_{23}xt + \lambda_{32}t^2]$$

$$+ 2\lambda_{33}xt^2 \tag{3.4.12}$$

The true spatial derivative of u can be found from

$$\left(\frac{\partial u}{\partial x}\right)_T = \sum_{i=0}^{\infty} \left(\frac{1}{i!}\right) \sum_{j=0}^{i} \binom{i}{j}\, j \frac{\partial^i u}{\partial x^j \partial t^{(i-j)}}\, x^{(j-1)}\, t^{(i-j)} \tag{3.4.13}$$

$$\left(\frac{\partial u}{\partial x}\right)_T = \left(\frac{\partial u}{\partial x}\right)_0$$

$$+ \frac{1}{2!}\left[2 \frac{\partial^2 u}{\partial x \partial t} t + 2 \frac{\partial^2 u}{\partial x^2} x\right]$$

$$+ \frac{1}{3!}\left[3 \frac{\partial^3 u}{\partial x^3} x^2 + 6 \frac{\partial^3 u}{\partial x^2 \partial t} xt + 3 \frac{\partial^3 u}{\partial x \partial t^2} t^2\right]$$

$$+ \frac{1}{4!} [4 \frac{\partial^4 u}{\partial x^4} x^3 + 12 \frac{\partial^4 u}{\partial x^3 \partial t} x^2 t + 12 \frac{\partial^4 4}{\partial x^2 \partial t^2} x t^2 + 4 \frac{\partial^4 u}{\partial x \partial t^3} t^3]$$

$$+ R_5(x,t) \qquad (3.4.14)$$

The coefficients of equation 3.4.12 are identical to those of equation 3.4.14 for the same powers of x and t. Subtracting equation 3.4.12 from 3.4.14

$$\left(\frac{\partial u}{\partial x}\right)_T - \left(\frac{\partial u}{\partial x}\right)_A = \frac{1}{3!} [3 \frac{\partial^3 u}{\partial x^3} x^2]$$

$$+ \frac{1}{4!} [4 \frac{\partial^4 u}{\partial x^4} x^3 + 12 \frac{\partial^4 u}{\partial x^3 \partial t} x^2 t + 4 \frac{\partial^4 u}{\partial x \partial t^3} t^3]$$

$$+ R_5(x,t) \qquad (3.4.15)$$

Which can be written as:

$$\left(\frac{\partial u}{\partial x}\right)_A = \left(\frac{\partial u}{\partial x}\right)_T + R^*_{total} \qquad (3.4.16)$$

where
$$R^*_{total} = - \frac{1}{3!} [3 \frac{\partial^3 u}{\partial x^3} x^2]$$

$$- \frac{1}{4!} [4 \frac{\partial^4 u}{\partial x^4} x^3 + 12 \frac{\partial^4 u}{\partial x^3 \partial t} x^2 t + 4 \frac{\partial^4 u}{\partial x \partial t^3} t^3]$$

$$- \sum_{i=5}^{\infty} \left(\frac{1}{i!}\right) \sum_{j=0}^{i} j \binom{i}{j} \frac{\partial^i u}{\partial x^j \partial t^{(i-j)}} x^{(j-1)} \, t^{(i-j)} \qquad (3.4.17)$$

Equation 3.4.1 can be rewritten as:

$$\phi_{A_j}^{n+1} = \tilde{\phi}_{A_j}^{n+1} - \int_{n\Delta t}^{(n+1)\Delta t} [\phi_A(t) \left(\frac{\partial u}{\partial x}\right)_A]dt$$

$$\phi_{A_j}^{n+1} = [\tilde{\phi}_{T_j}^{n+1} + KR_{total}]$$

$$- \int_{n\Delta t}^{(n+1)\Delta t} \{[\phi_T(t) + R^{+}_{total}][\left(\frac{\partial u}{\partial x}\right)_T + R^{*}_{total}]\}dt \qquad (3.4.18)$$

Where the substitutions above were obtained from equations 3.4.2, 3.4.9 and 3.4.16 respectively. Equation 3.4.18 can be expressed as:

$$\phi^{n+1}_{A_j} = \tilde{\phi}^{n+1}_{T_j} - \int_{n\Delta t}^{(n+1)\Delta t} [\phi_T(t)\left(\frac{\partial u}{\partial x}\right)_T]dt + S\phi \qquad (3.4.19)$$

where: $$S\phi = KR_{total} - \int_{n\Delta t}^{(n+1)\Delta t} \{R^{*}_{total}[\phi_T(t) + R^{+}_{total}] + R^{+}_{total}\,[\left(\frac{\partial u}{\partial x}\right)_T]\}dt \qquad (3.4.20)$$

The first two terms in equation 3.4.19 represent the true value of ϕ^{n+1}_j (by definition) we can thus write:

$$\phi^{n+1}_{A_j} = \phi^{n+1}_{T_j} + S\phi \qquad (3.4.21)$$

The above equation states that the approximate value of ϕ^{n+1}_j differs from its true value by an amount $S\phi$.

The expression for $S\phi$ (equations 3.4.20) is very complex. An idea of its behaviour in the limiting cases of small x and t can be obtained by considering the order of each of its components

$$\begin{aligned} S\phi = {} & K[O(\Delta x^5) + O(\Delta x^i \Delta t^j)] \\ & + O[\Delta t]*\{O[\Delta x^2][O[\phi_T] + O[\Delta t^5 \Delta x] + O[\Delta x^5]] \\ & + O[\Delta t^5 \Delta x] + O[\Delta x^5]\} \end{aligned} \qquad (3.4.22)$$

where $(i+j) = 4$

The important parameter here is not so much how big $S\phi$ is but rather how big it is in comparison to the true value of ϕ. Let

$|\phi_T| \simeq 1$, in the limiting case of small Δx

$$\rightarrow \qquad O[\phi_T] + O[\Delta t^5 \Delta x] + O[\Delta x^5] \simeq O(1) = 1$$

$$\therefore\ S\phi = K[O(\Delta x^5) + O(\Delta x^i \Delta t^j)]$$

$$O[\Delta x^2 \Delta t] + O[\Delta t^6 \Delta x] + O[\Delta x^5 \Delta t] \qquad \text{where } (i+j) = 4 \qquad (3.4.23)$$

Equation 3.4.23 represents the order of the relative error in the value of ϕ_j^{n+1} obtained by this method.

CHAPTER 4

COMPARISON TESTS

4.1 Modes of Comparison and Results

The method developed here has been used to solve the equation:

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u\phi)}{\partial x} = 0 \qquad (4.1.1)$$

The results were compared to two other solutions of the same equation:

(1) The true analytical solution

(2) The solution obtained by an upwind one sided finite difference scheme.

This comparison was done for three different problems:

(1) Velocity function of time only

(2) Velocity function of space only

(3) Fully variable velocity

The following parameters were used for all problems:

pipe length = 1 m

number of nodes = 10

mesh size = 0.1 m

time step = 0.1 secs

number of time steps = 50

The solution of equation 4.1.1 as given by the upwind one sided finite difference scheme used is:

$$\phi_j^{n+1} = \phi_j^n + \left(\frac{\Delta t}{\Delta X}\right)[u_j^n(\phi_{j-1}^n - \phi_j^n) + \phi_j^n(u_{j-1}^n - u_j^n)] \qquad (4.1.2)$$

The nature of the boundary and initial conditions will be specified for each case.

Ten plots were produced for each problem. Some of the points used to produce these plots are shown in Appendix 4.

4.2 Velocity Function of Time Only

For the velocity field:

$$u(t) = 0.4 \exp [0.180*t] \tag{4.2.1}$$

The solution of the homogeneous advection equation can be expressed as:

$$\phi(x,t) = k \exp[0.5*(x - u(t)/0.180)] \tag{4.2.2}$$

The boundary condition is:

$$\phi(x = 0,t) = k \exp[-0.5\ u(t)/0.180] \tag{4.2.3}$$

The initial condition is:

$$\phi(x,t = 0) = k \exp[0.5(x - 0.4/0.180)] \tag{4.2.4}$$

The value of k was chosen to be:

$$k = 1.0 * 10^6 \tag{4.2.5}$$

The results obtained in this section are shown on Figures 4.2.1 to 4.2.10.

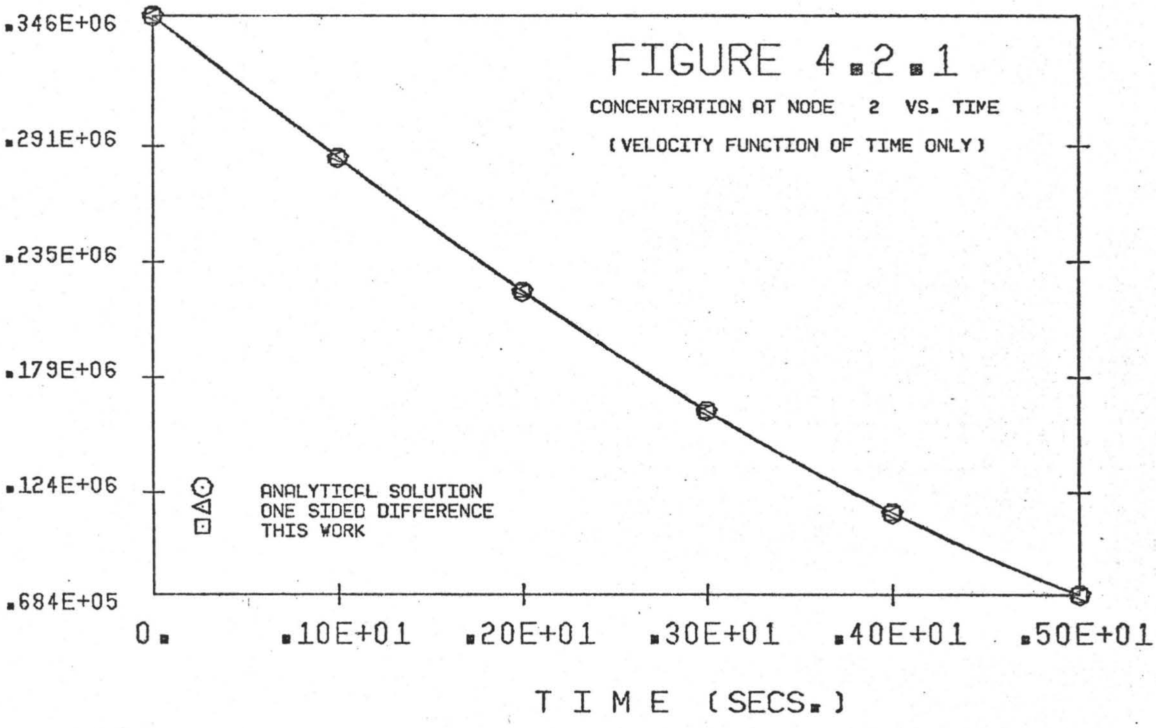


FIGURE 4.2.1
CONCENTRATION AT NODE 2 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
.346E+06
.291E+06
.235E+06
.179E+06
.124E+06
.684E+05
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

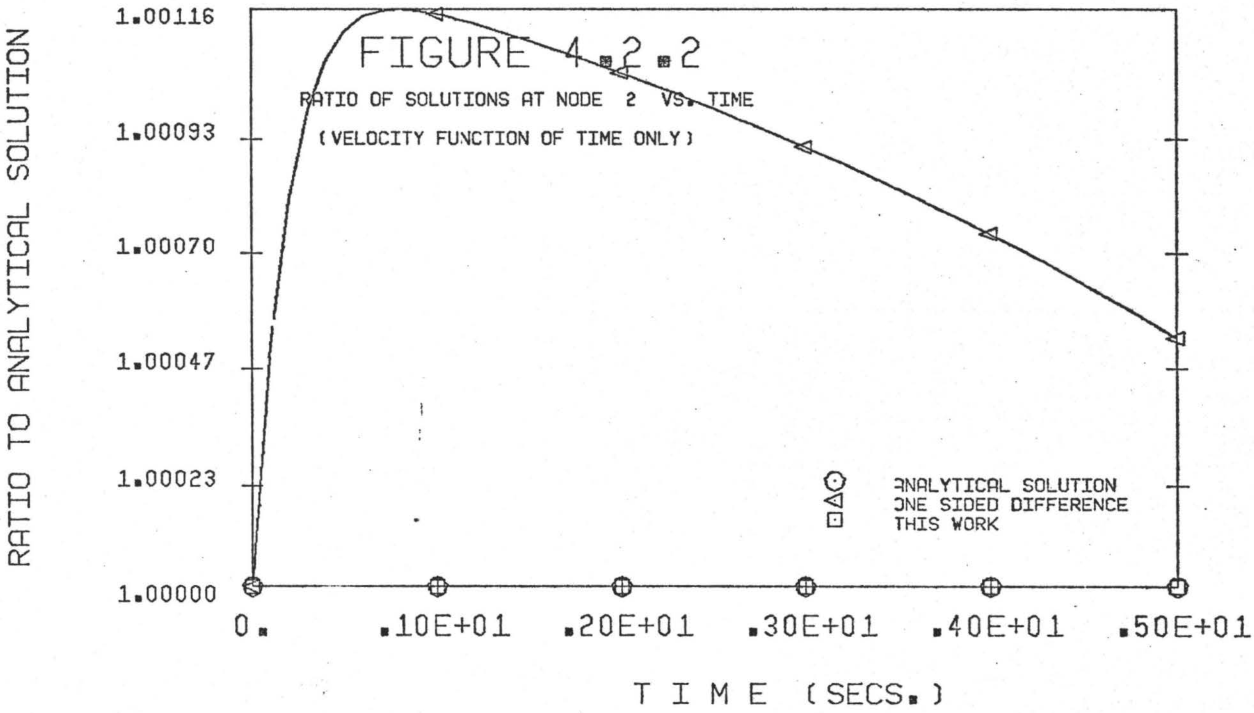


FIGURE 4.2.2
RATIO OF SOLUTIONS AT NODE 2 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00116
1.00093
1.00070
1.00047
1.00023
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

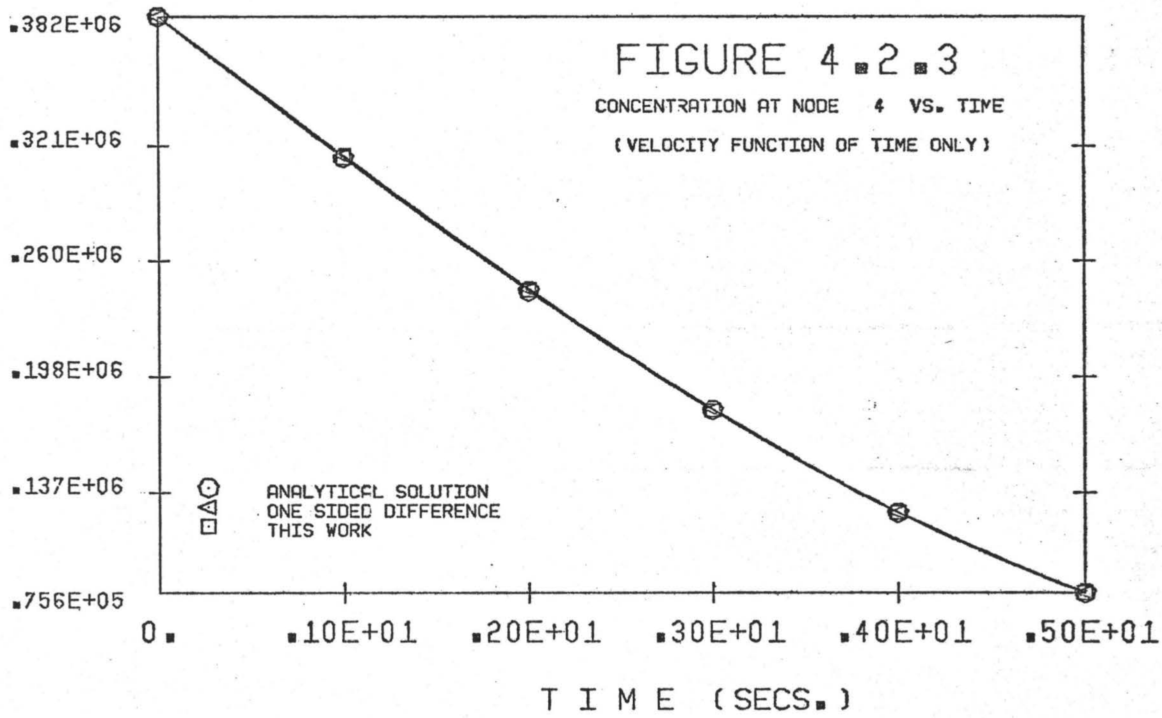


FIGURE 4.2.3
CONCENTRATION AT NODE 4 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
.382E+06
.321E+06
.260E+06
.198E+06
.137E+06
.756E+05
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

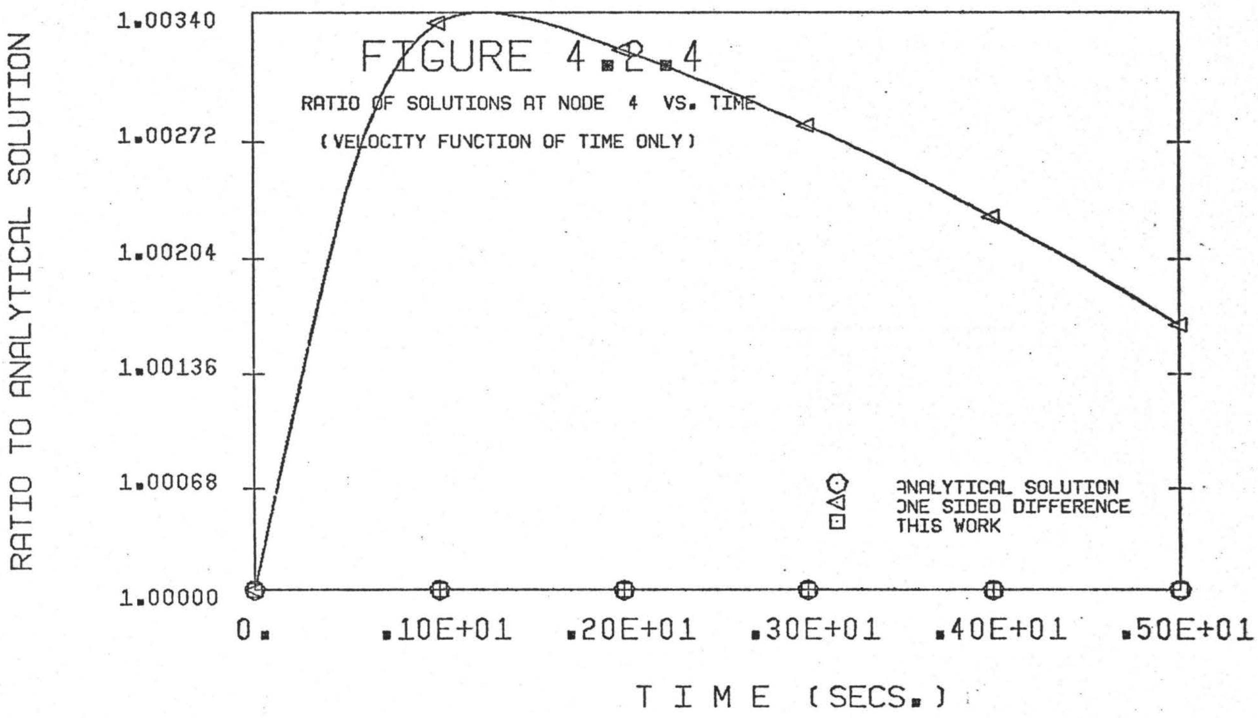


FIGURE 4.2.4
RATIO OF SOLUTIONS AT NODE 4 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00340
1.00272
1.00204
1.00136
1.00068
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

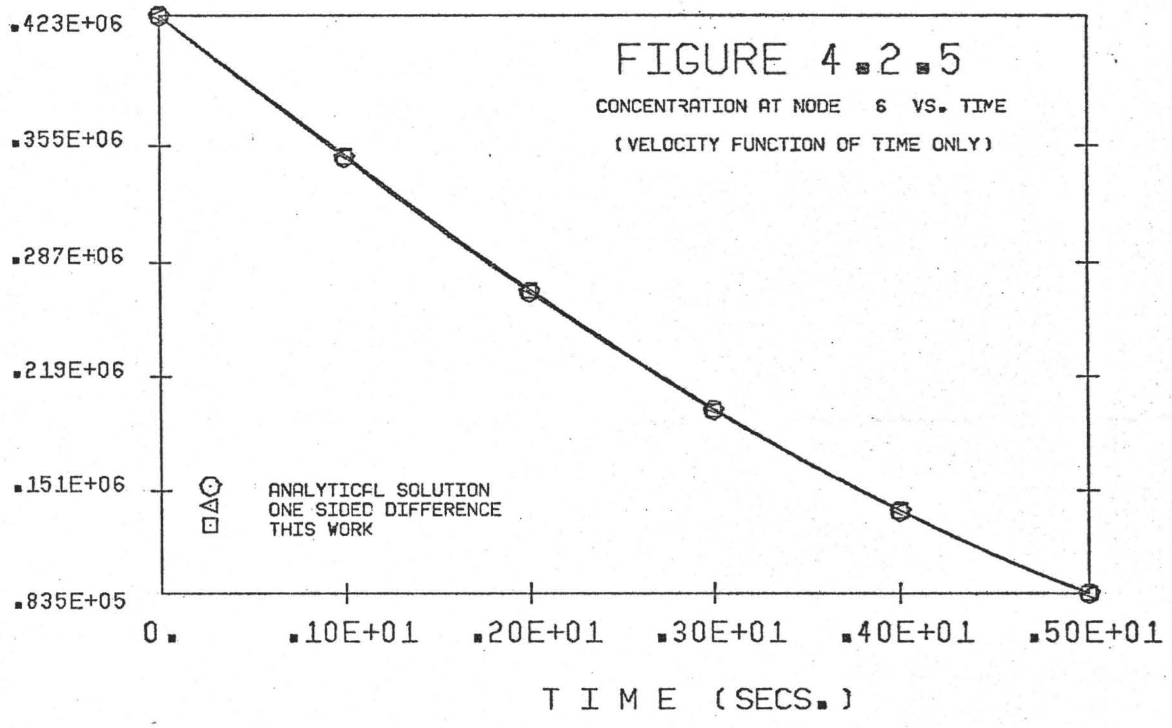


FIGURE 4.2.5
CONCENTRATION AT NODE 6 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
.423E+06
.355E+06
.287E+06
.219E+06
.151E+06
.835E+05
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

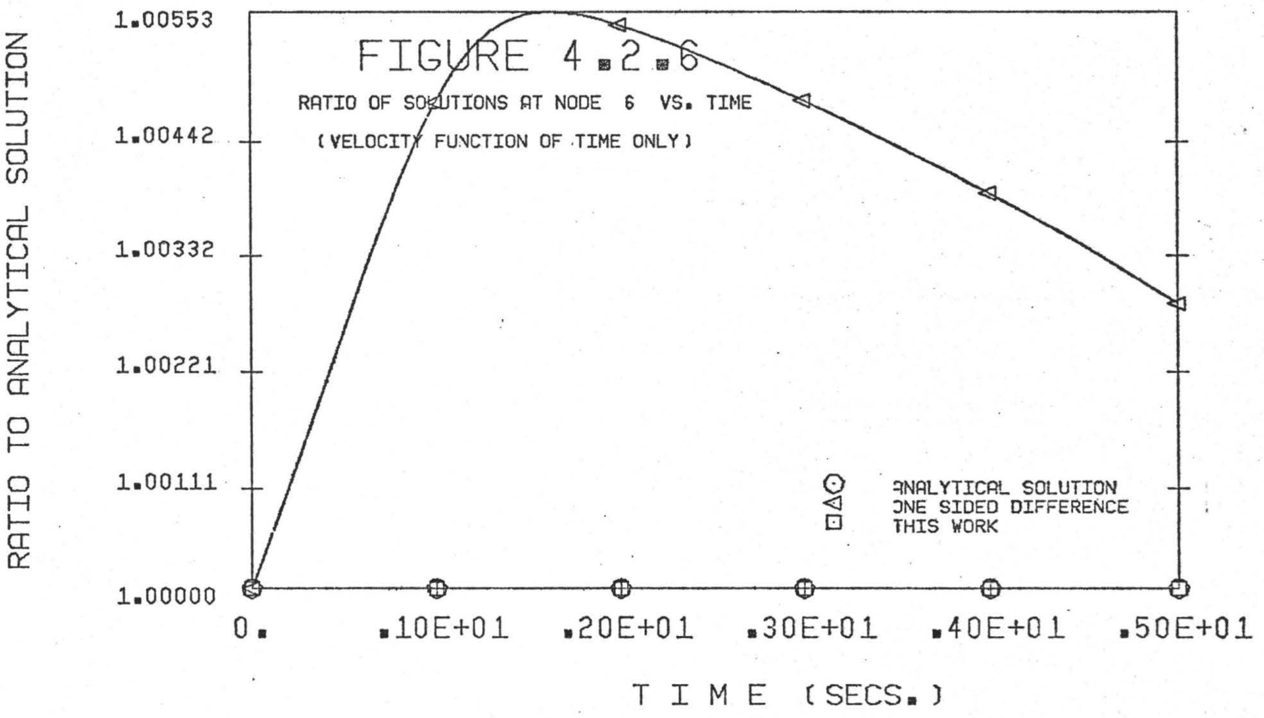


FIGURE 4.2.6
RATIO OF SOLUTIONS AT NODE 6 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00553
1.00442
1.00332
1.00221
1.00111
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

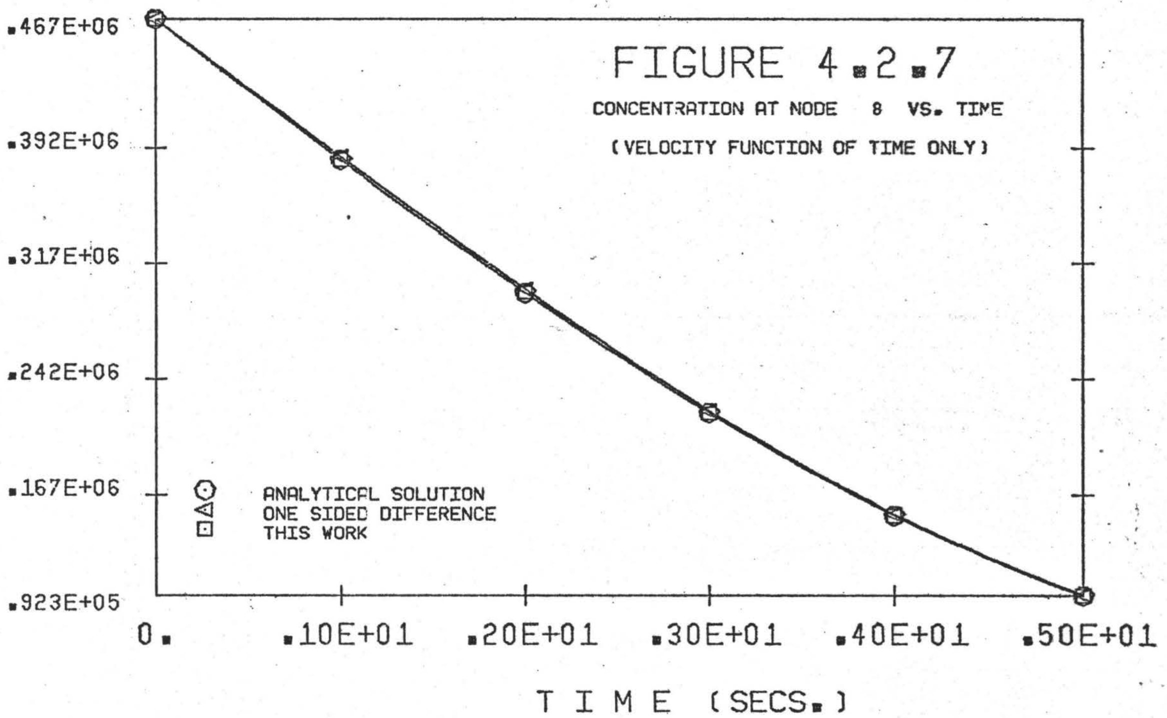


FIGURE 4.2.7
CONCENTRATION AT NODE 8 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
.467E+06
.392E+06
.317E+06
.242E+06
.167E+06
.923E+05
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

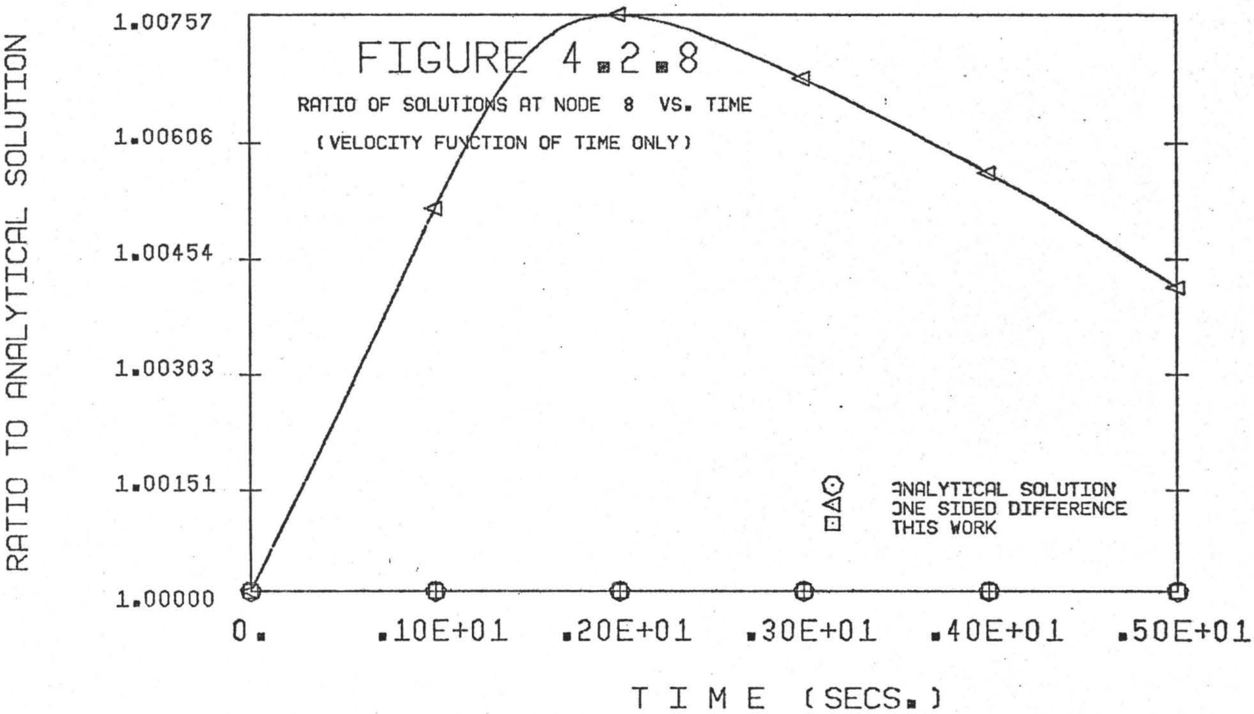


FIGURE 4.2.8
RATIO OF SOLUTIONS AT NODE 8 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00757
1.00606
1.00454
1.00303
1.00151
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

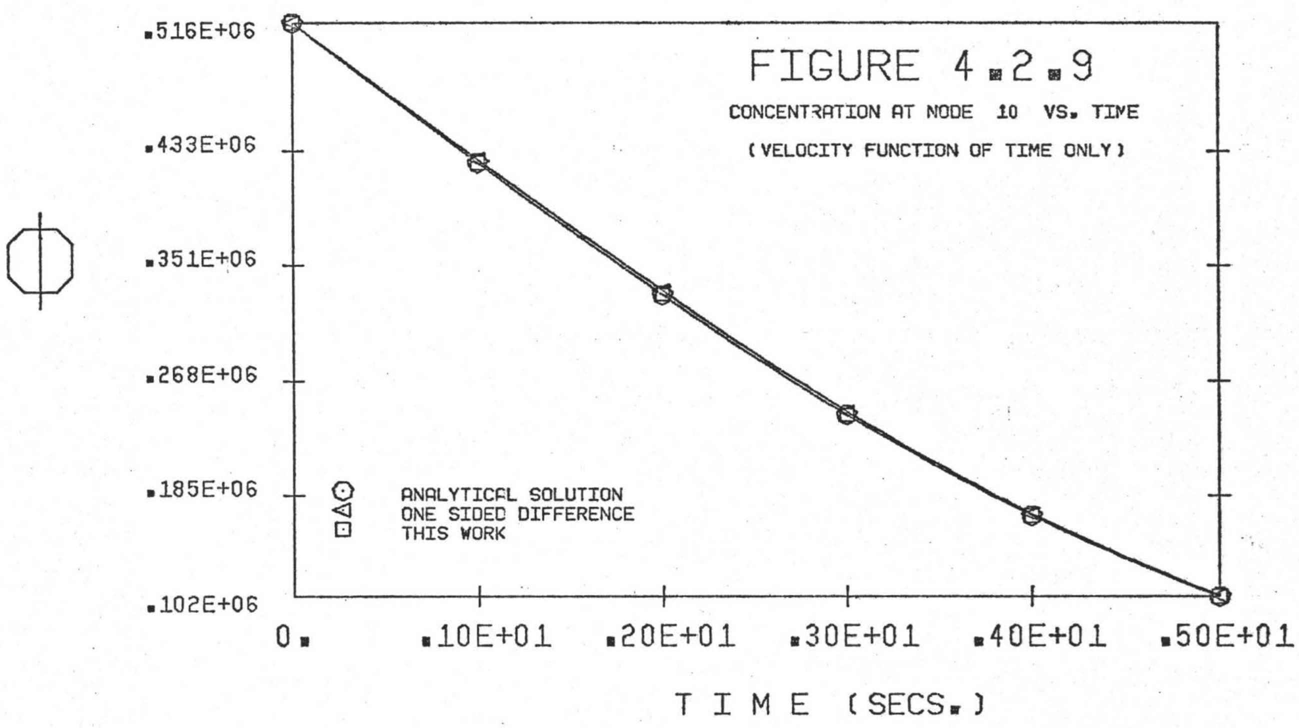


FIGURE 4.2.9
CONCENTRATION AT NODE 10 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
.516E+06
.433E+06
.351E+06
.268E+06
.185E+06
.102E+06
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

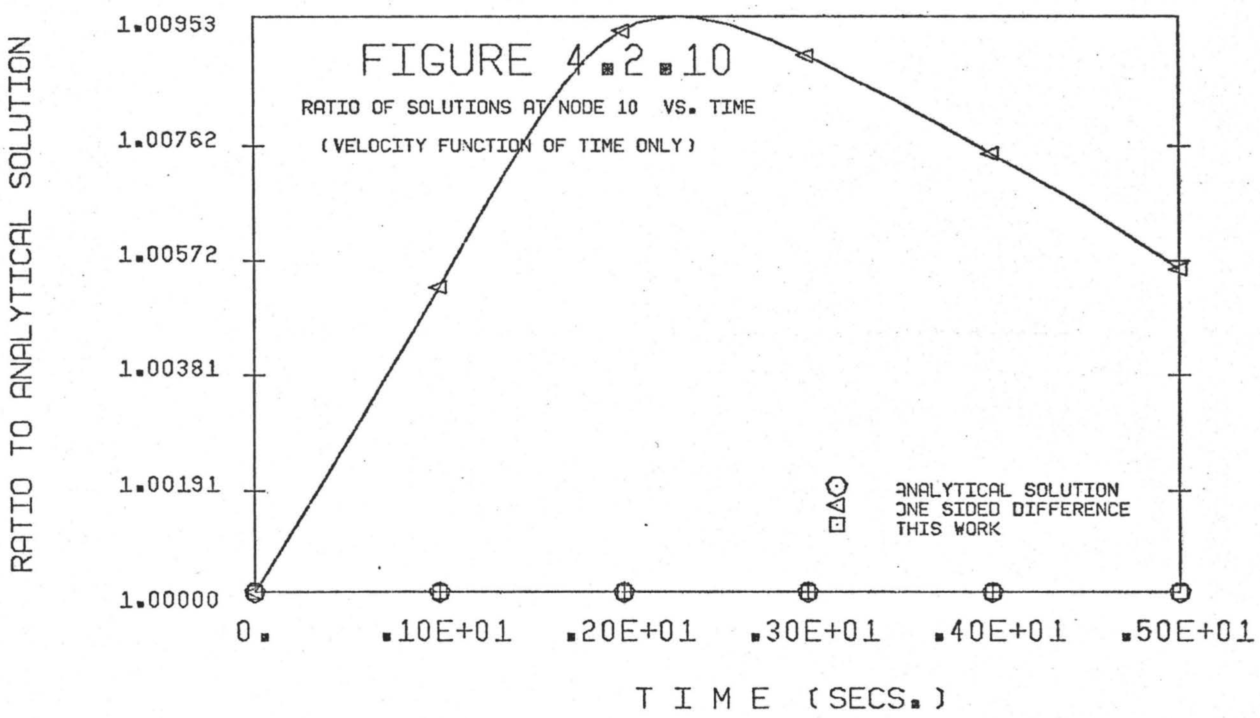


FIGURE 4.2.10
RATIO OF SOLUTIONS AT NODE 10 VS. TIME
(VELOCITY FUNCTION OF TIME ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00953
1.00762
1.00572
1.00381
1.00191
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

4.3 Velocity Function of Space Only

For the velocity field:

$$u(x) = \exp[\,0.4x] \tag{4.3.1}$$

The solution to the homogeneous advection equation can be expressed as:

$$\phi(x,t) = k \exp[1.0/u(x) + 0.2(x-t)] \tag{4.3.2}$$

The boundary condition is:

$$\phi(x=0,t) = k \exp[1.0-0.2t] \tag{4.3.3}$$

The initial condition is:

$$\phi(x,t=0) = k \exp[1.0/u(x) + 0.2x] \tag{4.3.4}$$

The value of k was chosen to be:

$$k = 1.0 * 10^6 \tag{4.3.5}$$

The comparison of the different solution schemes for this particular problem can be seen in Figures 4.3.1 to 4.3.10.

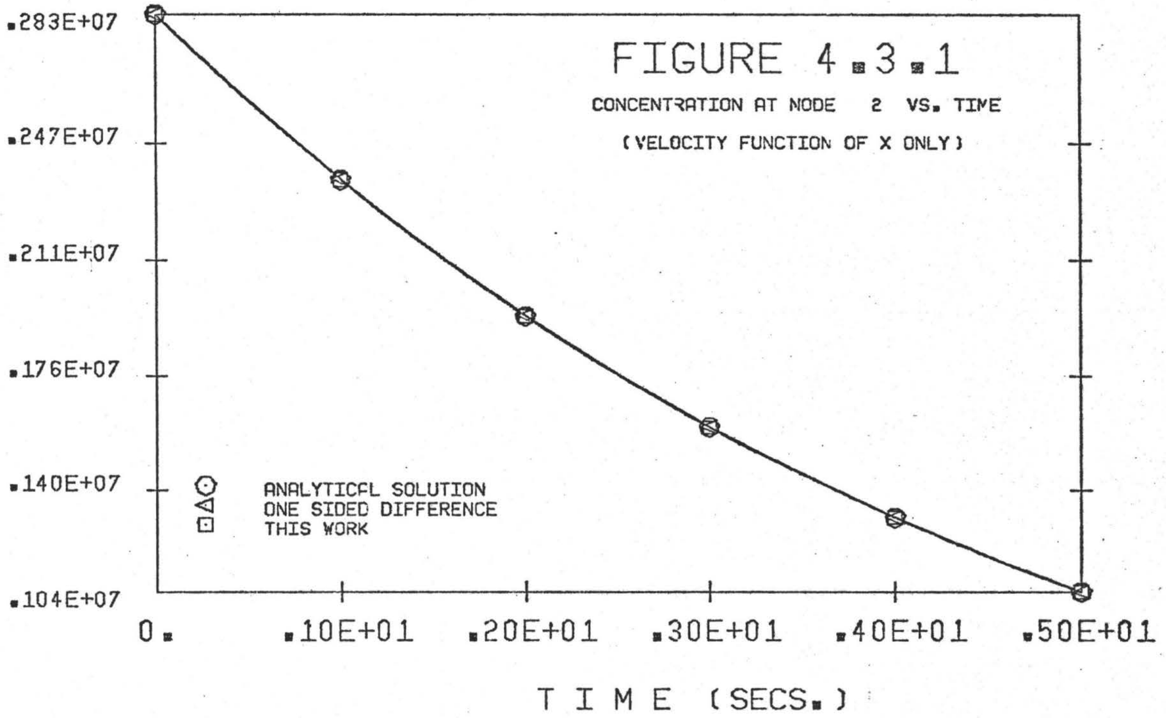


FIGURE 4.3.1
CONCENTRATION AT NODE 2 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
.283E+07
.247E+07
.211E+07
.176E+07
.140E+07
.104E+07
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

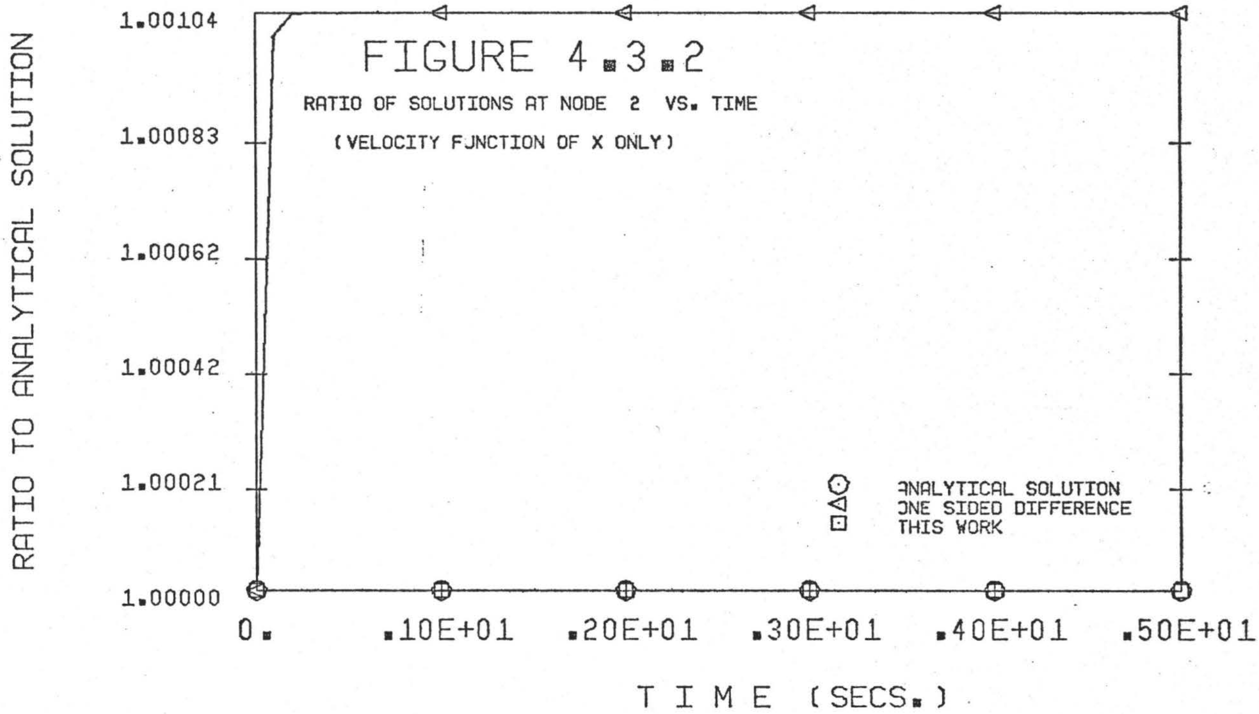


FIGURE 4.3.2
RATIO OF SOLUTIONS AT NODE 2 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00104
1.00083
1.00062
1.00042
1.00021
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

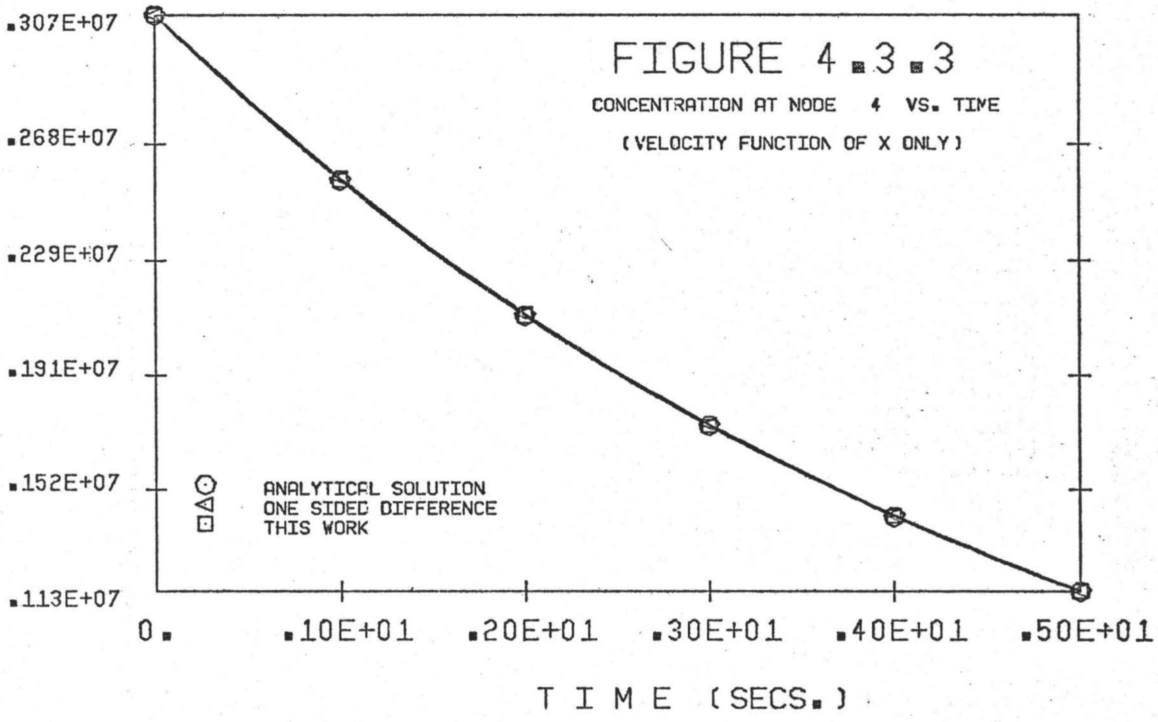


FIGURE 4.3.3
CONCENTRATION AT NODE 4 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
.307E+07
.268E+07
.229E+07
.191E+07
.152E+07
.113E+07
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

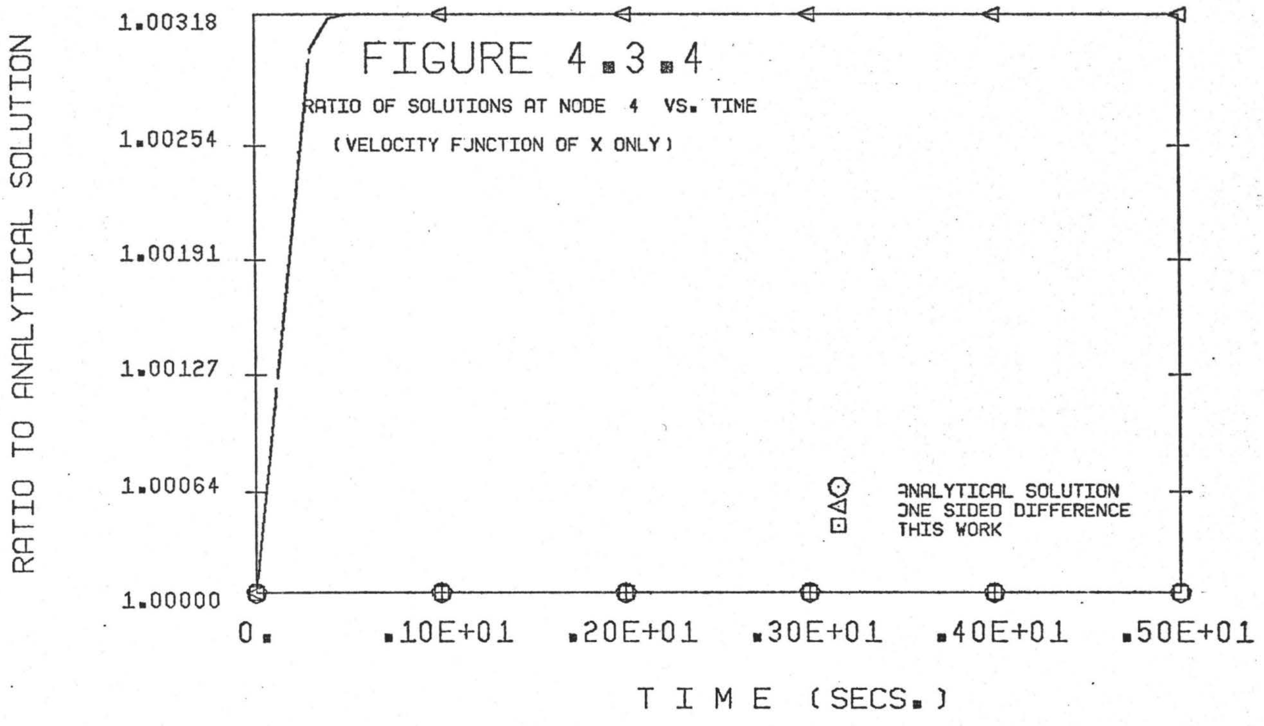


FIGURE 4.3.4
RATIO OF SOLUTIONS AT NODE 4 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00318
1.00254
1.00191
1.00127
1.00064
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

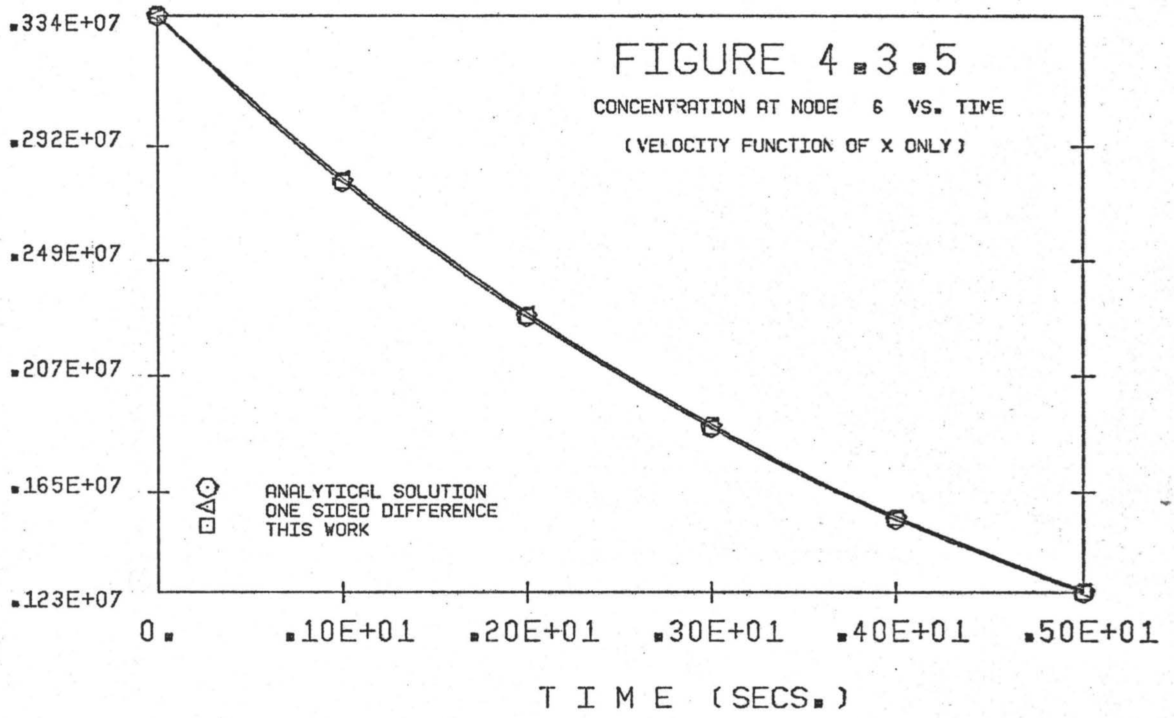


FIGURE 4.3.5
CONCENTRATION AT NODE 6 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
.334E+07
.292E+07
.249E+07
.207E+07
.165E+07
.123E+07
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

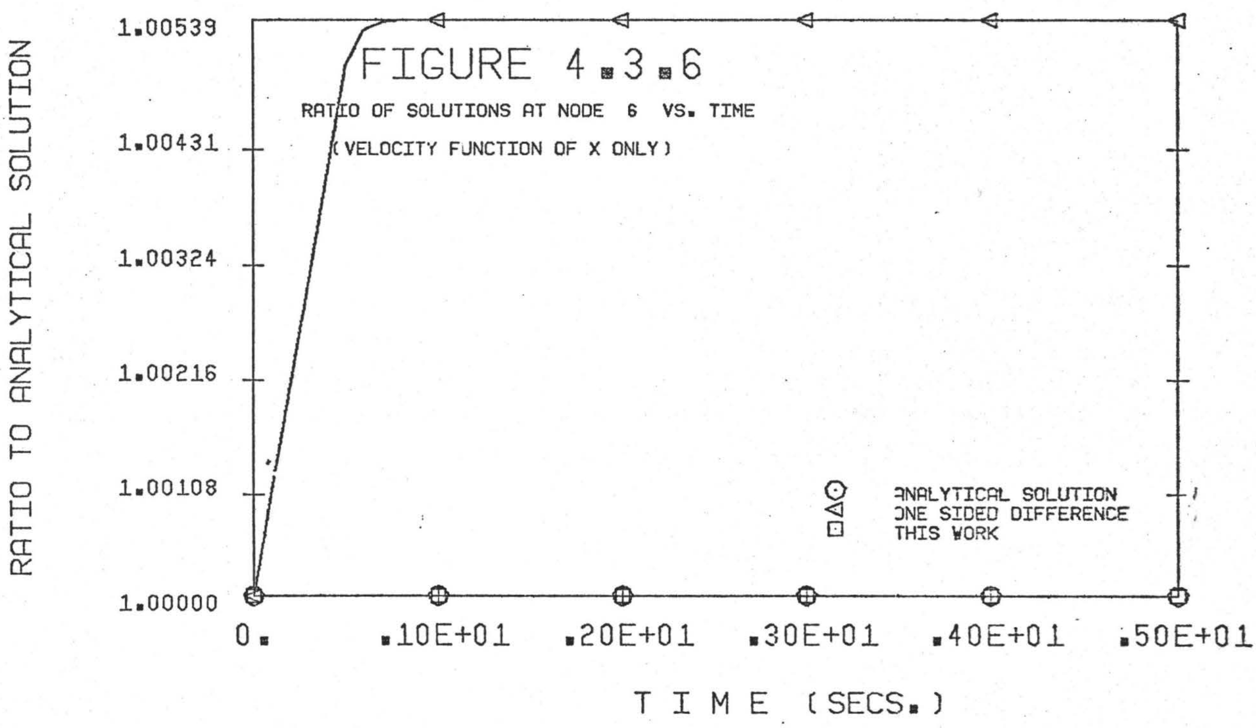


FIGURE 4.3.6
RATIO OF SOLUTIONS AT NODE 6 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00539
1.00431
1.00324
1.00216
1.00108
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
0.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

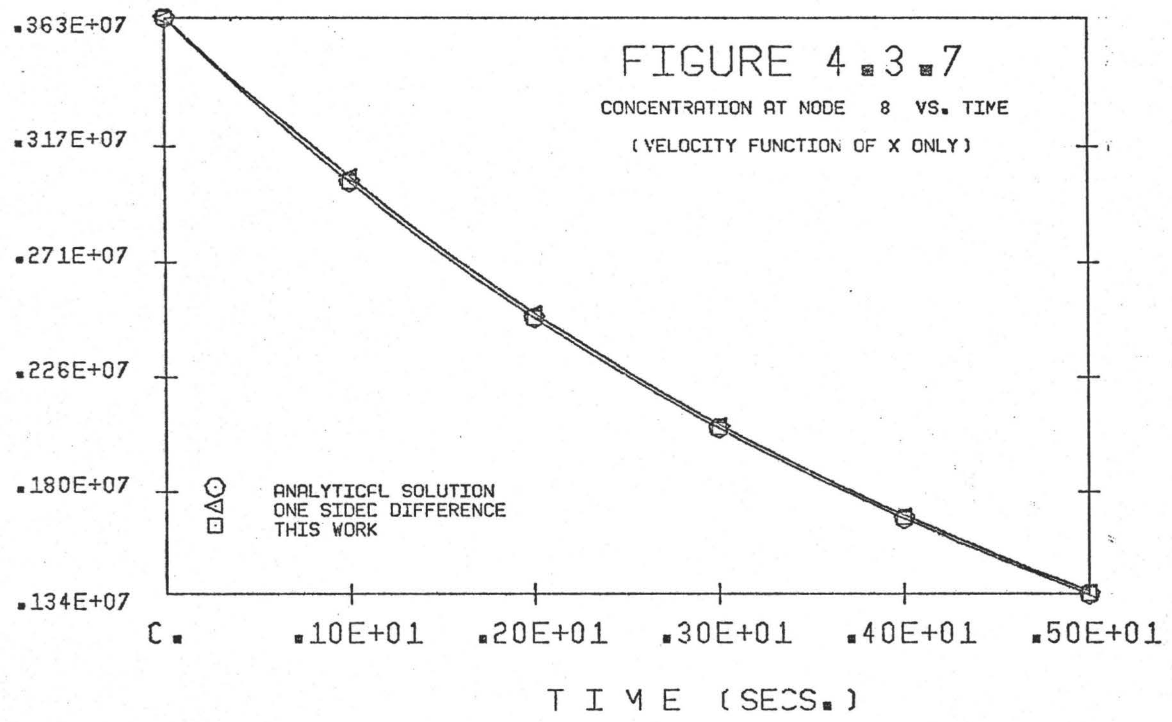


FIGURE 4.3.7
CONCENTRATION AT NODE 8 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
.363E+07
.317E+07
.271E+07
.226E+07
.180E+07
.134E+07
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

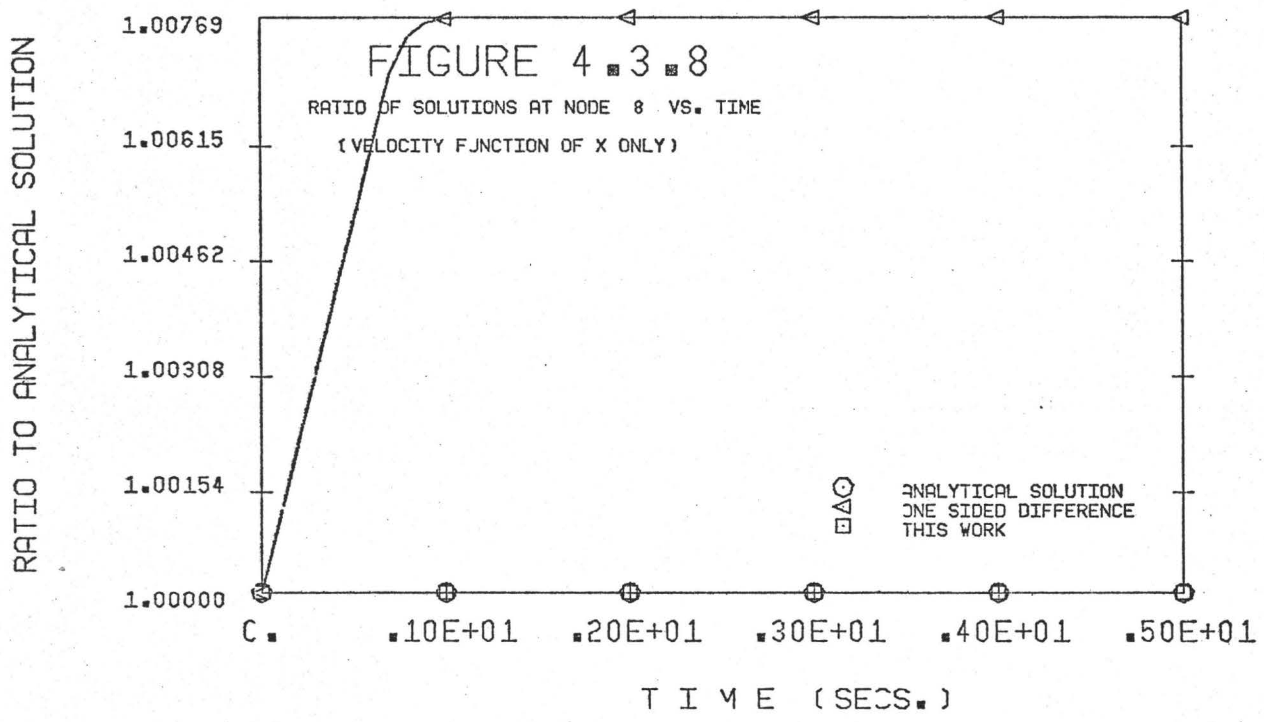


FIGURE 4.3.8
RATIO OF SOLUTIONS AT NODE 8 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
RATIO TO ANALYTICAL SOLUTION
1.00769
1.00615
1.00462
1.00308
1.00154
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

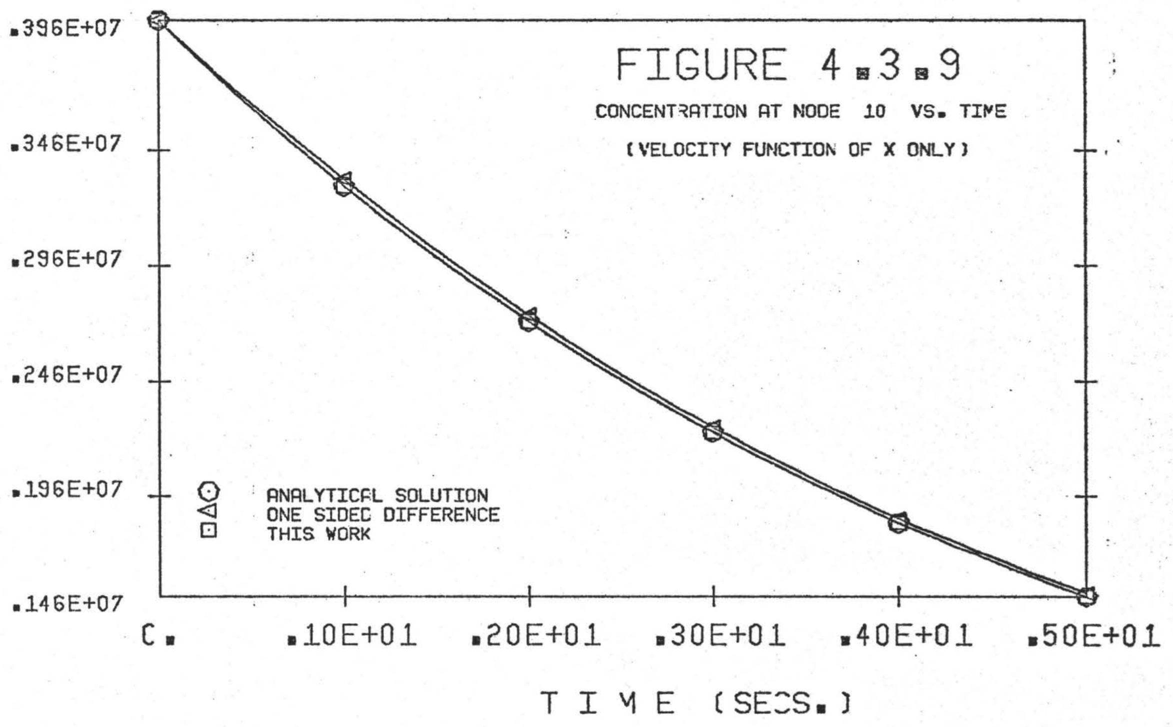


FIGURE 4.3.9
CONCENTRATION AT NODE 10 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
.396E+07
.346E+07
.296E+07
.246E+07
.196E+07
.146E+07
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK

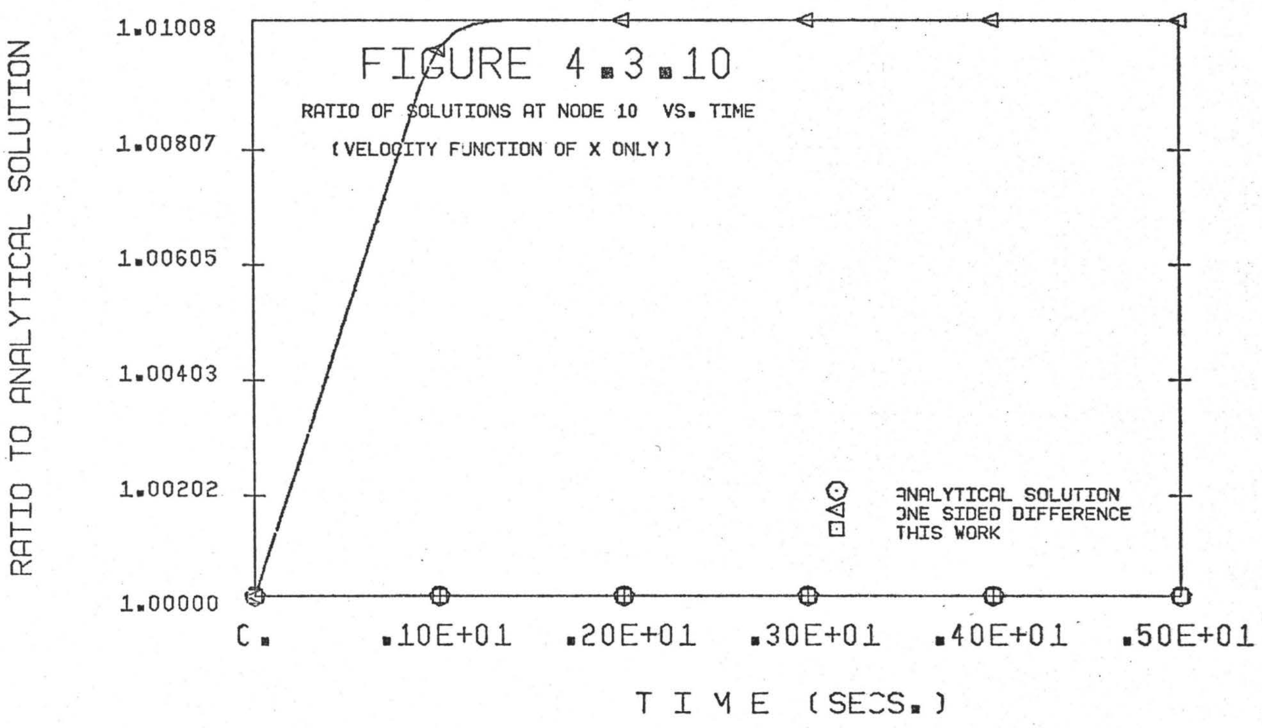


FIGURE 4.3.10
RATIO OF SOLUTIONS AT NODE 10 VS. TIME
(VELOCITY FUNCTION OF X ONLY)
RATIO TO ANALYTICAL SOLUTION
1.01008
1.00807
1.00605
1.00403
1.00202
1.00000
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK

4.4. Fully Variable Velcoity

For the velocity field:

$$u(x,t) = \frac{x}{3[10-t]} \tag{4.4.1}$$

The solution to the homogeneous advection equation can be expressed as:

$$\phi(x,t) = \frac{k\ x^2}{[10-t]} \tag{4.4.2}$$

The boundary conditon is:

$$\phi(x=0,t) = 0 \tag{4.4.3}$$

The initial condition is:

$$\phi(x,t=0) = \frac{k\ x^2}{10} \tag{4.4.4}$$

The value of k was chosen to be:

$$k = 1.0 * 10^6 \tag{4.4.5}$$

These results are shown on Figures 4.4.1 to 4.4.10.

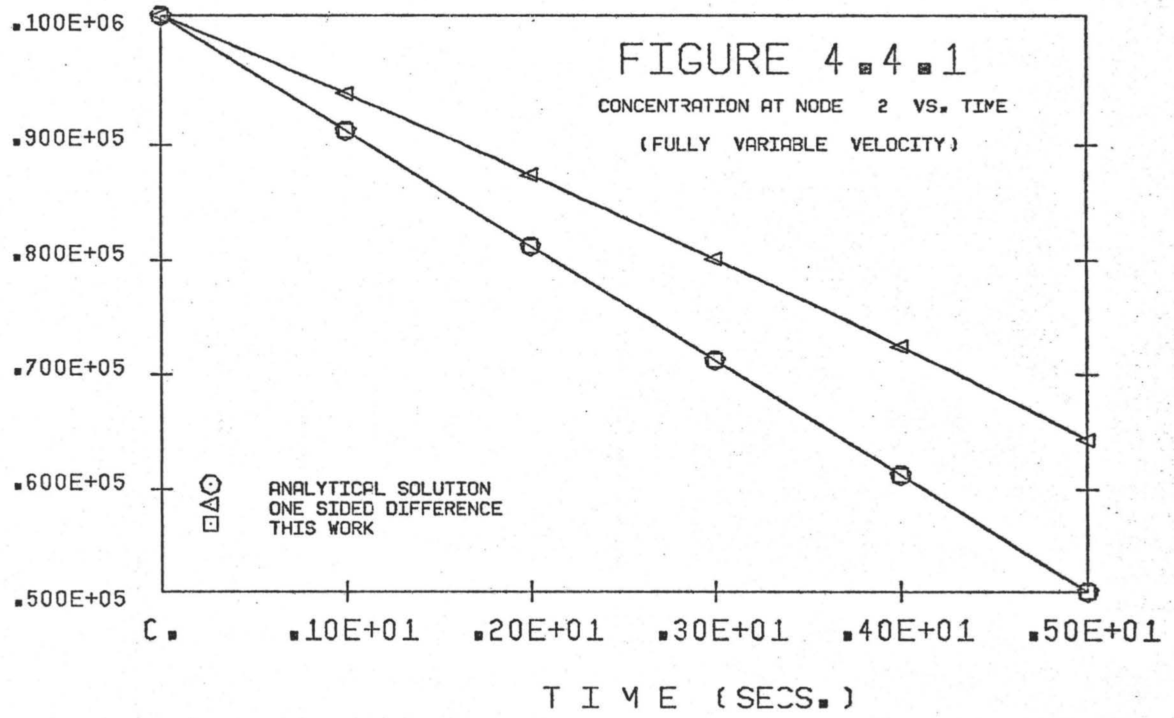


FIGURE 4.4.1
CONCENTRATION AT NODE 2 VS. TIME
(FULLY VARIABLE VELOCITY)
.100E+06
.900E+05
.800E+05
.700E+05
.600E+05
.500E+05
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

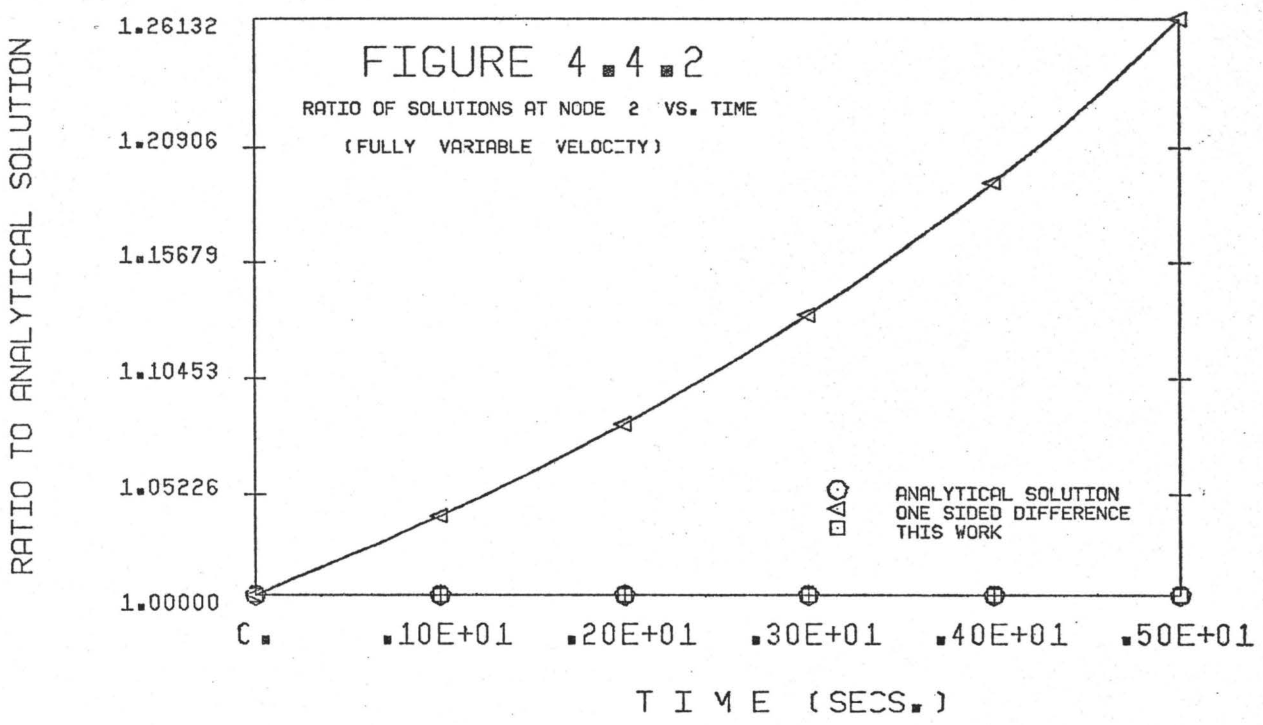


FIGURE 4.4.2
RATIO OF SOLUTIONS AT NODE 2 VS. TIME
(FULLY VARIABLE VELOCITY)
RATIO TO ANALYTICAL SOLUTION
1.26132
1.20906
1.15679
1.10453
1.05226
1.00000
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

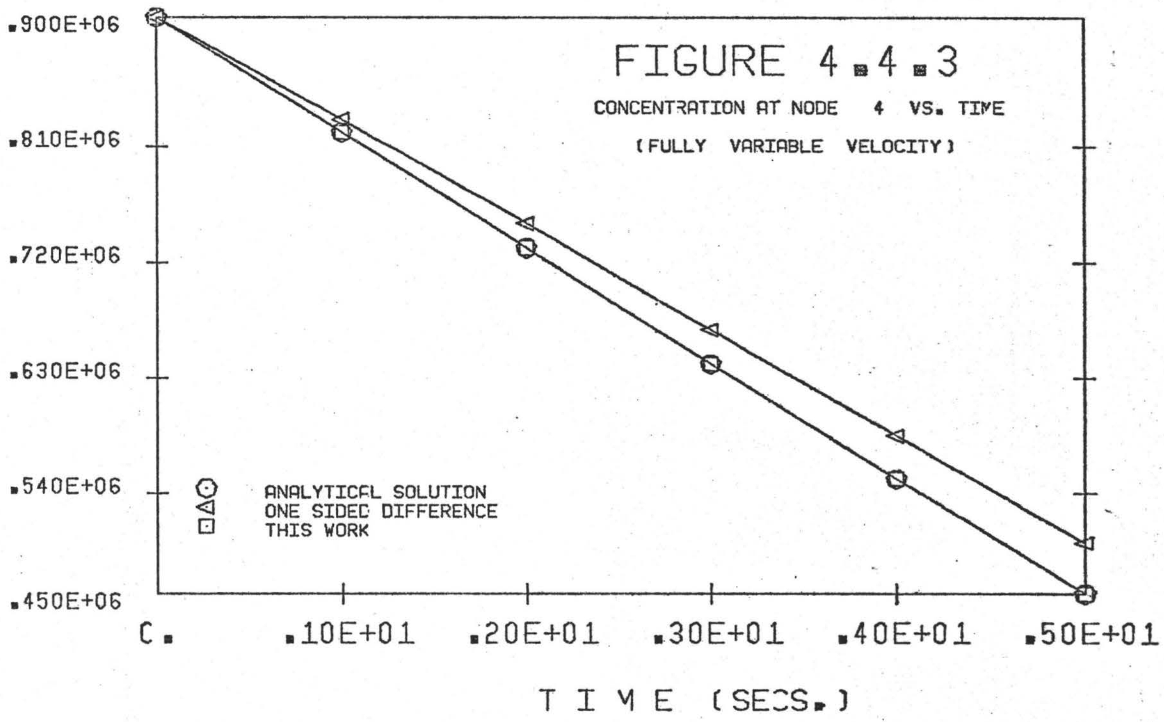


FIGURE 4.4.3
CONCENTRATION AT NODE 4 VS. TIME
(FULLY VARIABLE VELOCITY)
.900E+06
.810E+06
.720E+06
.630E+06
.540E+06
.450E+06
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

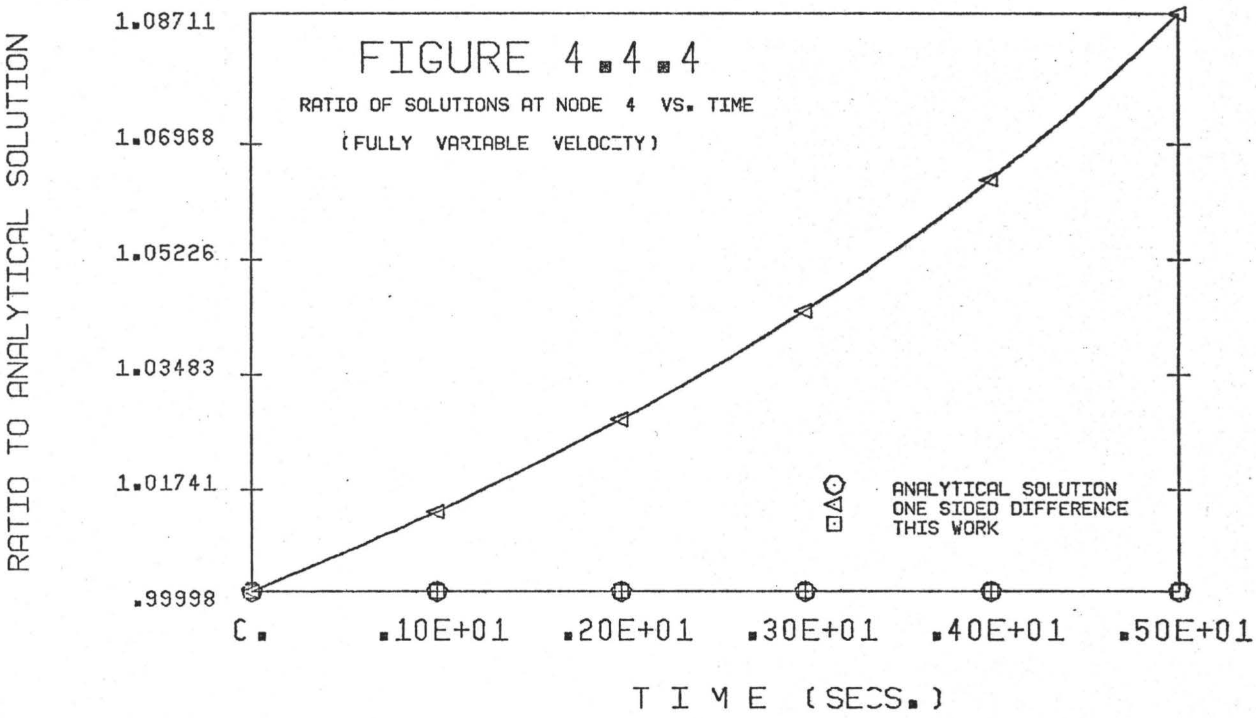


FIGURE 4.4.4
RATIO OF SOLUTIONS AT NODE 4 VS. TIME
(FULLY VARIABLE VELOCITY)
RATIO TO ANALYTICAL SOLUTION
1.08711
1.06968
1.05226
1.03483
1.01741
.99998
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

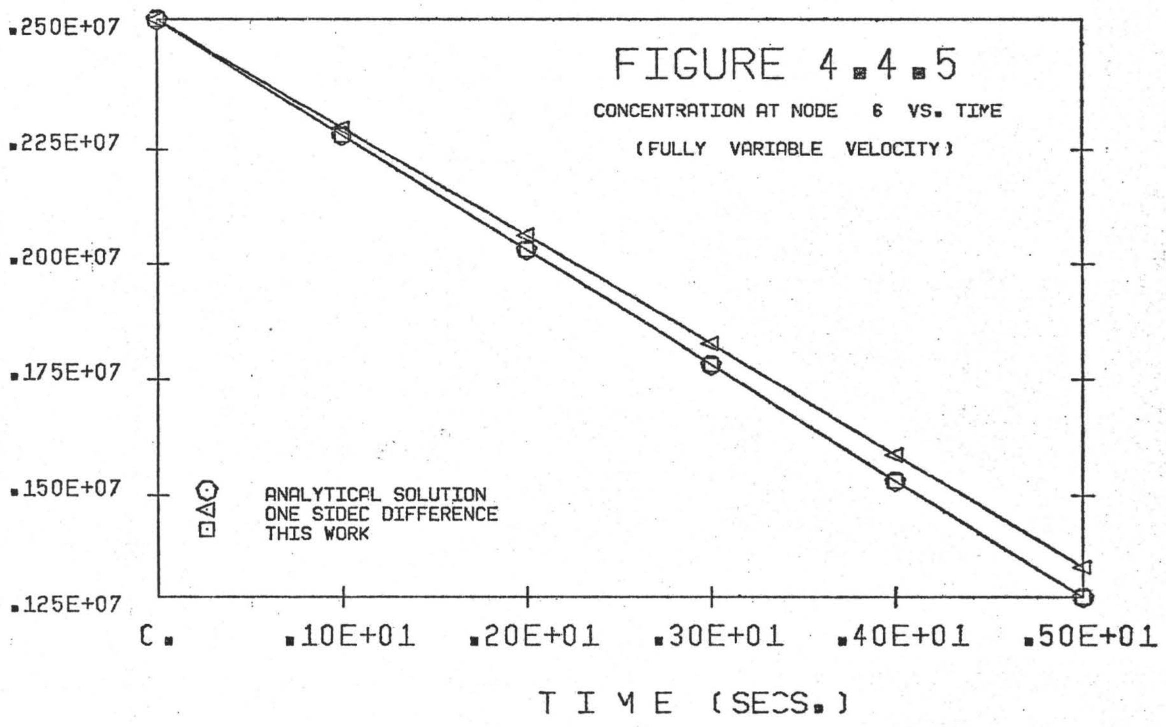


FIGURE 4.4.5
CONCENTRATION AT NODE 6 VS. TIME
(FULLY VARIABLE VELOCITY)
.250E+07
.225E+07
.200E+07
.175E+07
.150E+07
.125E+07
ANALYTICAL SOLUTION
ONE SIDEC DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

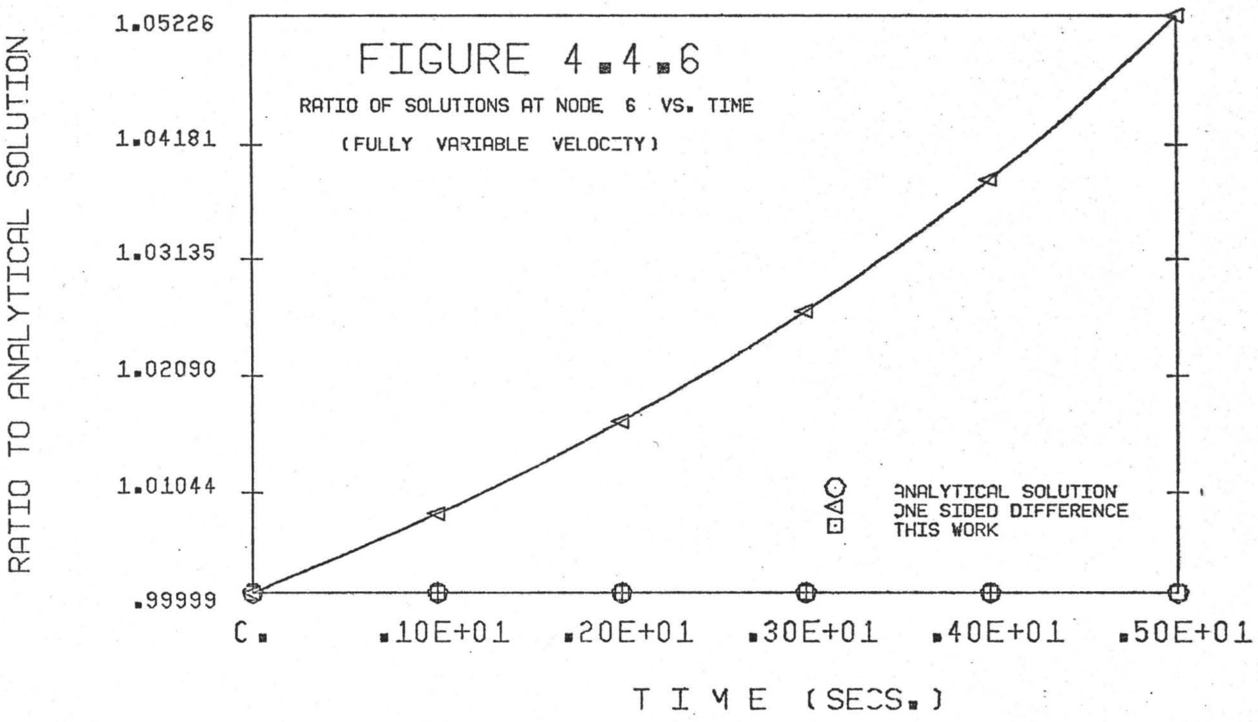


FIGURE 4.4.6
RATIO OF SOLUTIONS AT NODE 6 VS. TIME
(FULLY VARIABLE VELOCITY)
RATIO TO ANALYTICAL SOLUTION
1.05226
1.04181
1.03135
1.02090
1.01044
.99999
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
TIME (SECS.)

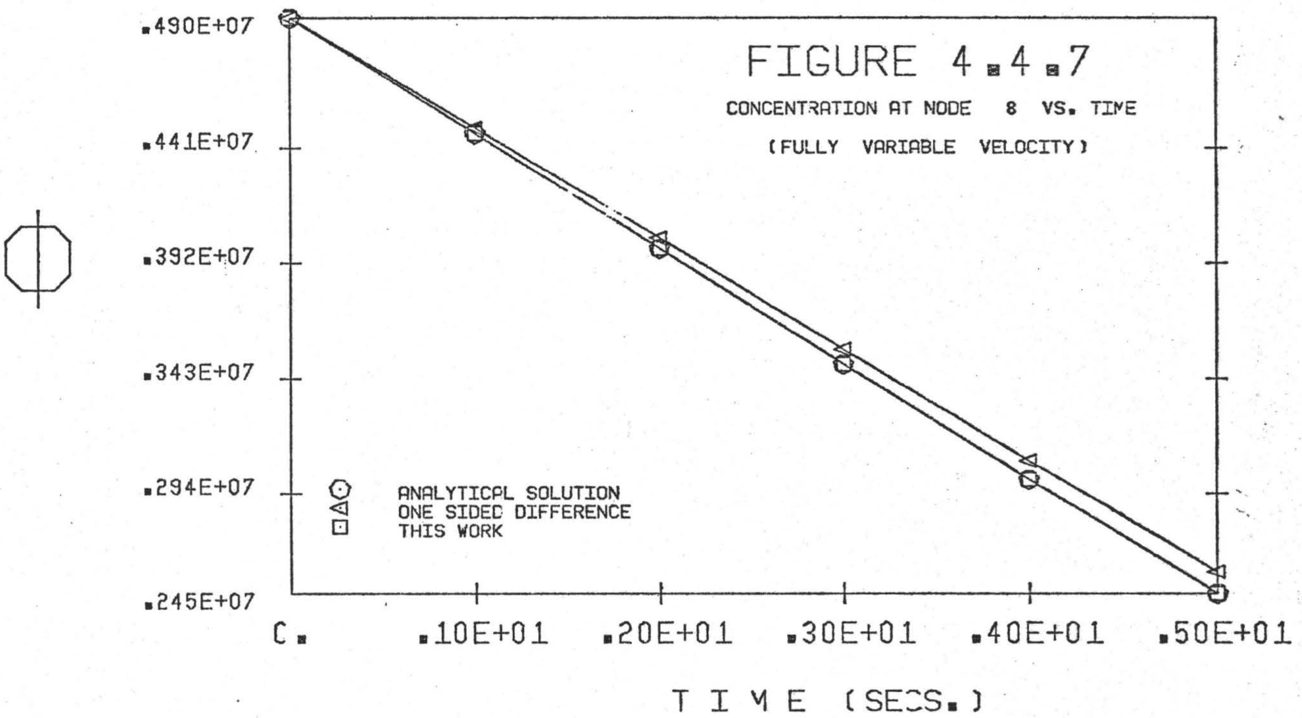


FIGURE 4.4.7
CONCENTRATION AT NODE 8 VS. TIME
(FULLY VARIABLE VELOCITY)
.490E+07
.441E+07
.392E+07
.343E+07
.294E+07
.245E+07
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

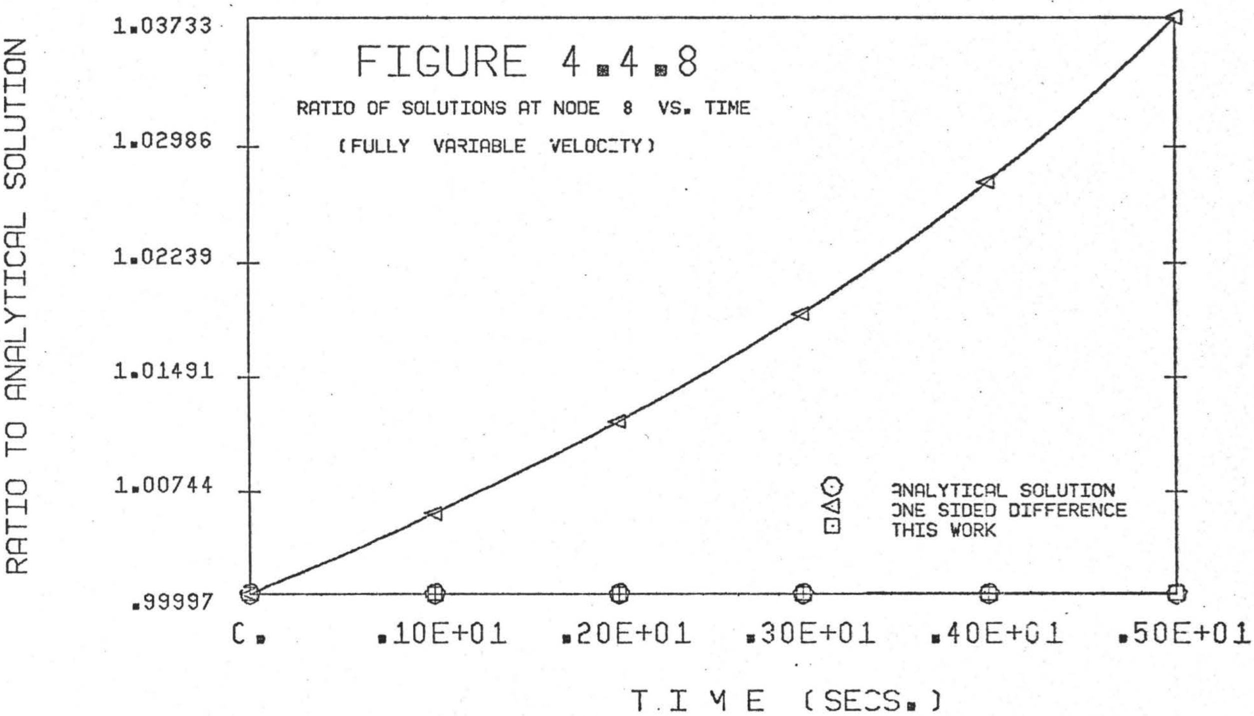


FIGURE 4.4.8
RATIO OF SOLUTIONS AT NODE 8 VS. TIME
(FULLY VARIABLE VELOCITY)
RATIO TO ANALYTICAL SOLUTION
1.03733
1.02986
1.02239
1.01491
1.00744
.99997
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

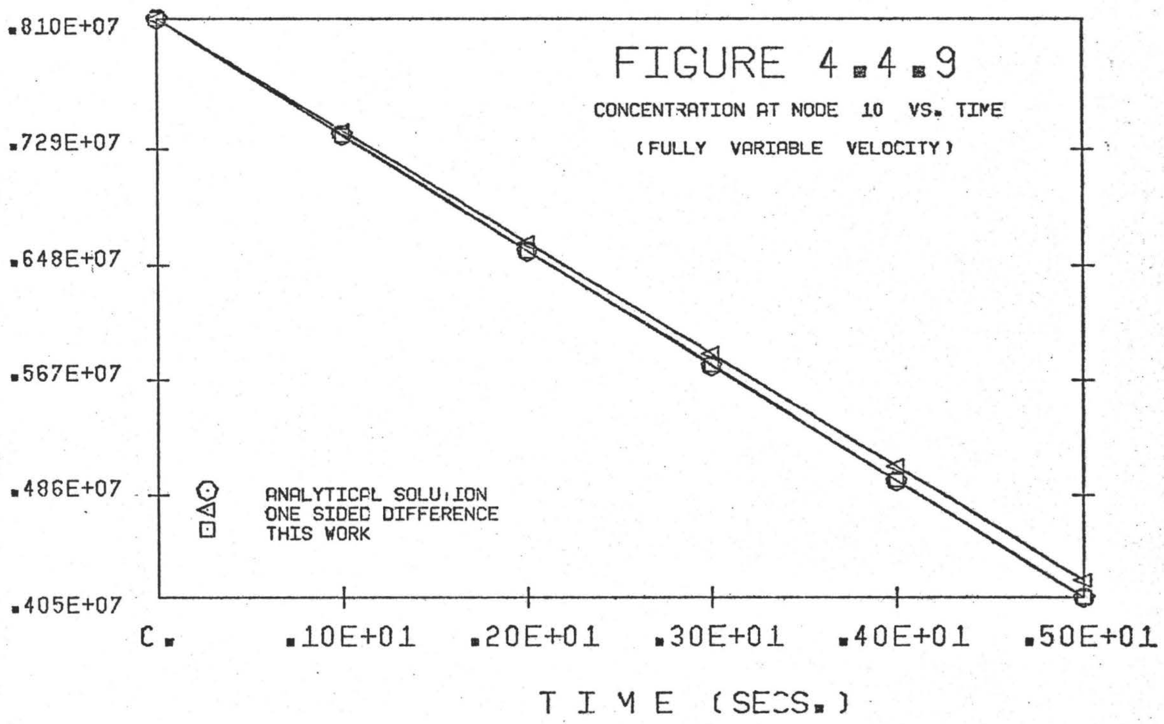


FIGURE 4.4.9
CONCENTRATION AT NODE 10 VS. TIME
(FULLY VARIABLE VELOCITY)
.810E+07
.729E+07
.648E+07
.567E+07
.486E+07
.405E+07
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

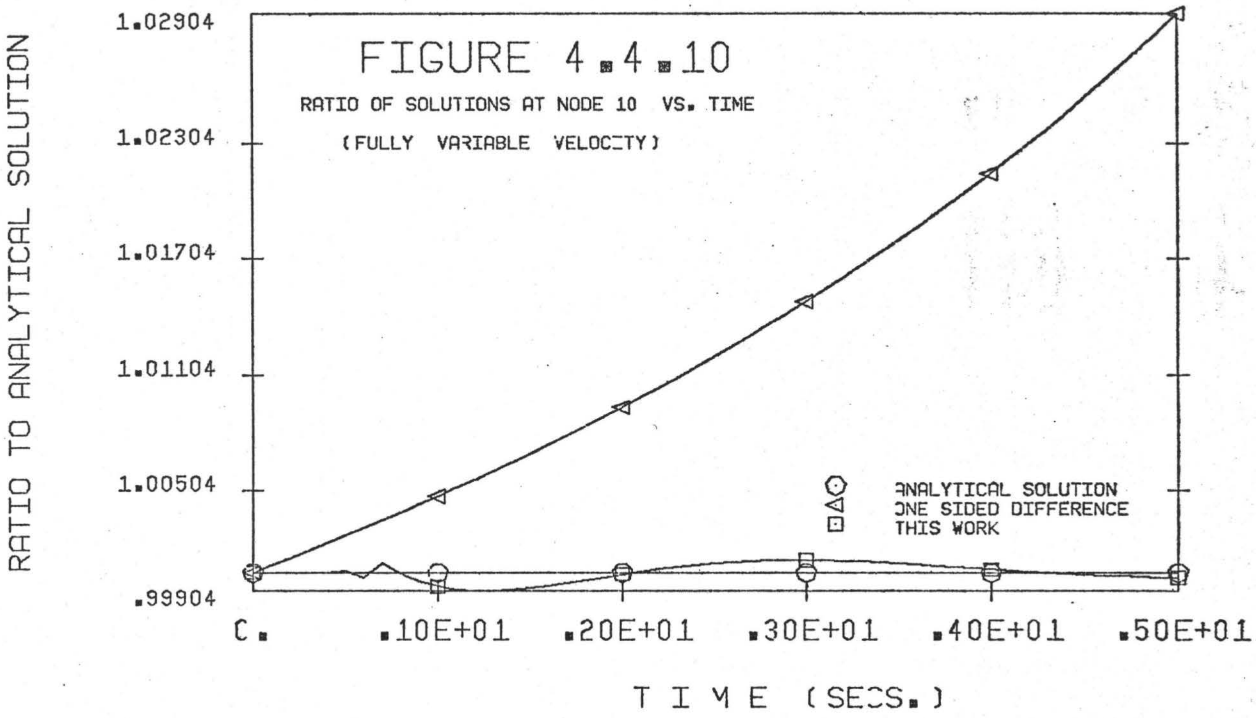


FIGURE 4.4.10
RATIO OF SOLUTIONS AT NODE 10 VS. TIME
(FULLY VARIABLE VELOCITY)
RATIO TO ANALYTICAL SOLUTION
1.02904
1.02304
1.01704
1.01104
1.00504
.99904
ANALYTICAL SOLUTION
ONE SIDED DIFFERENCE
THIS WORK
C.
.10E+01
.20E+01
.30E+01
.40E+01
.50E+01
T I M E (SECS.)

CHAPTER 5

CONCLUSIONS

The method developed here has been used to solve the advection equation with a high degree of accuracy.

Although this method in theory does not have any Courant number limitation, its accuracy will fall drastically for Courant numbers greater than unity. This is due to the fact that the method uses local power series expansion which are obtained by considering known values of the function in the surrounding nodes. If C_N is greater than unit then any value obtained by these expansions will be by extrapolation rather than interpolation and its accuracy in that case will fall tremendously, thus defeating the purpose of this method.

In the runs that were done in the McMaster University Computer Centre (CYBER 170) the time required was about 0.25 CPU seconds per node per time step. Thus for a ten node pipe the program required 2.5 seconds CPU time per time step.

Clearly this method is consideraly more expensive than most conventional numerical methods of lower accuracy, and should only be used for those cases where high accuracy is the governing criterion.

In actual comparison tests for particular cases with known analytical solution this method proved to be at least two orders of magnitude more accurate than the conventional upwind one sided difference scheme.

This method can now easily be extended to solve the general advection diffusion equation.

REFERENCES

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2. Noh, W.F., and Protter, M.H. (1963), "Difference Methods and the Equations of Hydrodynamics", Journal of Mathematics and Mechanics, Vol. 12, no. 2, pp. 149-191.

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APPENDIX I

A1.1 Coefficients of the Particle Path Function

Let the particle path equation about the point $(j\Delta X, n\Delta t)$ be given by:

$$X(t) = \sum_{i=1}^{5} \alpha_i t^{(i-1)} \tag{A1.1.1}$$

Let's choose five points in this particle path equally spaced in time as shown in Figure A1.1.1.

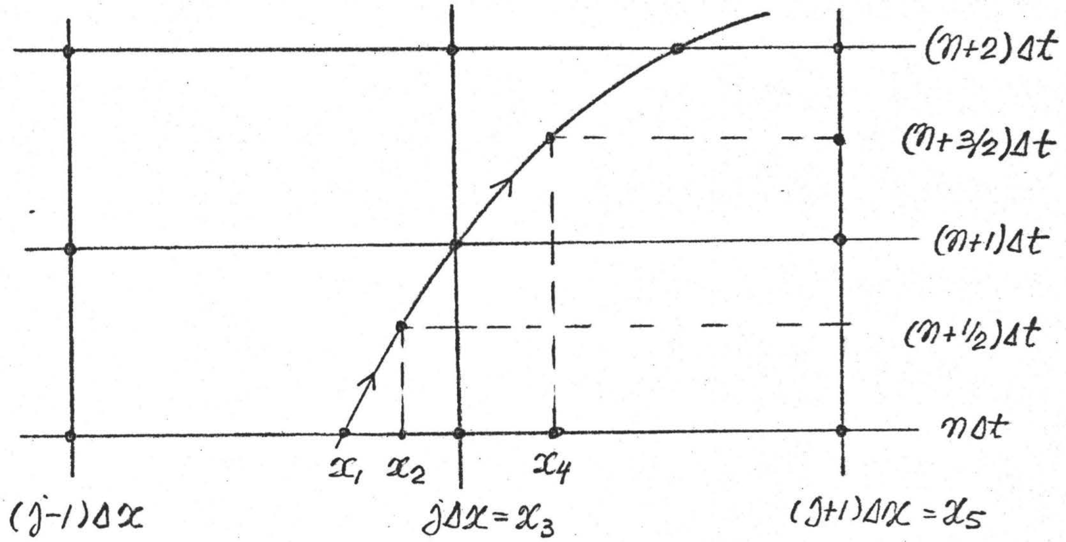

Figure A1.1.1: Equally spaced points in the particle path.

We can then construct five equations, as follows:

$$X_k = \sum_{i=1}^{5} \alpha_i \; t_k^{(i-1)}, \; k = 1,2,\ldots,5 \tag{A1.1.2}$$

where:

$t_1 = -\Delta t$

$t_2 = -\Delta t/2$

$t_3 = 0$

$t_4 = \Delta t/2$

$t_5 = \Delta t$

If we consider the point $(j\Delta X,(n+1)\Delta t)$ to be the origin of expansion then clearly $\alpha_1 = 0$ and we are left with only four equations:

$$X_R = \sum_{i=2}^{5} \alpha_i t_k^{(i-1)}; \; i = 1,2,4,5 \tag{A1.1.3}$$

Where the corresponding $t_k^{'s}$ are given above. In matrix notation we have

$$\begin{bmatrix} -\Delta t & \Delta t^2 & -\Delta t^3 & \Delta t^4 \\ -\Delta t/2 & \frac{1}{4}\Delta t^2 & -\frac{1}{8}\Delta t^3 & \frac{1}{16}\Delta t^4 \\ \Delta t/2 & \frac{1}{4}\Delta t^2 & \frac{1}{8}\Delta t^3 & \frac{1}{16}\Delta t^4 \\ \Delta t & \Delta t^2 & \Delta t^3 & \Delta t^4 \end{bmatrix} \begin{bmatrix} \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_4 \\ x_5 \end{bmatrix}$$

We can apply elementary row operations to reduce the above coefficient matrix to upper triangular.

$$\begin{array}{l} R_1 = R_1 \\ R_2 = 2R_2 - R_1 \\ R_3 = 2R_3 + R_1 \\ R_4 = R_4 + R_1 \end{array} \left[\begin{array}{cccc|c} -\Delta t & \Delta t^2 & -\Delta t^3 & \Delta t^4 & X_1 \\ 0 & -\frac{1}{2}\Delta t^2 & \frac{3}{4}\Delta t^3 & -\frac{7}{8}\Delta t^4 & 2X_2-X_1 \\ 0 & \frac{3}{2}\Delta t^2 & -\frac{3}{4}\Delta t^3 & \frac{9}{8}\Delta t^4 & 2X_4+X_1 \\ 0 & 2\Delta t^2 & 0 & 2\Delta t^4 & X_5+X_1 \end{array}\right]$$

$$\begin{array}{l} R_1 = R_1 \\ R_2 = R_2 \\ R_3 = R_3 + 3R_2 \\ R_4 = R_4+4R_2 \end{array} \left[\begin{array}{cccc|c} -\Delta t & \Delta t^2 & -\Delta t^3 & \Delta t^4 & X_1 \\ 0 & -\frac{1}{2}\Delta t^2 & \frac{3}{4}\Delta t^3 & -\frac{7}{8}\Delta t^4 & 2X_2-X_1 \\ 0 & 0 & \frac{3}{2}\Delta t^3 & -\frac{3}{2}\Delta t^4 & 2X_4+6X_2-2X_1 \\ 0 & 0 & 3\Delta t^3 & -\frac{3}{2}\Delta t^4 & X_5+8X_2-3X_1 \end{array}\right]$$

$$\begin{array}{l} R_1 = R_1 \\ R_2 = R_2 \\ R_3 = R_3 \\ R_4 = R_4 - 2R_3 \end{array} \quad \left[\begin{array}{cccc|c} -\Delta t & \Delta t^2 & -\Delta t^3 & \Delta t^4 & X_1 \\ 0 & -\frac{1}{2}\Delta t^2 & \frac{3}{4}\Delta t^3 & -\frac{7}{8}\Delta t^4 & 2X_2 - X_1 \\ 0 & 0 & \frac{3}{2}\Delta t^3 & -\frac{3}{2}\Delta t^4 & 2X_4 + 6X_2 - 2X_1 \\ 0 & 0 & 0 & \frac{3}{2}\Delta t^4 & X_5 - 4X_4 - 4X_2 + X_1 \end{array}\right]$$

We can now solve for the coefficients directly:

$$\alpha_2 = \left(\frac{1}{6\Delta t}\right) [-X_5 + 8X_4 - 8X_2 + X_1] \tag{A1.1.4}$$

$$\alpha_3 = \left(\frac{1}{6\Delta t^2}\right)[-X_5 + 16X_4 + 16X_2 - X_1] \tag{A1.1.5}$$

$$\alpha_4 = \left(\frac{2}{3\Delta t^3}\right)[X_5 - 2X_4 + 2X_2 - X_1] \tag{A1.1.6}$$

$$\alpha_5 = \left(\frac{2}{3\Delta t^4}\right)[X_5 - 4X_4 - 4X_2 + X_1] \tag{A1.1.7}$$

A1.2 Coefficients of $\phi(x)$ Along the Particle Path

Let the value of the variable $\phi(x,t)$ along the particle path be given by:

$$\phi(x) = \sum_{i=1}^{5} \beta_i t^{(i-1)} \tag{A1.2.1}$$

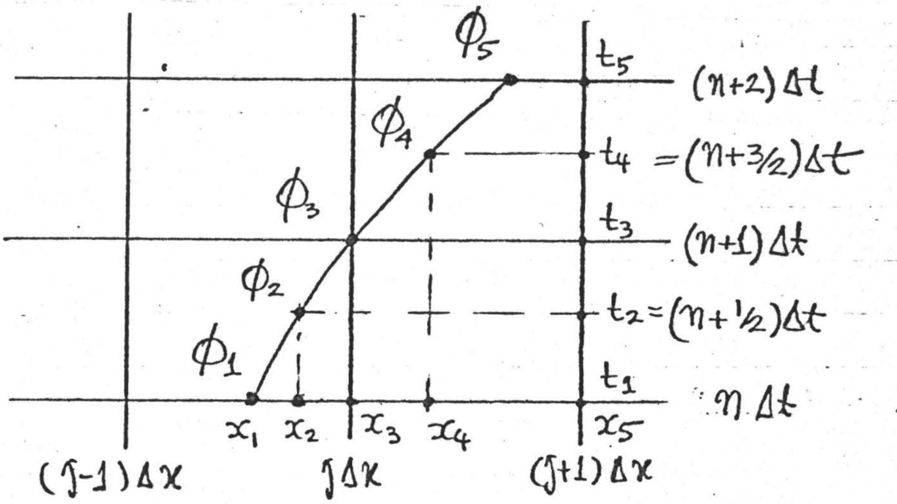

Figure A1.2.1: Values of ϕ at selected points along the particle data.

We choose five points along the particle path as shown on Figure A1.2.1. We can again construct five equations:

$$\phi_k = \phi(x_k) = \sum_{i=1}^{5} \beta_i t_k^{(i-1)}; \; k = 1,2,..,5 \qquad \text{(A1.2.2)}$$

Where the points (x_k, t_k) are:

$$t_1 = -\Delta t$$

$$t_2 = -\Delta t/2$$

$$t_3 = 0$$

$$t_4 = \Delta t/2$$

$$t_5 = \Delta t$$

and

$$x_k = \sum_{i=1}^{5} \alpha_i t_k^{(i-1)}$$

Where the summation above is the particle path equation.

If we choose the point $(j\Delta x, (n+1)\Delta t)$ as the origin of the expansion of equation (A1.2.1) we then get the value of β_1 directly.

i.e. $\beta_1 = \phi(x_3) = \phi_3$

The matrix representation of equation (A1.2.2) becomes:

$$\begin{bmatrix} x_1 & x_1^2 & x_1^3 & x_1^4 \\ x_2 & x_2^2 & x_2^3 & x_2^4 \\ x_4 & x_4^2 & x_4^3 & x_4^4 \\ x_5 & x_5^2 & x_5^3 & x_5^4 \end{bmatrix} \begin{bmatrix} \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \end{bmatrix} = \begin{bmatrix} \phi_1 - \phi_3 \\ \phi_2 - \phi_3 \\ \phi_4 - \phi_3 \\ \phi_5 - \phi_3 \end{bmatrix}$$

Performing elementary row operation on the above system we get:

1st Reduction

$\underline{R_1 = R_1}$

$\underline{R_2 = x_1R_2 - x_2R_1}$

$\rightarrow \quad a_{21} = 0$

$a_{22} = x_1x_2^2 - x_2x_1^2$

$a_{23} = x_1x_2^3 - x_2x_1^3$

$a_{24} = x_1x_2^4 - x_2x_1^4$

$b_2 = x_1(\phi_2-\phi_3) - x_2(\phi_1-\phi_3)$

$\underline{R_3 = X_1R_3 - X_4R_1}$

$\rightarrow \quad a_{31} = 0$

$a_{32} = x_1x_4^2 - x_4x_1^2$

$a_{33} = x_1x_4^3 - x_4x_1^3$

$a_{34} = x_1x_4^4 - x_4x_1^4$

$b_3 = x_1(\phi_4-\phi_3) - x_4(\phi_1-\phi_3)$

$\underline{R_4 = X_1R_4 - X_5R_1}$

$\rightarrow \quad a_{41} = 0$

$a_{42} = x_1x_5^2 - x_5x_1^2$

$a_{43} = x_1x_5^3 - x_5x_1^3$

$a_{44} = x_3x_5^4 - x_5x_1^4$

$b_4 = x_1(\phi_5-\phi_3) - x_5(\phi_1-\phi_3)$

2nd Reduction

$\underline{R_1 = R_1}$

$\underline{R_2 = R_2}$

$\underline{R_3 = a_{22}R_3 - a_{32}R_2}$

$\rightarrow$ $a_{31} = 0$

$a_{32} = 0$

$$a_{33} = (x_1x_2^2-x_2x_1^2)(x_1x_4^3-x_4x_1^3)$$
$$-(x_1x_4^2-x_4x_1^2)(x_1x_2^3-x_2x_1^3)$$
$$= x_1x_2x_4(x_1x_2x_4^2-x_1^3x_2-x_1^2x_4^2-x_1x_2^2x_4-x_1^3x_4-x_1^2x_2^2)$$

$$a_{34} = (x_1x_2^2-x_2x_1^2)(x_1x_4^4-x_4x_1^4)$$
$$-(x_1x_4^2-x_4x_1^2)(x_1x_2^4-x_2x_1^4)$$
$$= x_1x_2x_4(x_1x_2x_4^3-x_1^4x_2-x_1^2x_4^3-x_1x_2^3x_4-x_1^4x_4-x_1^2x_2^3)$$

$$b_3 = (x_1x_2^2-x_2x_1^2)[x_1(\phi_4-\phi_3)-x_4(\phi_1-\phi_3)]$$
$$-(x_1x_4^2-x_4x_1^2)[x_1(\phi_2-\phi_3)-x_2(\phi_1-\phi_3)]$$
$$= \phi_1[x_1x_2x_4(x_4-x_2)] + \phi_2[x_1x_4(x_1^2-x_1x_4)]$$
$$+ \phi_3[x_1^2x_4^4-x_1^3x_4-x_1x_2x_4^2+x_1x_2^2x_4+x_1x_1^2x_2-x_1^2x_2]$$
$$+ \phi_4[x_1^2x_2(x_2-x_1)]$$

$\underline{R_4 = a_{22}R_4 - a_{42}R_2}$

$\rightarrow$ $a_{41} = 0$

$a_{42} = 0$

$$a_{43} = (x_1x_2^2-x_2x_1^2)(x_1x_5^3-x_5x_1^3)$$
$$-(x_1x_5^2-x_5x_1^2)(x_1x_2^3-x_2x_1^3)$$
$$= x_1x_2x_5(x_1x_2x_5^2-x_1^3x_2-x_1^2x_5^2-x_1x_2^2x_5+x_1^3x_5+x_1^2x_2^2)$$

$$a_{44} = (x_1x_2^2-x_2x_1^2)(x_1x_5^4-x_5x_1^4)$$
$$-(x_1x_5^2-x_5x_1^2)(x_1x_2^4-x_2x_1^4)$$

$$= x_1x_2x_5(x_1x_2x_5^3-x_1^4x_2-x_1^2x_5^3-x_1x_2^3x_5+x_1^4x_5+x_1^2x_2^3)$$

$$b_4 = (x_1x_2^2-x_2x_1^2)[x_1(\phi_5-\phi_3)-x_5(\phi_1-\phi_3)]$$

$$-(x_1x_5^2-x_5x_1^2)[x_1(\phi_2-\phi_3)-x_2(\phi_1-\phi_3)]$$

$$= \phi_1[x_1x_2x_5(x_5-x_2)]$$

$$+ \phi_2[x_1^2x_5(x_1-x_5)]$$

$$+ \phi_3[x_1(x_2x_5(x_2-x_5)+x_1x_2(x_1-x_2)+x_1x_5(x_5-x_1))]$$

$$+ \phi_5[x_1^2x_2(x_2-x_1)]$$

We now have a system which has the following format:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} & a_{23} & a_{24} \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

The solution is given by:

$$\beta_5 = \left[\frac{1}{(a_{33}a_{44}-a_{34}a_{43})}\right]* [a_{33}b_4 - a_{43}b_3] \qquad \text{(A1.2.3)}$$

$$\beta_4 = \left[\frac{1}{a_{33}}\right]*[b_3 - a_{34}\beta_5] \qquad \text{(A1.2.4)}$$

$$\beta_3 = \left[\frac{1}{a_{22}}\right]*[b_2 - a_{24}\beta_5 - a_{23}\beta_4] \qquad \text{(A1.2.5)}$$

$$\beta_2 = \left[\frac{1}{a_{11}}\right]*[b_1 - a_{14}\beta_5 - a_{13}\beta_4 - a_{12}\beta_3] \qquad \text{(A1.2.6)}$$

where

$a_{11} = x_1$

$a_{12} = x_1^2$

$a_{13} = x_1^3$

$a_{14} = x_1^4$

$$b_1 = (\phi_1 - \phi_3)$$

$$a_{22} = x_1 x_2 (x_2 - x_1)$$

$$a_{23} = x_1 x_2 (x_2^2 - x_1^2)$$

$$a_{24} = x_1 x_2 (x_2^3 - x_1^3)$$

$$b_2 = \phi_1[-x_2] + \phi_2[x_1] + \phi_3[x_2 - x_1]$$

$$a_{33} = x_1 x_2 x_4 (x_1 x_2 x_4^2 - x_1^3 x_2 - x_1^2 x_4^2 - x_1 x_2^2 x_4 - x_1^3 x_4 - x_1^2 x_2^2)$$

$$a_{34} = x_1 x_2 x_4 (x_1 x_2 x_4^3 - x_4^4 x_2 - x_1^2 x_4^3 - x_1 x_2^3 x_4 - x_1^4 x_4 - x_1^2 x_2^3)$$

$$b_3 = \phi_1[x_1 x_2 x_4 (x_4 - x_2)] + \phi_2[x_1 x_4 (x_1^2 - x_1 x_4)]$$

$$+ \phi_3[x_1 x_2 x_4 (x_2 - x_4) - x_1^2 x_4 (x_1 - x_4) - x_1^2 x_2 (x_2 - x_1)]$$

$$+ \phi_4[x_1^2 x_2 (x_2 - x_1)]$$

$$a_{43} = x_1 x_2 x_5 (x_1 x_2 x_5^2 - x_1^3 \; x_2 - x_1^2 x_5^2 - x_1 x_2^2 x_5 + x_1^2 x_2^2)$$

$$a_{44} = x_1 x_2 x_5 (x_1 x_2 x_5^3 - x_1^4 x_2 - x_1^2 x_5^3 - x_1 x_2^3 x_5 + x_1^4 x_5 + x_1^2 x_2^3)$$

$$b_4 = \phi_1[x_1 x_2 x_5 (x_5 - x_2)] + \phi_2[x_1^2 x_5 (x_1 - x_5)]$$

$$+ \phi_3[x_1 (x_2 x_5 (x_2 - x_5) + x_1 x_2 (x_1 - x_2) + x_1 x_5 (x_5 - x_1))]$$

$$+ \phi_5[x_1^2 x_2 (x_2 - x_1)]$$

APPENDIX A2

A2.1 The Coefficients of $\partial u/\partial x(t)$ Along the Particle Path

The velocity field near the point ($j\Delta x$, $(n+1)\Delta t$ is given by:

$$u(x,t) = \sum_{i=1}^{3} \sum_{j=1}^{3} \lambda_{ij} x^{(j-1)} t^{(i-1)} \tag{A2.1.1}$$

The partial derivative of the velocity field w.v.t. x is given by:

$$\frac{\partial u}{\partial x} = \sum_{i=1}^{3} \sum_{j=2}^{3} \lambda_{ij}(j-1) x^{(j-2)} t^{(i-1)} \tag{A2.1.2}$$

If we substitute for the particle path equation ($x(t)$) we then have an expression for $\partial u/\partial x$ along the particle path which is a function of time only.

$$\frac{\partial u}{\partial x} = \sum_{i=1}^{3} \sum_{j=2}^{3} \lambda_{ij}(j-1)[x(t)]^{(j-2)} t^{(i-1)}$$

$$\rightarrow \qquad [\frac{du}{dx}](t) = \sum_{j=1}^{7} D_j \; t^{(j-1)} \tag{A2.1.3}$$

where the coefficients D_j are given by:

$$\begin{aligned}
D_1 &= \lambda_{12} \\
D_2 &= 2\lambda_{13}\alpha_2 + \lambda_{22} \\
D_3 &= 2\lambda_{13}\alpha_3 + 2\lambda_{23}\alpha_2 + \lambda_{32} \\
D_4 &= 2\lambda_{13}\alpha_4 + 2\lambda_{23}\alpha_3 + 2\lambda_{33}\alpha_2 \\
D_5 &= 2\lambda_{13}\alpha_5 + 2\lambda_{23}\alpha_4 + 2\lambda_{33}\alpha_3 \\
D_6 &= 2\lambda_{23}\alpha_5 + 2\lambda_{33}\alpha_4 \\
D_7 &= 2\lambda_{33}\alpha_5
\end{aligned} \tag{A2.1.4}$$

A2.2 The Coefficients of $\phi(t)$ Along the Particle Path

The value of ϕ near the point ($j\Delta u$, $(n+1)\Delta t$ is given by

$$\phi(x) = \sum_{i=1}^{5} \beta_i x^{(i=1)} \tag{A2.2.1}$$

Substituting for the particle path equation into the above equation we have:

$$\phi[x(t)] = \phi(t) = \sum_{i=1}^{5} \beta_i \left[\sum_{j=2}^{5} \alpha_j t^{(j-1)}\right]^{(i-1)}$$

$$= \beta_1 + \beta_2 \left[\sum_{j=2}^{5} \alpha_j t^{(j-1)}\right]$$

$$+ \beta_3 \left[\sum_{j=2}^{5} \alpha_j t^{(j-1)}\right]^2 + \beta_4 \left[\sum_{j=2}^{5} \alpha_j t^{(j-1)}\right]^3$$

$$+ \beta_5 \left[\sum_{j=2}^{5} \alpha_j t^{(j-1}\right]^4 \tag{A2.2.2}$$

Expanding the expression inside the square brackets and simplifying we get:

$$\left[\sum_{j=2}^{5} \alpha_j t^{(j-1)}\right]^2 = \sum_{j=3}^{9} A_j t^{(j-1)}$$

$$\left[\sum_{j=2}^{5} \alpha_j t^{(j-1)}\right]^3 = \sum_{j=4}^{13} B_j t^{(j-1)}$$

$$\left[\sum_{j=2}^{5} \alpha_j t^{(j-1)}\right]^4 = \sum_{j=5}^{17} C_j t^{(j-1)}$$

Where the coefficients of the above series are:

$$A_3 = \alpha_2^2$$

$$A_4 = 2\alpha_2\alpha_3$$

$$A_5 = 2\alpha_2\alpha_4 + \alpha_3^2$$

$$A_6 = 2\alpha_2\alpha_5 + 2\alpha_3\alpha_4$$

$$A_7 = 2\alpha_3\alpha_5 + \alpha_4^2$$

$$A_8 = 2\alpha_4\alpha_5$$

$$A_9 = \alpha_5^2$$

$$B_4 = \alpha_2 A_3$$

$$B_5 = \alpha_2 A_4 + \alpha_3 A_3$$

$$B_6 = \alpha_2 A_5 + \alpha_3 A_4 + \alpha_4 A_3$$

$$B_7 = \alpha_2 A_6 + \alpha_3 A_5 + \alpha_4 A_4 + \alpha_5 A_3$$

$$B_8 = \alpha_2 A_7 + \alpha_3 A_6 + \alpha_4 A_5 + \alpha_5 A_4$$

$$B_9 = \alpha_2 A_8 + \alpha_3 A_7 + \alpha_4 A_6 + \alpha_5 A_5$$

$$B_{10} = \alpha_2 A_9 + \alpha_3 A_8 + \alpha_4 A_7 + \alpha_5 A_6$$

$$B_{11} = \alpha_3 A_9 + \alpha_4 A_8 + \alpha_5 A_7$$

$$B_{12} = \alpha_4 A_9 + \alpha_5 A_8$$

$$B_{13} = \alpha_5 A_9$$

$$C_5 = \alpha_2 B_4$$

$$C_6 = \alpha_2 B_5 + \alpha_3 B_4$$

$$C_7 = \alpha_2 B_6 + \alpha_3 B_5 + \alpha_4 B_4$$

$$C_8 = \alpha_2 B_7 + \alpha_3 B_6 + \alpha_4 B_5 + \alpha_5 B_4$$

$$C_9 = \alpha_2 B_8 + \alpha_3 B_7 + \alpha_4 B_6 + \alpha_5 B_5$$

$$C_{10} = \alpha_2 B_9 + \alpha_3 B_8 + \alpha_4 B_7 + \alpha_5 B_6$$

$$C_{11} = \alpha_2 B_{10} + \alpha_3 B_9 + \alpha_4 B_8 + \alpha_5 B_7$$

$$C_{12} = \alpha_2 B_{11} + \alpha_3 B_{10} + \alpha_4 B_9 + \alpha_5 B_8$$

$$C_{13} = \alpha_2 B_{12} + \alpha_3 B_{11} + \alpha_4 B_{10} + \alpha_5 B_9$$

$$C_{14} = \alpha_2 B_{13} + \alpha_3 B_{12} + \alpha_4 B_{11} + \alpha_5 B_{10}$$

$$C_{15} = + \alpha_3 B_{13} + \alpha_4 B_{12} + \alpha_5 B_{11}$$

$$C_{16} = + \alpha_4 B_{13} + \alpha_5 B_{12}$$

$$C_{17} = + \alpha_5 B_{13}$$

Equation A2.2.3 can be rewritten as:

$$\phi(t) = \beta_1 + \beta_2 \left[\sum_{p=2}^{5} \alpha_p t^{(p-1)} \right]$$

$$+ \beta_3 \left[\sum_{j=3}^{9} A_j t^{(j-1)} \right] + \beta_4 \left[\sum_{j=4}^{13} B_j t^{(j-1)} \right]$$

$$+ \beta_5 \left[\sum_{j=5}^{17} C_j t^{(j-1)} \right] \qquad \text{(A2.2.4)}$$

The above equation can be further simplified by collecting equal powers of t and expressing $\phi(t)$ by only one power series in time.

$$\phi(t) = \sum_{j=1}^{17} \xi_j t^{(j-1)} \qquad \text{(A2.2.5)}$$

Where the coefficients ξ_j are:

$$\xi_1 = \beta_1$$

$$\begin{aligned}
\xi_2 &= \beta_2\alpha_2 \\
\xi_3 &= \beta_2\alpha_3 + \beta_3A_3 \\
\xi_4 &= \beta_2\alpha_4 + \beta_3A_4 + \beta_4B_4 \\
\xi_5 &= \beta_2\alpha_5 + \beta_3A_5 + \beta_4B_5 + \beta_5C_5 \\
\xi_6 &= \beta_3A_6 + \beta_4B_6 + \beta_5C_6 \\
\xi_7 &= \beta_3A_1 + \beta_4B_7 + \beta_5C_7 \\
\xi_8 &= \beta_3A_8 + \beta_4B_8 + \beta_5C_8 \\
\xi_9 &= \beta_3A_9 + \beta_4B_9 + \beta_5C_9 \\
\xi_{10} &= \beta_4B_{10} + \beta_5C_{10} \\
\xi_{11} &= \beta_4B_{11} + \beta_5C_{11} \\
\xi_{12} &= \beta_4B_{12} + \beta_5C_{12} \\
\xi_{13} &= \beta_4B_{13} + \beta_5C_{13} \\
\xi_{14} &= \beta_5C_{14} \\
\xi_{15} &= \beta_5C_{15} \\
\xi_{16} &= \beta_5C_{16} \\
\xi_{17} &= \beta_5C_{17}
\end{aligned} \qquad \text{(A2.2.6)}$$

A2.3 The coefficients of $[\phi\ \partial u/\partial x](t)$ Along the Particle Path

If we multiply equation A2.1.3 by equation A2.2.5 we get an expression for $\phi \frac{\partial u}{\partial x}$ along the particle path as a function of time only. The new expression becomes:

$$[\phi \frac{\partial u}{\partial x}](t) = \sum_{j=1}^{23} R_j t^{(j-1)} \qquad \text{(A2.3.1)}$$

Where the coefficients are:

$$R_1 = D_1\xi_1$$

$$R_2 = D_1\xi_2 + D_2\xi_1$$

$$R_3 = D_1\xi_3 + D_2\xi_2 + D_3\xi_1$$

$$R_4 = D_1\xi_4 + D_2\xi_3 + D_3\xi_2 + D_4\xi_1$$

$$R_5 = D_1\xi_5 + D_2\xi_4 + D_3\xi_3 + D_4\xi_2 + D_5\xi_1$$

$$R_6 = D_1\xi_6 + D_2\xi_5 + D_3\xi_4 + D_4\xi_3 + D_5\xi_2 + D_6\xi_1$$

$$R_7 = D_1\xi_7 + D_2\xi_6 + D_3\xi_5 + D_4\xi_4 + D_5\xi_3 + D_6\xi_2 + D_7\xi_1$$

$$R_8 = D_1\xi_8 + D_2\xi_7 + D_3\xi_6 + D_4\xi_5 + D_5\xi_4 + D_6\xi_3 + D_7\xi_2$$

$$R_9 = D_1\xi_9 + D_2\xi_8 + D_3\xi_7 + D_4\xi_6 + D_5\xi_5 + D_6\xi_4 + D_7\xi_3$$

$$R_{10} = D_1\xi_{10} + D_2\xi_9 + D_3\xi_8 + D_4\xi_7 + D_5\xi_6 + D_6\xi_5 + D_7\xi_4$$

$$R_{11} = D_1\xi_{11} + D_2\xi_{10} + D_3\xi_9 + D_4\xi_8 + D_5\xi_7 + D_6\xi_6 + D_7\xi_5$$

$$R_{12} = D_1\xi_{12} + D_2\xi_{11} + D_3\xi_{10} + D_4\xi_9 + D_5\xi_8 + D_6\xi_7 + D_7\xi_6$$

$$R_{13} = D_1\xi_{13} + D_2\xi_{12} + D_3\xi_{11} + D_4\xi_{10} + D_5\xi_9 + D_6\xi_8 + D_7\xi_7$$

$$R_{14} = D_1\xi_{14} + D_2\xi_{13} + D_3\xi_{12} + D_4\xi_{11} + D_5\xi_{10} + D_6\xi_9 + D_7\xi_8$$

$$R_{15} = D_1\xi_{15} + D_2\xi_{14} + D_3\xi_{13} + D_4\xi_{12} + D_5\xi_{11} + D_6\xi_{10} + D_7\xi_9$$

$$R_{16} = D_1\xi_{16} + D_2\xi_{15} + D_3\xi_{14} + D_4\xi_{13} + D_5\xi_{12} + D_6\xi_{11} + D_7\xi_{10}$$

$$R_{17} = D_1\xi_{17} + D_2\xi_{16} + D_3\xi_{15} + D_4\xi_{14} + D_5\xi_{13} + D_6\xi_{12} + D_7\xi_{11}$$

$$R_{18} = D_2\xi_{17} + D_3\xi_{16} + D_4\xi_{15} + D_5\xi_{14} + D_6\xi_{13} + D_7\xi_{12}$$

$$R_{19} = D_3\xi_{17} + D_4\xi_{16} + D_5\xi_{15} + D_6\xi_{14} + D_7\xi_{13}$$

$$R_{20} = D_4\xi_{17} + D_5\xi_{16} + D_6\xi_{15} + D_7\xi_{14}$$

$$+ \lambda_{i3}[\alpha_2^2 t^2 + 2\alpha_2\alpha_3 t^3 + (2\alpha_2\alpha_4+\alpha_3^2)t^4$$

$$+ 2(\alpha_2\alpha_5+\alpha_3\alpha_4)t^5 + (2\alpha_3\alpha_5+\alpha_4^2)t^6$$

$$+ 2\alpha_4\alpha_5 t^7 + \alpha_5^2 t^8]\}t^{(i-1)}$$

$$\rightarrow \quad u(t) = \sum_{j=1}^{11} e_j t^{(j-1)} \tag{A2.3.3}$$

Where:

$$
\begin{aligned}
e_1 &= \lambda_{11} \\
e_2 &= \lambda_{21} + \lambda_{12}\alpha_2 \\
e_3 &= \lambda_{31} + \lambda_{12}\alpha_3 + \lambda_{22}\alpha_2 + \lambda_{13}\alpha_2^2 \\
e_4 &= \lambda_{12}\alpha_4 + \lambda_{22}\alpha_3 + \lambda_{32}\alpha_2 + 2\lambda_{13}\alpha_2\alpha_3 + \lambda_{23}\alpha_2^2 \\
e_5 &= \lambda_{12}\alpha_5 + \lambda_{22}\alpha_4 + \lambda_{32}\alpha_3 + \lambda_{13}(2\alpha_2\alpha_4+\alpha_3^2) + 2\lambda_{23}\alpha_2\alpha_3 + \lambda_{33}\alpha_2^2 \\
e_6 &= \lambda_{22}\alpha_5 + \lambda_{32}\alpha_4 + 2\lambda_{13}(\alpha_2\alpha_5+\alpha_3\alpha_4)+\lambda_{23}(2\alpha_2\alpha_4+\alpha_3^2) + 2\lambda_{33}\alpha_2\alpha_3 \\
e_7 &= \lambda_{32}\alpha_5 + \lambda_{13}(2\alpha_3\alpha_5+\alpha_4^2) + 2\lambda_{23}(\alpha_2\alpha_5+\alpha_3\alpha_4) + \lambda_{33}(2\alpha_2\alpha_4+\alpha_3^2) \\
e_8 &= 2\lambda_{13}\alpha_4\alpha_5 + \lambda_{23}(2\alpha_3\alpha_5+\alpha_4^2) + 2\lambda_{33}(\alpha_2\alpha_5+\alpha_3\alpha_4) \\
e_9 &= \lambda_{13}\alpha_5^2 + 2\lambda_{23}\alpha_4\alpha_5 + \lambda_{33}(2\alpha_3\alpha_5+\alpha_4^2) \\
e_{10} &= \lambda_{23}\alpha_5^2 + 2\lambda_{33}\alpha_4\alpha_5 \\
e_{11} &= \lambda_{33}\alpha_5^2
\end{aligned}
\tag{A2.3.4}
$$

APPENDIX 3

A3.1 The Elements of the Jacobian Matrix

The elements of the Jacobian matrix of equation 2.3.12 can be found by differentiating equation 2.3.8 which is reproduced below:

$$H_k = x_k - x_1 - \sum_{i=1}^{11} \left[\frac{e_i(x_1,x_2,x_4,x_5)}{i} (t_k^i - t_1^i)\right] = 0 \qquad \text{(A3.1.1)}$$

$$\therefore \frac{\partial H_k}{\partial x_j} = \frac{\partial x_k}{\partial x_j} - \frac{\partial x_1}{\partial x_j} - \sum_{i=1}^{11} \left[\frac{(t_k^i - t_1^i)}{i} \frac{\partial e_i}{\partial x_j}\right] \qquad \text{(A3.1.2)}$$

where $\frac{\partial x_\ell}{\partial x_m} = \begin{cases} 1 \text{ if } \ell = m \\ 0 \text{ if } \ell \neq m \end{cases}$

and $\frac{\partial e_n}{\partial x_j}$ can be evaluated by taking the partial derivatives of e_n as given by equation A2.3.4 in Appendix 2.

Now

$$e_i = e_i(\lambda_{\ell m}, \alpha_j(x_1,x_2,x_4,x_5))$$

where ℓ, m = 1, 2, 3 and j = 1, 2, 3, 4, 5. Thus the partial derivative of e_i with respect to x_j is given by:

$$\frac{\partial e_i}{\partial x_j} = \sum_{\ell=1}^{5} \frac{\partial e_i}{\partial \alpha_\ell} \frac{\partial \alpha_\ell}{\partial x_j} \qquad \text{(A3.1.3)}$$

Where the partial derivatives $\frac{\partial \alpha_\ell}{\partial x_j}$ can be found by differentiating equations A1.1.4 to A1.1.7.

$$\frac{\partial \alpha_1}{\partial x_j} = 0 \qquad j = 1, 2, 4, 5$$

$$\frac{\partial\alpha_2}{\partial x_1} = \frac{1}{6\Delta t}$$

$$\frac{\partial\alpha_2}{\partial x_2} = \frac{-8}{6\Delta t} = \frac{-4}{3\Delta t}$$

$$\frac{\partial\alpha_2}{\partial x_4} = \frac{-1}{6\Delta t}$$

$$\frac{\partial\alpha_3}{\partial x_1} = \frac{-1}{6\Delta t^2}$$

$$\frac{\partial\alpha_3}{\partial x_2} = \frac{16}{6\Delta t^2} = \frac{8}{3\Delta t^2}$$

$$\frac{\partial\alpha_3}{\partial x_5} = \frac{16}{6\Delta t^2} = \frac{8}{3\Delta t^2}$$

$$\frac{\partial\alpha_3}{\partial x_5} = \frac{-1}{6\Delta t^2}$$

$$\frac{\partial\alpha_4}{\partial x_1} = \frac{-2}{3\Delta t^3}$$

$$\frac{\partial\alpha_4}{\partial x_2} = \frac{4}{3\Delta t^3}$$

$$\frac{\partial\alpha_4}{\partial x_4} = \frac{-4}{3\Delta t^3}$$

$$\frac{\partial\alpha_4}{\partial x_5} = \frac{2}{3\Delta t^3}$$

$$\frac{\partial\alpha_5}{\partial x_1} = \frac{2}{3\Delta t^4}$$

$$\frac{\partial\alpha_5}{\partial x_2} = \frac{-8}{3\Delta t^4}$$

$$\frac{\partial \alpha_5}{\partial x_4} = \frac{-8}{3\Delta t^4}$$

$$\frac{\partial \alpha_5}{\partial x_5} = \frac{2}{3\Delta t^4}$$

And the partial derivatives of e_i w.r.t. α_ℓ can be found by differentiating e_i as given in equation A2.3.4 in Appendix 2.

$$\frac{\partial e_i}{\partial \alpha_1} = 0 \qquad i = 1, 2, \ldots, 11.$$

$$\frac{\partial e_1}{\partial \alpha_2} = 0$$

$$\frac{\partial e_2}{\partial \alpha_2} = \lambda_{12}$$

$$\frac{\partial e_3}{\partial \alpha_2} = \lambda_{22} + 2\lambda_{13}\alpha_2$$

$$\frac{\partial e_4}{\partial \alpha_2} = \lambda_{32} + 2\lambda_{13}\alpha_3 + 2\lambda_{23}\alpha_2$$

$$\frac{\partial e_5}{\partial \alpha_2} = 2\lambda_{13}\alpha_4 + 2\lambda_{23}\alpha_3 + 2\lambda_{33}\alpha_2$$

$$\frac{\partial e_6}{\partial \alpha_2} = 2\lambda_{13}\alpha_5 + 2\lambda_{23}\alpha_4 + 2\lambda_{33}\alpha_3$$

$$\frac{\partial e_7}{\partial \alpha_2} = 2\lambda_{23}\alpha_5 + 2\lambda_{33}\alpha_4$$

$$\frac{\partial e_8}{\partial \alpha_2} = 2\lambda_{33}\alpha_5$$

$$\frac{\partial e_9}{\partial \alpha_2} = 0$$

$$\frac{\partial e_{10}}{\partial \alpha_2} = 0$$

$$\frac{\partial e_{11}}{\partial \alpha_2} = 0$$

And the partial derivatives of e_i w.r.t. the other alphas can be easily computed by the formula

$$\frac{\partial e_i}{\partial \alpha_j} \begin{cases} \dfrac{\partial e_\ell}{\partial \alpha_2} & \text{for } i \geq j \\ 0 & \text{for } i < j \end{cases}$$

where $i = 1, 2, 3, \ldots, 11$

$j = 3, 4, 5$

and $\ell = (i+2-j)$

A3.2 The Elements of the Linear System of ϕ_k

The elements of the linear system of equation 2.3.27 can be found by differentiating the homogeneous function S_k w.r.t. ϕ_j

$$\frac{\partial S_k}{\partial \phi_j} = \frac{\partial \phi_k}{\partial \phi_j} - \frac{\partial \phi_1}{\partial \phi_j} + \sum_{i=1}^{23} \{\frac{1}{i} \frac{\partial R_i}{\partial \phi_j} [t_k^i - t_1^i]\} \qquad \text{A3.2.1}$$

where:

$$\frac{\partial \phi_\ell}{\partial \phi_j} = \begin{cases} 1 \text{ if } \ell = j \\ 0 \text{ if } \ell \neq j \end{cases}$$

and $\frac{\partial R_i}{\partial \phi_j}$ can be found by differentiating the coefficients R_i given in Appendix 2.

As it can be seen in Appendix 2 (Section 3)

$$R_i = D_j \xi_\ell(\beta_1, \beta_2, \ldots, \beta_5) \tag{A3.2.2}$$

where $j = 1, 2, \ldots, 7$ and $\ell = 1, 2, \ldots, 17.$

and $$\beta_m = \beta_m(\phi_1, \phi_2, \ldots, \phi_5) \tag{A3.2.3}$$

Thus the partial derivative of R_i w.r.t. the variable ϕ_j will be given by:

$$\frac{\partial R_i}{\partial \phi_j} = \sum_{\ell=1}^{17} \frac{\partial R_i}{\partial \xi_\ell} [\sum_{m=1}^{5} \frac{\partial \xi_\ell}{\partial \beta_m} \frac{\partial \beta_m}{\partial \phi_j}] \tag{A3.2.3}$$

where:

$$\frac{\partial \beta_1}{\partial \phi_j} = \begin{cases} 1 \text{ if } j = 1 \\ 0 \text{ if } j \neq 0 \end{cases}$$

$$\frac{\partial \beta_5}{\partial \phi_j} = \left[\frac{1}{(a_{33}a_{44} - a_{34}a_{43})} \right] * \left[a_{33} \frac{\partial b_4}{\partial \phi_j} - a_{43} \frac{\partial b_3}{\partial \phi_j} \right]$$

$$\frac{\partial B_4}{\partial \phi_j} = \left[\frac{1}{a_{33}} \right] \left[\frac{\partial b_3}{\partial \phi_j} - a_{34} \frac{\partial \beta_5}{\partial \phi_j} \right]$$

$$\frac{\partial \beta_3}{\partial \phi_j} = \left[\frac{1}{a_{22}} \right] * \left[\frac{\partial b_2}{\partial \phi_j} - a_{24} \frac{\partial \beta_5}{\partial \phi_j} - a_{23} \frac{\partial \beta_4}{\partial \phi_j} \right]$$

$$\frac{\partial \beta_2}{\partial \phi_j} = \left[\frac{1}{a_{11}} \right] * \left[\frac{\partial b_1}{\partial \phi_j} - a_{14} \frac{\partial \beta_5}{\partial \phi_j} - a_{13} \frac{\partial \beta_4}{\partial \phi_j} - a_{12} \frac{\partial \beta_3}{\partial \phi_j} \right]$$

The above expressions were obtained by differentiating equations A1.2.3 to A1.2.6 in Appendix 1 (Section 2).

The partial derivatives of ξ_ℓ w.r.t. β_m can be found by differentiating the expressions for ξ_m as given in equation A2.2.6 in Appendix 2. I turns out to be:

$$\frac{\partial \xi_\ell}{\partial \beta_m} = \begin{cases} 1 & \text{if } \ell = 1 \text{ and } m = 1 \\ \alpha_\ell & \text{if } 2 \leq \ell \leq 5 \text{ and } m = 2 \\ A_\ell & \text{if } 3 \leq \ell \leq 9 \text{ and } m = 3 \\ B_\ell & \text{if } 4 \leq \ell \leq 13 \text{ and } m = 4 \\ C_\ell & \text{if } 5 \leq \ell \leq 17 \text{ and } m = 5 \end{cases}$$

And finally the partial derivatives of R_i w.r.t ξ_ℓ are given by:

$$\frac{\partial R_i}{\partial \xi_\ell} = \begin{cases} D_{1+1-\ell} & \text{if } i \geq \ell \\ 0 & \text{if } i < \ell \end{cases}$$

which can be verified by inspection if one refers to the expressions for $R_2 = R_i(\xi_m)$ as given in Appendix 2 (Section 2).

APPENDIX 4

T A B L E 1

C O M P A R I S O N ... AFTER 0 TIME STEPS

TOTAL TIME ELAPSED = 0.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.32919299E+06	.32919299E+06	.10000000E+01	.32919299E+06	.10000000E+01
2	.34607107E+06	.34607107E+06	.10000000E+01	.34607107E+06	.10000000E+01
3	.36381452E+06	.36381452E+06	.10000000E+01	.36381452E+06	.10000000E+01
4	.38246769E+06	.38246769E+06	.10000000E+01	.38246769E+06	.10000000E+01
5	.40207722E+06	.40207722E+06	.10000000E+01	.40207722E+06	.10000000E+01
6	.42269216E+06	.42269216E+06	.10000000E+01	.42269216E+06	.10000000E+01
7	.44436405E+06	.44436405E+06	.10000000E+01	.44436405E+06	.10000000E+01
8	.46714709E+06	.46714709E+06	.10000000E+01	.46714709E+06	.10000000E+01
9	.49109823E+06	.49109823E+06	.10000000E+01	.49109823E+06	.10000000E+01
10	.51627737E+06	.51627737E+06	.10000000E+01	.51627737E+06	.10000000E+01

(VELOCITY FUNCTION OF TIME ONLY)

T A B L E 2

C O M P A R I S O N ... AFTER 10 TIME STEPS

TOTAL TIME ELAPSED = 1.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.26441339E+06	.26441339E+06	.10000000E+01	.26441339E+06	.10000000E+01
2	.27797016E+06	.27797018E+06	.10000001E+01	.27829079E+06	.10011535E+01
3	.29222199E+06	.29222203E+06	.10000001E+01	.29289251E+06	.10022945E+01
4	.30720454E+06	.30720457E+06	.10000001E+01	.30822890E+06	.10033345E+01
5	.32295525E+06	.32295525E+06	.10000000E+01	.32429566E+06	.10041505E+01
6	.33951352E+06	.33951352E+06	.99999999E+00	.34109857E+06	.10046686E+01
7	.35692075E+06	.35692075E+06	.10000000E+01	.35867727E+06	.10049213E+01
8	.37522047E+06	.37522047E+06	.10000000E+01	.37710082E+06	.10050113E+01
9	.39445843E+06	.39445844E+06	.10000000E+01	.39644384E+06	.10050332E+01
10	.41468275E+06	.41468248E+06	.99999936E+00	.41677129E+06	.10050365E+01

(VELOCITY FUNCTION OF TIME ONLY)

T A B L E 3

C O M P A R I S O N ... AFTER 20 TIME STEPS

TOTAL TIME ELAPSED = 2.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.20339849E+06	.20339849E+06	.10000000E+01	.20339849E+06	.10000000E+01
2	.21382695E+06	.21382697E+06	.10000001E+01	.21404806E+06	.10010341E+01
3	.22479009E+06	.22479011E+06	.10000001E+01	.22526073E+06	.10020937E+01
4	.23631533E+06	.23631535E+06	.10000001E+01	.23706641E+06	.10031783E+01
5	.24843147E+06	.24843150E+06	.10000001E+01	.24949610E+06	.10042854E+01
6	.26116883E+06	.26116885E+06	.10000001E+01	.26258059E+06	.10054056E+01
7	.27455924E+06	.27455926E+06	.10000001E+01	.27634817E+06	.10065156E+01
8	.28863619E+06	.28863622E+06	.10000001E+01	.29082186E+06	.10075724E+01
9	.30343489E+06	.30343493E+06	.10000001E+01	.30601887E+06	.10085158E+01
10	.31899232E+06	.31899230E+06	.99999993E+00	.32195445E+06	.10092859E+01

(VELOCITY FUNCTION OF TIME ONLY)

T A B L E 4

C O M P A R I S O N ... AFTER 30 TIME STEPS

TOTAL TIME ELAPSED = 3.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.14857368E+06	.14857368E+06	.10000000E+01	.14857368E+06	.10000000E+01
2	.15619121E+06	.15619122E+06	.10000001E+01	.15632951E+06	.10008854E+01
3	.16419931E+06	.16419932E+06	.10000001E+01	.16449420E+06	.10017959E+01
4	.17261799E+06	.17261800E+06	.10000001E+01	.17308951E+06	.10027316E+01
5	.18146830E+06	.18146832E+06	.10000001E+01	.18213838E+06	.10036925E+01
6	.19077238E+06	.19077240E+06	.10000001E+01	.19166497E+06	.10046788E+01
7	.20055349E+06	.20055351E+06	.10000001E+01	.20169475E+06	.10056906E+01
8	.21083609E+06	.21083611E+06	.10000001E+01	.21225449E+06	.10067275E+01
9	.22164588E+06	.22164591E+06	.10000001E+01	.22337224E+06	.10077888E+01
10	.23300991E+06	.23300990E+06	.99999997E+00	.23507708E+06	.10088716E+01

(VELOCITY FUNCTION OF TIME ONLY)

T A B L E 5

C O M P A R I S O N ... AFTER 40 TIME STEPS

TOTAL TIME ELAPSED = 4.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.10200805E+06	.10200805E+06	.10000000E+01	.10200805E+06	.10000000E+01
2	.10723811E+06	.10723812E+06	.10000001E+01	.10731407E+06	.10007083E+01
3	.11273633E+06	.11273633E+06	.10000001E+01	.11289879E+06	.10014411E+01
4	.11851644E+06	.11851645E+06	.10000001E+01	.11877699E+06	.10021984E+01
5	.12459291E+06	.12459292E+06	.10000001E+01	.12496425E+06	.10029804E+01
6	.13098093E+06	.13098094E+06	.10000001E+01	.13147697E+06	.10037872E+01
7	.13769646E+06	.13759648E+06	.10000001E+01	.13833246E+06	.10046188E+01
8	.14475631E+06	.14475633E+06	.10000001E+01	.14554891E+06	.10054754E+01
9	.15217813E+06	.15217815E+06	.10000002E+01	.15314553E+06	.10063571E+01
10	.15998046E+06	.15998046E+06	.99999996E+00	.16114254E+06	.10072639E+01

(VELOCITY FUNCTION OF TIME ONLY)

T A B L E 6

C O M P A R I S O N ... AFTER 50 TIME STEPS

TOTAL TIME ELAPSED = 5.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.65030925E+05	.65030925E+05	.10000000E+01	.65030925E+05	.10000000E+01
2	.68365132E+05	.68365135E+05	.10000000E+01	.68399132E+05	.10004973E+01
3	.71870288E+05	.71870291E+05	.10000000E+01	.71943491E+05	.10010185E+01
4	.75555156E+05	.75555161E+05	.10000001E+01	.75673303E+05	.10015637E+01
5	.79428952E+05	.79428960E+05	.10000001E+01	.79598367E+05	.10021329E+01
6	.83501361E+05	.83501372E+05	.10000001E+01	.83729005E+05	.10027262E+01
7	.87782568E+05	.87782583E+05	.10000002E+01	.88076089E+05	.10033437E+01
8	.92283276E+05	.92283296E+05	.10000002E+01	.92651072E+05	.10039855E+01
9	.97014741E+05	.97014765E+05	.10000003E+01	.97466019E+05	.10046516E+01
10	.10198879E+06	.10198879E+06	.99999999E+00	.10253364E+06	.10053422E+01

(VELOCITY FUNCTION OF TIME ONLY)

T A B L E 7

C O M P A R I S O N ... AFTER 0 TIME STEPS

TOTAL TIME ELAPSED = 0.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.27182818E+07	.27182818E+07	.10000000E+01	.27182818E+07	.10000000E+01
2	.28297867E+07	.28297867E+07	.10000000E+01	.28297867E+07	.10000000E+01
3	.29470680E+07	.29470680E+07	.10000000E+01	.29470680E+07	.10000000E+01
4	.30704881E+07	.30704881E+07	.10000000E+01	.30704881E+07	.10000000E+01
5	.32004361E+07	.32004361E+07	.10000000E+01	.32004361E+07	.10000000E+01
6	.33373294E+07	.33373294E+07	.10000000E+01	.33373294E+07	.10000000E+01
7	.34816170E+07	.34816170E+07	.10000000E+01	.34816170E+07	.10000000E+01
8	.36337813E+07	.36337813E+07	.10000000E+01	.36337813E+07	.10000000E+01
9	.37943415E+07	.37943415E+07	.10000000E+01	.37943415E+07	.10000000E+01
10	.39638563E+07	.39638563E+07	.10000000E+01	.39638563E+07	.10000000E+01

(VELOCITY FUNCTION OF POSITION ONLY)

T A B L E 8

C O M P A R I S O N ... AFTER 10 TIME STEPS

TOTAL TIME ELAPSED = 1.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.22255409E+07	.22255409E+07	.10000000E+01	.22255409E+07	.10000000E+01
2	.23168334E+07	.23168334E+07	.10000000E+01	.23192446E+07	.10010407E+01
3	.24128552E+07	.24128554E+07	.10000001E+01	.24179219E+07	.10020999E+01
4	.25139031E+07	.25139036E+07	.10000002E+01	.25218922E+07	.10031780E+01
5	.26202954E+07	.26202962E+07	.10000003E+01	.26314991E+07	.10042757E+01
6	.27323742E+07	.27323757E+07	.10000005E+01	.27471116E+07	.10053936E+01
7	.28505069E+07	.28505087E+07	.10000006E+01	.28691242E+07	.10065312E+01
8	.29750885E+07	.29750914E+07	.10000010E+01	.29979269E+07	.10076765E+01
9	.31065441E+07	.31065476E+07	.10000011E+01	.31337447E+07	.10087559E+01
10	.32453310E+07	.32453380E+07	.10000021E+01	.32763427E+07	.10095558E+01

(VELOCITY FUNCTION OF POSITION ONLY)

T A B L E 9

C O M P A R I S O N ... AFTER 20 TIME STEPS

TOTAL TIME ELAPSED = 2.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.18221188E+07	.18221188E+07	.10000000E+01	.18221188E+07	.10000000E+01
2	.18968628E+07	.18958628E+07	.10000000E+01	.18988369E+07	.10010407E+01
3	.19754788E+07	.19754789E+07	.10000001E+01	.19796270E+07	.10020999E+01
4	.20582097E+07	.20582102E+07	.10000002E+01	.20647507E+07	.10031780E+01
5	.21453164E+07	.21453171E+07	.10000003E+01	.21544892E+07	.10042757E+01
6	.22370788E+07	.22370800E+07	.10000005E+01	.22491449E+07	.10053937E+01
7	.23337977E+07	.23337992E+07	.10000006E+01	.23490433E+07	.10065325E+01
8	.24357965E+07	.24357988E+07	.10000009E+01	.24545350E+07	.10076930E+01
9	.25434232E+07	.25434261E+07	.10000012E+01	.25659979E+07	.10088757E+01
10	.26570523E+07	.26570579E+07	.10000021E+01	.26838395E+07	.10100815E+01

(VELOCITY FUNCTION OF POSITION ONLY)

T A B L E 10

C O M P A R I S O N ... AFTER 30 TIME STEPS

TOTAL TIME ELAPSED = 3.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.14918247E+07	.14918247E+07	.10000000E+01	.14918247E+07	.10000000E+01
2	.15530199E+07	.15530199E+07	.10000000E+01	.15546362E+07	.10010407E+01
3	.16173852E+07	.16173853E+07	.10000001E+01	.16207815E+07	.10020999E+01
4	.16851196E+07	.16851200E+07	.10000002E+01	.16904749E+07	.10031780E+01
5	.17564365E+07	.17564371E+07	.10000003E+01	.17639466E+07	.10042757E+01
6	.18315652E+07	.18315662E+07	.10000005E+01	.18414441E+07	.10053937E+01
7	.19107519E+07	.19107532E+07	.10000007E+01	.19232340E+07	.10065325E+01
8	.19942615E+07	.19942633E+07	.10000009E+01	.20096033E+07	.10076930E+01
9	.20823788E+07	.20823812E+07	.10000012E+01	.21008614E+07	.10088757E+01
10	.21754105E+07	.21754150E+07	.10000021E+01	.21973419E+07	.10100815E+01

(VELOCITY FUNCTION OF POSITION ONLY)

T A B L E 11

C O M P A R I S O N ... AFTER 40 TIME STEPS

TOTAL TIME ELAPSED = 4.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.12214028E+07	.12214028E+07	.10000000E+01	.12214028E+07	.10000000E+01
2	.12715051E+07	.12715051E+07	.10000000E+01	.12728284E+07	.10010407E+01
3	.13242030E+07	.13242031E+07	.10000001E+01	.13269837E+07	.10020999E+01
4	.13796592E+07	.13796595E+07	.10000002E+01	.13840438E+07	.10031780E+01
5	.14380486E+07	.14380491E+07	.10000003E+01	.14441973E+07	.10042757E+01
6	.14995588E+07	.14995595E+07	.10000005E+01	.15076469E+07	.10053937E+01
7	.15643914E+07	.15643924E+07	.10000007E+01	.15746108E+07	.10065325E+01
8	.16327632E+07	.16327647E+07	.10000009E+01	.16453240E+07	.10076930E+01
9	.17049075E+07	.17049095E+07	.10000012E+01	.17200398E+07	.10088757E+01
10	.17810754E+07	.17810792E+07	.10000021E+01	.17990314E+07	.10100815E+01

(VELOCITY FUNCTION OF POSITION ONLY)

T A B L E 12

C O M P A R I S O N ... AFTER 50 TIME STEPS

TOTAL TIME ELAPSED = 5.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	.10000000E+07	.10000000E+07	.10000000E+01	.10000000E+07	.10000000E+01
2	.10410204E+07	.10410204E+07	.10000000E+01	.10421038E+07	.10010407E+01
3	.10841657E+07	.10841658E+07	.10000001E+01	.10864423E+07	.10020999E+01
4	.11295695E+07	.11295697E+07	.10000002E+01	.11331592E+07	.10031780E+01
5	.11773746E+07	.11773750E+07	.10000003E+01	.11824087E+07	.10042757E+01
6	.12277349E+07	.12277355E+07	.10000005E+01	.12343569E+07	.10053937E+01
7	.12808153E+07	.12808162E+07	.10000007E+01	.12891823E+07	.10065325E+01
8	.13367935E+07	.13367947E+07	.10000009E+01	.13470774E+07	.10076930E+01
9	.13958602E+07	.13958619E+07	.10000012E+01	.14082495E+07	.10088757E+01
10	.14582212E+07	.14582243E+07	.10000021E+01	.14729223E+07	.10100815E+01

(VELOCITY FUNCTION OF POSITION ONLY)

T A B L E 13

C O M P A R I S O N ... AFTER 0 TIME STEPS

TOTAL TIME ELAPSED = 0.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	0.	0.	.10000000E+01	0.	.10000000E+01
2	.12345679E+06	.12345679E+06	.10000000E+01	.12345679E+06	.10000000E+01
3	.49382716E+06	.49382716E+06	.10000000E+01	.49382716E+06	.10000000E+01
4	.11111111E+07	.11111111E+07	.10000000E+01	.11111111E+07	.10000000E+01
5	.19753086E+07	.19753086E+07	.10000000E+01	.19753086E+07	.10000000E+01
6	.30864198E+07	.30864198E+07	.10000000E+01	.30864198E+07	.10000000E+01
7	.44444444E+07	.44444444E+07	.10000000E+01	.44444444E+07	.10000000E+01
8	.60493827E+07	.60493827E+07	.10000000E+01	.60493827E+07	.10000000E+01
9	.79012346E+07	.79012346E+07	.10000000E+01	.79012346E+07	.10000000E+01
10	.10000000E+08	.10000000E+08	.10000000E+01	.10000000E+08	.10000000E+01

(FULLY VARIABLE VELOCITY)

TABLE 14

COMPARISON ... AFTER 10 TIME STEPS

TOTAL TIME ELAPSED = 1.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	0.	0.	.10000000E+01	0.	.10000000E+01
2	.90000000E+05	.90000024E+05	.10000003E+01	.93228498E+05	.10358722E+01
3	.36000000E+06	.36000008E+06	.10000002E+01	.36645700E+06	.10179361E+01
4	.81000000E+06	.80999958E+06	.99999948E+00	.81968549E+06	.10119574E+01
5	.14400000E+07	.14400014E+07	.10000010E+01	.14529140E+07	.10089680E+01
6	.22500000E+07	.22499956E+07	.99999804E+00	.22661425E+07	.10071744E+01
7	.32400000E+07	.32400121E+07	.10000037E+01	.32593710E+07	.10059787E+01
8	.44100000E+07	.44099691E+07	.99999299E+00	.44325995E+07	.10051246E+01
9	.57600000E+07	.57600674E+07	.10000117E+01	.57858280E+07	.10044840E+01
10	.72900000E+07	.72846191E+07	.99926188E+00	.73190565E+07	.10039858E+01

(FULLY VARIABLE VELOCITY)

T A B L E 15

C O M P A R I S O N ... AFTER 20 TIME STEPS

TOTAL TIME ELAPSED = 2.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	0.	0.	.10000000E+01	0.	.10000000E+01
2	.80000000E+05	.80000125E+05	.10000016E+01	.86201359E+05	.10775170E+01
3	.32000000E+06	.32000033E+06	.10000010E+01	.33240272E+06	.10387585E+01
4	.72000000E+06	.71999823E+06	.99999754E+00	.73860408E+06	.10258390E+01
5	.12800000E+07	.12800059E+07	.10000046E+01	.13048054E+07	.10193792E+01
6	.20000000E+07	.19999822E+07	.99999111E+00	.20310068E+07	.10155034E+01
7	.28800000E+07	.28800474E+07	.10000165E+01	.29172082E+07	.10129195E+01
8	.39200000E+07	.39198832E+07	.99997021E+00	.39634095E+07	.10110739E+01
9	.51200000E+07	.51202612E+07	.10000510E+01	.51696109E+07	.10096896E+01
10	.64800000E+07	.64793250E+07	.99989583E+00	.65358122E+07	.10086130E+01

(FULLY VARIABLE VELOCITY)

T A B L E 16

C O M P A R I S O N ... AFTER 30 TIME STEPS

TOTAL TIME ELAPSED = 3.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	0.	0.	.10000000E+01	0.	.10000000E+01
2	.70000000E+05	.70000347E+05	.10000050E+01	.78874952E+05	.11267850E+01
3	.28000000E+06	.28000071E+06	.10000025E+01	.29774990E+06	.10633925E+01
4	.63000000E+06	.62999645E+06	.99999436E+00	.65662486E+06	.10422617E+01
5	.11200000E+07	.11200102E+07	.10000091E+01	.11554998E+07	.10316963E+01
6	.17500000E+07	.17499761E+07	.99998635E+00	.17943748E+07	.10253570E+01
7	.25200000E+07	.25200415E+07	.10000165E+01	.25732497E+07	.10211308E+01
8	.34300000E+07	.34299615E+07	.99998877E+00	.34921247E+07	.10181121E+01
9	.44800000E+07	.44799153E+07	.99998110E+00	.45509996E+07	.10158481E+01
10	.56700000E+07	.56735917E+07	.10006335E+01	.57498746E+07	.10140872E+01

(FULLY VARIABLE VELOCITY)

TABLE 17

COMPARISON ... AFTER 40 TIME STEPS

TOTAL TIME ELAPSED = 4.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	0.	0.	.10000000E+01	0.	.10000000E+01
2	.60000000E+05	.60000762E+05	.10000127E+01	.71190657E+05	.11865110E+01
3	.24000000E+06	.24000118E+06	.10000049E+01	.25238131E+06	.10932555E+01
4	.54000000E+06	.53999464E+06	.99999007E+00	.57357197E+06	.10621703E+01
5	.96000000E+06	.96001222E+06	.10000127E+01	.10047626E+07	.10466277E+01
6	.15000000E+07	.14999807E+07	.99998712E+00	.15559533E+07	.10373022E+01
7	.21600000E+07	.21600080E+07	.10000037E+01	.22271439E+07	.10310852E+01
8	.29400000E+07	.29400581E+07	.10000198E+01	.30183346E+07	.10266444E+01
9	.38400000E+07	.38397816E+07	.99994313E+00	.39295253E+07	.10233139E+01
10	.48600000E+07	.48607850E+07	.10001615E+01	.49607159E+07	.10207234E+01

(FULLY VARIABLE VELOCITY)

T A B L E 18

C O M P A R I S O N ... AFTER 50 TIME STEPS

TOTAL TIME ELAPSED = 5.0000 SECS.

NODE NUMBER	ANALYTICAL SOLUTION	THIS WORK	RATIO TO ANALYTICAL SOLUTION	ONE SIDED DIFFERENCE	RATIO TO ANALYTICAL SOLUTION
1	0.	0.	.10000000E+01	0.	.10000000E+01
2	.50000000E+05	.50001497E+05	.10000299E+01	.63066202E+05	.12613240E+01
3	.20000000E+06	.20000169E+06	.10000084E+01	.22613240E+06	.11306620E+01
4	.45000000E+06	.44999309E+06	.99998465E+00	.48919861E+06	.10871080E+01
5	.80000000E+06	.80001169E+06	.10000146E+01	.85226481E+06	.10653310E+01
6	.12500000E+07	.12499906E+07	.99999249E+00	.13153310E+07	.10522648E+01
7	.18000000E+07	.17999834E+07	.99999078E+00	.18783972E+07	.10435540E+01
8	.24500000E+07	.24500570E+07	.10000233E+01	.25414634E+07	.10373320E+01
9	.32000000E+07	.31999695E+07	.99999047E+00	.33045296E+07	.10326655E+01
10	.40500000E+07	.40489600E+07	.99974320E+00	.41675958E+07	.10290360E+01

(FULLY VARIABLE VELOCITY)

APPENDIX 5

```
C     PROGRAM     A  S  A  E

C     AUTHOR .... DURVAL DUARTE

C                 DEPT. OF ENGINEERING PHYSICS

C                 MCMASTER UNIVERSITY

C                 HAMILTON,ONTARIO,

C                 CANADA    L8S 4M1

C                 TEL. (416) 525-9140 EXT.2010

C     SUPERVISOR  DR. S. BANERJEE

C                 SAME ADDRESS AS ABOVE

C                 TEL. (416) 525-9140 EXT.4545

C     PURPOSE ....THIS PROGRAM CAN BE USED TO SOLVE THE GENERAL ADVECTION

C                 EQUATION . THE MAIN FEATURES OF THE METHOD EMPLOYED HERE ARE

C                        1. HIGH ORDER ACCURACY

C                        2. LOW DISPERSION AND DIFFUSION
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C       ************************************************************************

        PROGRAM ASAE(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)

        COMMON / BLOCK1 / PHI(50,3),PHIBAR(50,3),PHIHAT(50,3),
       2   PHIUSED(50,3),PHITRUE(50,3),RU(50,3),D1(50,3),D2(50,3)
       3,DUDX(50,3),S(50,3)
        COMMON / BLOCK2 / RL,JJ,DT,DX,TIME,TIMEF,NTS
        COMMON / BLOCK3 / UCOEF(3,3,50),PCOEF(5,50),SCOEF(3,3,50)
        COMMON / BLOCK4 / PHIPLOT(5,3,51)


C       BRIEF DESCRIPTION OF THE VARIABLES USED .....

C          PHI(J,N) ..... VALUE OF PHI AT THE JTH NODE GIVEN BY THIS WORK

C          PHIBAR(J,N) .. VALUE OF PHI AT THE INTERSECTION OF THE PARTICLE PATH

C                         WITH THE LINE N*DT

C          PHIHAT(J,N) .. VALUE OF PHI AT THE INTERSECTION OF THE PARTICLE PATH

C                         WITH THE LINE (N+2)*DT

C          PHIUSED(J,N) . VALUE OF PHI AT THE JTH NODE GIVEN BY THE ONE SIDED

C          PHITRUE(J,N) . THE TRUE VALUE OF PHI AT THE JTH NODE AS GIVEN BY THE

C                         ANALYTICAL SOLUTION
```

```
C         RU(J,N) ...... VELOCITY AT THE JTH NODE

C         D1(J,N) ...... THE DISTANCE FROM THE INTERSECTION OF THE PARTICLE

C                        PATH WITH THE LINE N*DT TO THE POINT J*DX

C         D2(J,N) ...... THE DISTANCE FROM THE INTERSECTION OF THE PARTICLE

C                        PATH WITH THE LINE (N+2)*DT TO THE POINT J*DX

C         DUDX(J,N) .... THE SPATIAL DERIVATIVE OF THE VELOCITY AT THE JTH NODE

C         RL ........... THE TOTAL LENGTH OF THE PIPE

C         JJ ........... THE TOTAL NUMBER OF NODES IN THE PIPE

C         DT ........... THE TIME STEP

C         TIME ......... THE REAL TIME OF THE CALCULATION

C         TIMEF ........ THE TOTAL REAL TIME OF THE CALCULATION

C         NTS .......... TOTAL NUMBER OF TIME STEPS

C         UCOEF(3,3,J) . COEFFICIENTS OF THE LOCAL VELOCITY EXPANSION

C         PCOEF(5,J) ... COEFFICIENTS OF THE LOCAL PARTICLE PATH FUNCTION

C         PHIPLOT(*,*,*) ARRAY CONTAINING SELECTED VALUES OF PHI TO BE PLOTTED


C         RL IS THE LENGTH OF THE PIPE
```

```
      RL=1.0

C        JJ IS THE TOTAL NUMBER OF NODES

      JJ=10
      DX=RL/FLOAT(JJ)

C        DT IS THE TIME STEP

      DT=0.1

C        TIMEF IS THE REAL TIME OF THE CALCULATION

      TIMEF=5.0

C        IFLAG DESIGNATES THE TYPE OF SOLUTION
C             1 ... PHI FUNCTION OF  TIME  ONLY
C             2 ... PHI FUNCTION OF SPACE  ONLY
C             3 ... PHI FUNCTION OF BOTH SPACE AND TIME
C             4 ... ALL THREE SOLUTIONS

      IFLAG=1
      ISOL1=ISOL2=IFLAG
      IF(IFLAG.NE.4) GOTO 5
      ISOL1=1
      ISOL2=3
5     CONTINUE
```

```
      NTS=IFIX(TIMEF/DT+1.0E-5)
      JM=JJ/2


      DO 10 ISOL=ISOL1,ISOL2


      NN=1
      TIME=0.
      CALL UPDATE(ISOL)
      CALL PRINT(ISOL,NN)


      NT1=NTS+1
      DO 20 NN=1,NT1


      IF(NN.EQ.1) GOTO 15
      TIME=TIME+DT
      CALL FIT
      CALL PPATH
      CALL PHIBARS
      CALL SOLVE
      CALL UPDATE(ISOL)
      CALL PRINT(ISOL,NN)
15    CONTINUE
      DO 30 IP=1,5
      IP2=2*IP
      PHIPLOT(IP,1,NN)=PHITRUE(IP2,1)
      PHIPLOT(IP,2,NN)=PHIUSED(IP2,1)
      PHIPLOT(IP,3,NN)=PHI(IP2,1)
30    CONTINUE


20    CONTINUE
```

```
      CALL PLOTR(ISOL)


10    CONTINUE
      CALL PLOT(1.0,1.0,999)

      STOP
      END
```

```
      SUBROUTINE UPDATE(ISOL)
      COMMON / BLOCK1 / PHI(50,3),PHIBAR(50,3),PHIHAT(50,3),
     2   PHIUSED(50,3),PHITRUE(50,3),RU(50,3),D1(50,3),D2(50,3)
     3,DUDX(50,3),S(50,3)
      COMMON / BLOCK2 / RL,JJ,DT,DX,TIME,TIMEF,NTS
      COMMON / BLOCK3 / UCOEF(3,3,50),PCOEF(5,50),SCOEF(3,3,50)




      DO 10 N=1,3



      RT=TIME+FLOAT(N-1)*DT


      DO 20 J=1,JJ



C        THE SOURCE TERM

      S(J,N)=0.


      RX=FLOAT(J-1)*DX
      GOTO(30,40,50) , ISOL

30    CONTINUE

C     ******************************************************************************
```

```
C        VELOCITY FUNCTION OF TIME ONLY

      RK1=1.0E+6
      RK2=0.5
      RK3=0.180
      RK4=0.400
      RU(J,N)=RK4*EXP(RK3*RT)
      DUDX(J,N)=0.
      PHITRUE(J,N)=RK1*EXP(RK2*(RX-RK4*EXP(RK3*RT)/RK3))

C     ************************************************************************

      GOTO 60

40    CONTINUE

C     ************************************************************************

C        VELOCITY FUNCTION OF POSITION ONLY

      RK1=0.2
      RK3=1.0E+6
      RK4=-0.2
      RU(J,N)=EXP(RK4*RX)
      DUDX(J,N)=RK4*RU(J,N)
      DUMMY=-RK1*EXP(-RK4*RX)/RK4-RK4*RX
      PHITRUE(J,N)=RK3*EXP(DUMMY -RK1*RT)

C     ************************************************************************

      GOTO 60

50    CONTINUE

C     ************************************************************************
```

```
C        FULLY VARIABLE VELOCITY

      RK1=1.0
      RK2=10.0
      RK3=1.0E+6
      RU(J,N)=RK1*RX/(3.0*(RK2-RK1*RT))
      DUDX(J,N)=RU(J,N)/RX
      PHITRUE(J,N)=RK3*RX*RX*(RK2-RK1*RT)

C     ***************************************************************************

60    CONTINUE

      IF(TIME.EQ.(0.)) GOTO 18
      DUDX(J,3)=UCOEF(1,2,J)
      IF(N.EQ.3)  GOTO 18
      PHIHAT(J,N)=PHIHAT(J,N+1)
      D2(J,N)=D2(J,N+1)
      IF(N.NE.1) GOTO 18
      PHI(J,N)=PHI(J,N+1)
      PHIUSED(J,N)=PHIUSED(J,N+1)
18    CONTINUE
      IF(TIME.GT.(0.)) GOTO 20
      D1(J,N)=D2(J,N)=PHIBAR(J,N)=PHIHAT(J,N)=0.
      IF(N.GT.1) GOTO 20
      PHI(J,1)=PHIUSED(J,1)=PHITRUE(J,1)
      DUDX(1,3)=DUDX(JJ,3)=0.

20    CONTINUE

      PHI(1,N)=PHIUSED(1,N)=PHITRUE(1,N)
```

```
10      CONTINUE

        RETURN
        END
```

```
      SUBROUTINE FIT
      COMMON / BLOCK1 / PHI(50,3),PHIBAR(50,3),PHIHAT(50,3),
     2   PHIUSED(50,3),PHITRUE(50,3),RU(50,3),D1(50,3),D2(50,3)
     3,DUDX(50,3),S(50,3)
      COMMON / BLOCK2 / RL,JJ,DT,DX,TIME,TIMEF,NTS
      COMMON / BLOCK3 / UCOEF(3,3,50),PCOEF(5,50),SCOEF(3,3,50)
      DIMENSION A(9,9),B(9),X(9),WORKM(9,9),C(9),Y(9)



      JJ1=JJ-1



      DO 10 J=2,JJ1



      DELTAT=-DT



      DO 20 N=1,3



      DELTAX=-DX
```

```
      DO 30 I=1,3



      DO 40 L=1,3


      DO 50 K=1,3

      DXP=DTP=0.
      IF(L.EQ.1.AND.DELTAX.EQ.(0.)) DXP=1.0
      IF(K.EQ.1.AND.DELTAT.EQ.(0.)) DTP=1.0
      IF(DXP.EQ.(1.0)) GOTO 52
      DXP=DELTAX**(L-1)
52    CONTINUE
      IF(DTP.EQ.(1.0)) GOTO 54
      DTP=DELTAT**(K-1)
54    CONTINUE
      KL=3*(L-1)+K
      IN=3*(N-1)+I
      A(IN,KL)=DXP*DTP


50    CONTINUE


40    CONTINUE
```

```
      KB=3*(N-1)+I
      B(KB)=RU(J-2+I,N)
      C(KB)=S(J-2+I,N)
      DELTAX=DELTAX+DX

30    CONTINUE

      DELTAT=DELTAT+DT

20    CONTINUE

      CALL MV(A,9,9,B,X,DET,IDET,WORKM)
      CALL MV(A,9,9,C,Y,DET,IDET,WORKM)

      DO 60 N=1,3

      DO 70 I=1,3

      IN=3*(N-1)+I
      UCOEF(I,N,J)=X(IN)
      SCOEF(I,N,J)=Y(IN)
```

```
70    CONTINUE

60    CONTINUE

10    CONTINUE

      RETURN
      END
```

```
      SUBROUTINE PPATH
      COMMON / BLOCK1 / PHI(50,3),PHIBAR(50,3),PHIHAT(50,3),
     2   PHIUSED(50,3),PHITRUE(50,3),RU(50,3),D1(50,3),D2(50,3)
     3,DUDX(50,3),S(50,3)
      COMMON / BLOCK2 / RL,JJ,DT,DX,TIME,TIMEF,NTS
      COMMON / BLOCK3 / UCOEF(3,3,50),PCOEF(5,50),SCOEF(3,3,50)
      DIMENSION E(11),DEDA(11,5),DEDX(11,5),DHDX(11,5),H(5),A(4,4),B(4),
     2WORKM(4,4),X(4),XX(5)
      DIMENSION RLAMBDA(3,3),ALPHA(5),DADX(5,5)

      RR=1.0/(6.0*DT)
      DADX(2,1)=RR
      DADX(2,2)=-8.0*RR
      DADX(2,4)=+8.0*RR
      DADX(2,5)=-RR
      RR=RR/DT
      DADX(3,1)=DADX(3,5)=-RR
      DADX(3,2)=DADX(3,4)=16.0*RR
      RR=2.0/(3.0*(DT**3))
      DADX(4,1)=-RR
      DADX(4,2)=2.0*RR
      DADX(4,4)=-2.0*RR
      DADX(4,5)=RR
      RR=RR/DT
      DADX(5,1)=DADX(5,5)=RR
      DADX(5,2)=DADX(5,4)=-4.0*RR

      DO 5 I=1,5
      DADX(I,3)=DADX(1,I)=0.
5     CONTINUE

      JJ1=JJ-1
```

```
      DO 10 J=2,JJ1



      DO 17 I=1,3
      DO 19 N=1,3
      RLAMBDA(I,N)=UCOEF(I,N,J)
19    CONTINUE
17    CONTINUE

      XX(1)=-DT*RU(J,2)
      XX(2)=-0.5*DT*RU(J,2)
      XX(3)=0.
      XX(4)= 0.5*DT*RU(J,2)
      XX(5)=DT*RU(J,2)
      ALPHA(1)=ALPHA(3)=ALPHA(4)=ALPHA(5)=0.
      ALPHA(2)=RU(J,2)


      DO 30 ITER=2,5
      IF(ITER.GT.2) ALPHA(ITER)=10.0**(-ITER)

      DO 20 K=1,10



      E(1)=RLAMBDA(1,1)
      E(2)=RLAMBDA(2,1)+RLAMBDA(1,2)*ALPHA(2)
      E(3)=RLAMBDA(3,1)+RLAMBDA(1,2)*ALPHA(3)+RLAMBDA(2,2)*ALPHA(2)+
     2RLAMBDA(1,3)*(ALPHA(2)**2)
      E(4)=RLAMBDA(1,2)*ALPHA(4)+RLAMBDA(2,2)*ALPHA(3)+RLAMBDA(3,2)*
     2ALPHA(2)+2.0*RLAMBDA(1,3)*ALPHA(2)*ALPHA(3)+RLAMBDA(2,3)*
     3(ALPHA(2)**2)
      E(5)=RLAMBDA(1,2)*ALPHA(5)+RLAMBDA(2,2)*ALPHA(4)+RLAMBDA(3,2)*
```

```
     2ALPHA(3)+RLAMBDA(1,3)*(2.0*ALPHA(2)*ALPHA(4)+(ALPHA(3)**2))+
     32.0*RLAMBDA(2,3)*ALPHA(2)*ALPHA(3)+RLAMBDA(3,3)*(ALPHA(2)**2)
      E(6)=RLAMBDA(2,2)*ALPHA(5)+RLAMBDA(3,2)*ALPHA(4)+2.0*RLAMBDA(1,3)*
     2(ALPHA(2)*ALPHA(5)+ALPHA(3)*ALPHA(4))+RLAMBDA(2,3)*(2.0*ALPHA(2)*
     3ALPHA(4)+(ALPHA(3)**2))+2.0*RLAMBDA(3,3)*ALPHA(2)*ALPHA(3)
      E(7)=RLAMBDA(3,2)*ALPHA(5)+RLAMBDA(1,3)*(2.0*ALPHA(3)*ALPHA(5)+
     2(ALPHA(4)**2))+2.0*RLAMBDA(2,3)*(ALPHA(2)*ALPHA(5)+ALPHA(3)*
     3ALPHA(4))+RLAMBDA(3,3)*(2.0*ALPHA(2)*ALPHA(4)+(ALPHA(3)**2))
      E(8)=2.0*RLAMBDA(1,3)*ALPHA(4)*ALPHA(5)+RLAMBDA(2,3)*(2.0*ALPHA(3)
     2*ALPHA(5)+(ALPHA(4)**2))+2.0*RLAMBDA(3,3)*(ALPHA(2)*ALPHA(5)+
     3ALPHA(3)*ALPHA(4))
      E(9)=RLAMBDA(1,3)*(ALPHA(5)**2)+2.0*RLAMBDA(2,3)*ALPHA(4)*ALPHA(5)
     2+RLAMBDA(3,3)*(2.0*ALPHA(3)*ALPHA(5)+(ALPHA(4)**2))
      E(10)=RLAMBDA(2,3)*(ALPHA(5)**2)+2.0*RLAMBDA(3,3)*ALPHA(4)*
     2ALPHA(5)
      E(11)=RLAMBDA(3,3)*(ALPHA(5)**2)

C          THE PARTIAL DERIVATIVES OF THE VELOCITY COEFFICIENTS

      DEDA(1,2)=0.
      DEDA(2,2)=RLAMBDA(1,2)
      DEDA(3,2)=RLAMBDA(2,2)+2.0*RLAMBDA(1,3)*ALPHA(2)
      DEDA(4,2)=RLAMBDA(3,2)+2.0*RLAMBDA(1,3)*ALPHA(3)+2.0*RLAMBDA(2,3)*
     2ALPHA(2)
      DEDA(5,2)=2.0*(RLAMBDA(1,3)*ALPHA(4)+RLAMBDA(2,3)*ALPHA(3)+
     2RLAMBDA(3,3)*ALPHA(2))
      DEDA(6,2)=2.0*(RLAMBDA(1,3)*ALPHA(5)+RLAMBDA(2,3)*ALPHA(4)+
     2RLAMBDA(3,3)*ALPHA(3))
      DEDA(7,2)=2.0*(RLAMBDA(2,3)*ALPHA(5)+RLAMBDA(3,3)*ALPHA(4))
      DEDA(8,2)=2.0*RLAMBDA(3,3)*ALPHA(5)
      DEDA(9,2)=DEDA(10,2)=DEDA(11,2)=0.
      DEDA(1,1)=0.
```

```
      DO 6 INDEXI=2,11
      DEDA(INDEXI,1)=0.
      DO 8 INDEXJ=3,5
      DEDA(1,INDEXJ)=0.
      DEDA(INDEXI,INDEXJ)=0.
      IF(INDEXI.LT.INDEXJ) GOTO 8
      DEDA(INDEXI,INDEXJ)=DEDA(INDEXI+2-INDEXJ,2)
8     CONTINUE
6     CONTINUE
      DO 50 KK=1,11
      DO 50 LL=1,5
      DEDX(KK,LL)=0.
      DO 50 MM=2,ITER
```

```
      DEDX(KK,LL)=DEDX(KK,LL)+DEDA(KK,MM)*DADX(MM,LL)
50    CONTINUE
      RT=-DT
      DO 60 KK=2,5
      RT=RT+0.5*DT
      DO 70 LL=1,5
      DHDX(KK,LL)=H(KK)=0.
      DO 70 MM=1,11
      DUMMY=((-DT)**MM-(RT**MM))/FLOAT(MM)
      DHDX(KK,LL)=DHDX(KK,LL)+DEDX(MM,LL)*DUMMY
      H(KK)=H(KK)+E(MM)*DUMMY
70    CONTINUE
      DHDX(KK,1)=DHDX(KK,1)-1.0
      DHDX(KK,KK)=DHDX(KK,KK)+1.0
      H(KK)=H(KK)+XX(KK)-XX(1)
```

```
60    CONTINUE
      DO 80 II=1,4
      KK=II+1
      DO 90 I1=1,4
      LL=I1
      IF(I1.GE.3) LL=I1+1
      A(II,I1)=DHDX(KK,LL)
90    CONTINUE
      B(II)=-H(KK)
80    CONTINUE
C         SOLVE FOR NEW VALUES OF XX
      CALL MV(A,4,4,B,X,DET,IDET,WORKM)
      XX(1)=XX(1)+X(1)
      XX(2)=XX(2)+X(2)
      XX(4)=XX(4)+X(3)
```

```
      XX(5)=XX(5)+X(4)

C          RE-DEFINE COEFFICIENTS OF PARTICLE PATH

      DO 18 III=2,ITER

      ALPHA(III)=0.

      DO 18 JJJ=1,5

      ALPHA(III)=ALPHA(III)+DADX(III,JJJ)*XX(JJJ)

18    CONTINUE

      RINC=ABS(X(1)/XX(1))+ABS(X(2)/XX(2))+ABS(X(3)/XX(4))+ABS(X(4)/
     2XX(5))
      DELTA=1.0E-12
      IF(RINC.LT.DELTA) GOTO 22

20    CONTINUE

      WRITE(6,9050)
9050  FORMAT(///,30X,"W A R N I N G   ..... ITERATION OF PARTICLE PATH H
     2AS NOT CONVERGED")
22    CONTINUE
30    CONTINUE

C          DEFINE THE INTERSECTION OF THE PARTICLE PATH WITH THE X-AXIS
```

```
      D1(J,1)=-XX(1)
      D2(J,3)=XX(5)

      DO 16 I=1,5
      PCOEF(I,J)=ALPHA(I)
16    CONTINUE


10    CONTINUE


      RETURN
      END
```

```
      SUBROUTINE PHIBARS
      COMMON / BLOCK1 / PHI(50,3),PHIBAR(50,3),PHIHAT(50,3),
     2   PHIUSED(50,3),PHITRUE(50,3),RU(50,3),D1(50,3),D2(50,3)
     3,DUDX(50,3),S(50,3)
      COMMON / BLOCK2 / RL,JJ,DT,DX,TIME,TIMEF,NTS
      COMMON / BLOCK3 / UCOEF(3,3,50),PCOEF(5,50),SCOEF(3,3,50)
      DIMENSION A(6,6),B(6),X(6),WORKM(6,6)


      JJ1=JJ-1
      TT=2.0*DT
      IF(TIME.LE.TT) GOTO 100

      DO 10 K=1,5

      A(1,K)=(-0.5*DX)**(K-1)
      A(2,K)=(0.5*DX)**(K-1)
      A(3,K)=(0.5*DX+D2(2,1))**(K-1)
      A(4,K)=(1.5*DX)**(K-1)
      A(5,K)=(1.5*DX+D2(3,1))**(K-1)
      A(6,K)=(0.5*DX-D1(2,1))**(K-1)
      A(K,6)=0.

10    CONTINUE

      A(6,6)=-1.0
      B(1)=PHI(1,1)
      B(2)=PHI(2,1)
      B(4)=PHI(3,1)
      B(3)=PHIHAT(2,1)
      B(5)=PHIHAT(3,1)
      B(6)=0.
      CALL MV(A,6,6,B,X,DET,IDET,WORKM)
      PHIBAR(2,1)=X(6)
```

```
      DO 20 J=3,JJ1


      DO 30 K=1,5

      A(1,K)=(-1.5*DX)**(K-1)
      A(2,K)=(-0.5*DX)**(K-1)
      A(3,K)=( 0.5*DX)**(K-1)
      A(4,K)=(-0.5*DX+D2(J-1,1))**(K-1)
      A(5,K)=(-1.5*DX+D2(J-2,1))**(K-1)
      IF(J.NE.3) GOTO 35
      A(5,K)=(0.5*DX+D2(J,1))**(K-1)
35    CONTINUE
      A(6,K)=(0.5*DX-D1(J,1))**(K-1)
      A(K,6)=0.
      B(K)=PHI(J-3+K,1)

30    CONTINUE

      A(6,6)=-1.0
      B(4)=PHIHAT(J-1,1)
      B(5)=PHIHAT(J-2,1)
      IF(J.NE.3) GOTO 45
      B(5)=PHIHAT(J,1)
45    CONTINUE
      B(6)=0.

      CALL MV(A,6,6,B,X,DET,IDET,WORKM)
      PHIBAR(J,1)=X(6)

20    CONTINUE

      GOTO 200

100   CONTINUE
```

```
      DO 110 K=1,5

      A(1,K)=(-0.5*DX)**(K-1)
      A(2,K)=(0.5*DX)**(K-1)
      A(3,K)=(1.5*DX)**(K-1)
      A(4,K)=(2.5*DX)**(K-1)
      A(5,K)=(3.5*DX)**(K-1)
      A(6,K)=(0.5*DX-D1(2,1))**(K-1)
      A(K,6)=0.
      B(K)=PHI(K,1)

110   CONTINUE

      A(6,6)=-1.0
      B(6)=0.

      CALL MV(A,6,6,B,X,DET,IDET,WORKMD

      PHIBAR(2,1)=X(6)

      DO 120 J=3,JJ1

      DO 130 K=1,5

      A(1,K)=(-1.5*DX)**(K-1)
      A(2,K)=(-0.5*DX)**(K-1)
      A(3,K)=(+0.5*DX)**(K-1)
      A(4,K)=(+1.5*DX)**(K-1)
      A(6,K)=(0.5*DX-D1(J,1))**(K-1)
      A(K,6)=0.
      B(K)=PHI(J-3+K,1)
      IF(J.NE.JJ1.OR.TIME.NE.TT) GOTO 140
```

```
      A(4,K)=(-3.5*DX)**(K-1)
140   CONTINUE
      IF(J.NE.3) GOTO 500
      A(5,K)=(2.5*DX)**(K-1)
      GOTO 130
500   CONTINUE
      A(5,K)=(-2.5*DX)**(K-1)
130   CONTINUE

      A(6,6)=-1.0
      B(6)=0.
      IF(J.NE.JJ1.OR.TIME.NE.TT) GOTO 640
      B(4)=PHI(J-4,1)
640   CONTINUE
      IF(J.NE.3) GOTO 600
      B(5)=PHI(J+2,1)
      GOTO 630
600   CONTINUE
      B(5)=PHI(J-3,1)
630   CONTINUE

      CALL MV(A,6,6,B,X,DET,IDET,WORKM)

      PHIBAR(J,1)=X(6)

120   CONTINUE


200   CONTINUE

      RETURN
      END
```

```
      SUBROUTINE SOLVE
      COMMON / BLOCK1 / PHI(50,3),PHIBAR(50,3),PHIHAT(50,3),
     2   PHIUSED(50,3),PHITRUE(50,3),RU(50,3),D1(50,3),D2(50,3)
     3,DUDX(50,3),S(50,3)
      COMMON / BLOCK2 / RL,JJ,DT,DX,TIME,TIMEF,NTS
      COMMON / BLOCK3 / UCOEF(3,3,50),PCOEF(5,50),SCOEF(3,3,50)
      DIMENSION AA(4,4),BB(4,4),X(4),WORKM(4,4),A(12),B(16),C(17),D(7),
     2DRDE(23,17),DEDB(23,5),DSDP(5,5),DRDP(23,5),
     3AAA(6,6),BBB(6),XXX(6),WORKMM(6,6)
      DIMENSION DB(4,5),DG(5,5)
      DIMENSION RLAMBDA(3,3),ALPHA(5)
      DIMENSION TJ(5)


      JJ1=JJ-1


      DO 50 J=2,JJ1


      DO 17 I=1,5
      DO 19 N=1,3
      IF(I.GT.3) GOTO 19
      RLAMBDA(I,N)=UCOEF(I,N,J)
19    CONTINUE
      ALPHA(I)=PCOEF(I,J)
17    CONTINUE


      D(1)=RLAMBDA(1,2)
      D(2)=2.0*RLAMBDA(1,3)*ALPHA(2)+RLAMBDA(2,2)
      D(3)=2.0*(RLAMBDA(1,3)*ALPHA(3)+RLAMBDA(2,3)*ALPHA(2)) +
     2RLAMBDA(3,2)
```

```
 D(4)=2.0*(RLAMBDA(1,3)*ALPHA(4)+RLAMBDA(2,3)*ALPHA(3)+RLAMBDA(3,3)
2*ALPHA(2))
 D(5)=2.0*(RLAMBDA(1,3)*ALPHA(5)+RLAMBDA(2,3)*ALPHA(4)+RLAMBDA(3,3)
2*ALPHA(3))
 D(6)=2.0*(RLAMBDA(2,3)*ALPHA(5)+RLAMBDA(3,3)*ALPHA(4))
 D(7)=2.0*RLAMBDA(3,3)*ALPHA(5)


 A(1)=A(2)=A(11)=A(12)=A(10)=0.
 A(3)=ALPHA(2)**2
 A(4)=2.0*ALPHA(2)*ALPHA(3)
 A(5)=2.0*ALPHA(2)*ALPHA(4)+(ALPHA(3)**2)
 A(6)=2.0*ALPHA(2)*ALPHA(5)+2.0*ALPHA(3)*ALPHA(4)
 A(7)=2.0*ALPHA(3)*ALPHA(5)+(ALPHA(4)**2)
 A(8)=2.0*ALPHA(4)*ALPHA(5)
 A(9)=ALPHA(5)**2


 B(1)=B(2)=B(3)=B(14)=B(15)=B(16)=0.


 DO 3 I=5,13


 B(I)=ALPHA(2)*A(I-1)+ALPHA(3)*A(I-2)+ALPHA(4)*A(I-3)+ALPHA(5)*
2A(I-4)


3       CONTINUE


 B(4)=ALPHA(2)*A(3)


 C(1)=C(2)=C(3)=C(4)=0.
```

```
      DO 5 I=5,17

      C(I)=ALPHA(2)*B(I-1)+ALPHA(3)*B(I-2)+ALPHA(4)*B(I-3)+ALPHA(5)*
     2B(I-4)

5     CONTINUE



      W=-0.5*D1(J,1)
      Z=0.5*D2(J,3)
      TW=W/RU(J,2)
      TW=-0.5*DT
      TZ=Z/RU(J,2)
      TZ= 0.5*DT
      DO 16 ITER=1,50
      H1=H2=DH1=DH2=0.
      DO 14 I=2,5
      H1=H1+ALPHA(I)*(TW**(I-1))
      H2=H2+ALPHA(I)*(TZ**(I-1))
      DH1=DH1+FLOAT(I-1)*ALPHA(I)*(TW**(I-2))
      DH2=DH2+FLOAT(I-1)*ALPHA(I)*(TZ**(I-2))
14    CONTINUE
      H1=H1-W
      H2=H2-Z
      TW=TW-(H1/DH1)
      TZ=TZ-(H2/DH2)
      DUMMY=ABS(H1/DH1)+ABS(H2/DH2)
      IF(DUMMY.LT.(1.0E-12)) GOTO 18
16    CONTINUE
      WRITE(6,22)
22    FORMAT(5(/),30X,"W A R N I N G  ...  THE TIME SEARCH FOR THE PARTI
     2CLE PATH HAS NOT CONVERGED")
18    CONTINUE
      TJ(1)=-DT
      TJ(2)=TW
```

```
TJ(3)=0.
TJ(4)=TZ
TJ(5)=DT
W=0.5*D1(J,1)
A11=-2.0*W
A12=4.0*(W**2)
A13=-8.0*(W**3)
A14=16.0*(W**4)
A22=-2.0*(W**2)
A23=6.0*(W**3)
A24=-14.0*(W**4)
A33=8.0*(W**5)*Z+12.0*(W**4)*(Z**2)+4.0*(W**3)*(Z**3)
A34=-24.0*(W**6)*Z-28.0*(W**5)*(Z**2)+4.0*(W**3)*(Z**4)
A43=8.0*(W**5)*Z+24.0*(W**4)*(Z**2)+16.0*((W*Z)**3)
A44=-24.0*(W**6)*Z-56.0*(W**5)*(Z**2)+32.0*(W**3)*(Z**4)
DB(4,1)=-2.0*(W**2)*Z-4.0*W*(Z**2)
DB(4,2)=8.0*W*Z*(W+Z)
DB(4,3)=-2.0*W*(W**2+3.0*W*Z+2.0*(Z**2))
DB(4,4)=0.
DB(4,5)=2.0*(W**3)
DB(3,1)=-2.0*W*Z*(W+Z)
DB(3,2)=4.0*W*Z*(Z+2.0*W)
DB(3,3)=-2.0*W*(2.0*(W**2)+3.0*W*Z+Z**2)
DB(3,4)=4.0*(W**3)
DB(3,5)=0.
DB(2,1)=DB(2,3)=-1.0
DB(2,2)=2.0
DB(2,4)=DB(2,5)=0.
DB(1,1)=1.0
DB(1,3)=-1.0
DB(1,2)=DB(1,4)=DB(1,5)=0.
DO 8 K=1,5
DG(5,K)=(A33*DB(4,K)-A43*DB(3,K))/(A33*A44-A43*A34)
DG(4,K)=(DB(3,K)-A34*DG(5,K))/A33
DG(3,K)=(DB(2,K)-A24*DG(5,K)-A23*DG(4,K))/A22
```

```
      DG(2,K)=(DB(1,K)-A14*DG(5,K)-A13*DG(4,K)-A12*DG(3,K))/A11
      DG(1,K)=0.
8     CONTINUE
      DG(1,3)=1.0

      DO 100 K=1,23

      DO 200 KJ=1,17

      DRDE(K,KJ)=0.
      INDEXI=K+1-KJ
      IF(INDEXI.LT.1.OR.INDEXI.GT.7) GOTO 200
      DRDE(K,KJ)=D(INDEXI)

200   CONTINUE

      IF(K.GT.17) GOTO 100
      DEDB(K,1)=DEDB(K,2)=DEDB(K,3)=DEDB(K,4)=DEDB(K,5)=0.
      IF(K.EQ.1) DEDB(K,1)=1.0
      IF(K.GE.2.AND.K.LE.5) DEDB(K,2)=ALPHA(K)
      IF(K.GE.3.AND.K.LE.9) DEDB(K,3)=A(K)
      IF(K.GE.4.AND.K.LE.13)DEDB(K,4)=B(K)
      IF(K.GE.5.AND.K.LE.17)DEDB(K,5)=C(K)
```

```
100   CONTINUE

      DO 300 K=1,23

      DO 400 KJ=1,5

      DUMMY2=0.

      DO 500 M=1,17

      DUMMY1=0.

      DO 600 MS=1,5

      DUMMY1=DUMMY1+DEDB(M,MS)*  DG(MS,KJ)

600   CONTINUE

      DUMMY2=DUMMY2+DRDE(K,M)*DUMMY1

500   CONTINUE

      DRDP(K,KJ)=DUMMY2

400   CONTINUE
```

```
300   CONTINUE


      DO 1000 L=2,5

      RT=TJ(L)

      DO 1100 IP=1,5


      DUMMY=0.

      DO 1200 K=1,23

      RRTT=0.
      IF(ABS(RT).LT.1.0E-10) GOTO 1250
      RRTT=RT**K
1250  CONTINUE
      DUMMY=DUMMY+DRDP(K,IP)*(RRTT-(-DT)**K)/FLOAT(K)

1200  CONTINUE

      DSDP(L,IP)=DUMMY


1100  CONTINUE


      DSDP(L,L)=DSDP(L,L)+1.0
      DSDP(L,1)=DSDP(L,1)-1.0



1000  CONTINUE
```

```
      DO 1500 K=1,4


      DO 1600 L=1,4

      AA(K,L)=DSDP(K+1,L+1)

1600  CONTINUE

      BB(K)=-DSDP(K+1,1)*PHIBAR(J,1)


1500  CONTINUE



      CALL MV(AA,4,4,BB,X,DET,IDET,WORKM)

      PHI(J,2)=X(2)
      PHIHAT(J,3)=X(4)


50    CONTINUE


      DO 2000 K=1,5

      AAA(2,K)=(-1.5*DX)**(K-1)
      AAA(4,K)=(-.5*DX)**(K-1)
      AAA(6,K)=(0.5*DX)**(K-1)
      AAA(K,6)=0.
```

```
      IF(TIME.LE.DT) GOTO 2100
      AAA(5,K)=(-.5*DX+D2(JJ-1,2))**(K-1)
      AAA(3,K)=(-1.5*DX+D2(JJ-2,2))**(K-1)
      AAA(1,K)=(-2.5*DX+D2(JJ-3,2))**(K-1)
      GOTO 2000
2100  CONTINUE
      AAA(5,K)=(-4.5*DX)**(K-1)
      AAA(3,K)=(-3.5*DX)**(K-1)
      AAA(1,K)=(-2.5*DX)**(K-1)

2000  CONTINUE

      BBB(2)=PHI(JJ-2,2)
      BBB(4)=PHI(JJ-1,2)
      BBB(6)=0.
      AAA(6,6)=-1.0
      IF(TIME.LE.DT) GOTO 2200
      BBB(1)=PHIHAT(JJ-3,2)
      BBB(3)=PHIHAT(JJ-2,2)
      BBB(5)=PHIHAT(JJ-1,2)
      GOTO 2300
2200  CONTINUE
      BBB(5)=PHI(JJ-5,2)
      BBB(3)=PHI(JJ-4,2)
      BBB(1)=PHI(JJ-3,2)
2300  CONTINUE

      CALL MV(AAA,6,6,BBB,XXX,DET,IDET,WORKMM)

      PHI(JJ,2)=XXX(6)

      N=2
      DO 5000 I=2,JJ
      PHIUSED(I,2)=PHIUSED(I,1)-DT*(RU(I,1)*((PHIUSED(I,1) -
     2PHIUSED(I-1,1))/DX)+PHIUSED(I,1)*((RU(I,1)-RU(I-1,1))/DX))
```

```
5000  CONTINUE

      RETURN
      END
```

```
      SUBROUTINE PRINT(ISOL,NN)
      COMMON / BLOCK1 / PHI(50,3),PHIBAR(50,3),PHIHAT(50,3),
     2   PHIUSED(50,3),PHITRUE(50,3),RU(50,3),D1(50,3),D2(50,3)
     3,DUDX(50,3),S(50,3)
      COMMON / BLOCK2 / RL,JJ,DT,DX,TIME,TIMEF,NTS
      COMMON / BLOCK3 / UCOEF(3,3,50),PCOEF(5,50),SCOEF(3,3,50)
      WRITE(6,20) TIME
20    FORMAT(1H1,40X,"T  I  M  E  =     ",F8.4,5X,"SECONDS",/////)
      WRITE(6,30)
30    FORMAT(1X,"NODE NUMBER",11X,"PHI",10X,
     1                            "PHIBAR",8X,"PHIHAT",8X,"DELTA1",8X,
     2"DELTA2",7X,"VELOCITY",7X,"DUDX",10X,"ALPHA",///)
      DO 10 I=1,JJ
      WRITE(6,40) I,PHI(I,1),PHIBAR(I,1),PHIHAT(I,1),D1(I,1),D2(I,1),
     1RU(I,1),DUDX(I,1) ,DUDX(I,3)
40    FORMAT(  7X,I2,7X,8(E14.7,1X))
10    CONTINUE
      ITN=6*(ISOL-1)+1+(NN-1)/10
      WRITE(6,3000) ITN
3000  FORMAT(1H1,10(/),47X,"T   A   B   L   E       ",I2)
      WRITE(6,1100) (NN-1)
1100  FORMAT(     9(/),38X,"C O M P A R I S O N ... AFTER",2X,I2,2X,"TIME
     1 STEPS",/////)
      WRITE(6,1150) TIME
1150  FORMAT(41X,"TOTAL  TIME  ELAPSED  =",F8.4,3X,"SECS.",////)
      WRITE(6,1200)
1200  FORMAT(15X,"NODE",6X,"ANALYTICAL",7X,"   THIS    ",6X," RATIO TO ",
     27X,"   ONE     ",6X," RATIO TO ",/,14X,"NUMBER",5X," SOLUTION",8X,
     3"   WORK    ",6X,"ANALYTICAL",7X,"  SIDED    ",6X,"ANALYTICAL",5X,
     4/,58X," SOLUTION ",7X,"DIFFERENCE",6X," SOLUTION ",//)
      K=1
      DO 1400 I=1,JJ
      DUMMY=FLOAT(I-1)*DX
      DUMMY1=(PHI(I,K)+1.0E-20)/(PHITRUE(I,1)+1.0E-20)
      DUMMY2=(PHIUSED(I,1)+1.0E-20)/(PHITRUE(I,1)+1.0E-20)
```

```
      WRITE(6,1500)I,PHITRUE(I,1),PHI(I,K),DUMMY1,PHIUSED(I,1),DUMMY2
1500  FORMAT(15X,I3,3X,E15.8,3X,2(E15.8,E15.8,3X))
      CALL PLOTPT(DUMMY,PHITRUE(I,1),21)
      CALL PLOTPT(DUMMY,PHI(I,K),22)
      CALL PLOTPT(DUMMY,PHIUSED(I,1),23)
1400  CONTINUE
      GOTO (2100,2200,2300) , ISOL
2100  WRITE(6,2150)
2150  FORMAT(////,43X,"( VELOCITY FUNCTION OF TIME ONLY )")
      GOTO 2400
2200  WRITE(6,2250)
2250  FORMAT(////,43X,"( VELOCITY FUNCTION OF POSITION ONLY )")
      GOTO 2400
2300  WRITE(6,2350)
2350  FORMAT(////,47X,"( FULLY VARIABLE VELOCITY )")
2400  CONTINUE
      CALL OUTPLOT
      RETURN
      END
```

```
      SUBROUTINE PLOTR(ISOL)
      COMMON / BLOCK1 / PHI(50,3),PHIBAR(50,3),PHIHAT(50,3),
     2   PHIUSED(50,3),PHITRUE(50,3),RU(50,3),D1(50,3),D2(50,3)
     3,DUDX(50,3)
      COMMON / BLOCK2 / RL,JJ,DT,DX,TIME,TIMEF,NTS
      COMMON / BLOCK4 / PHIPLOT(5,3,51)
      DIMENSION YMIN(5,2),YMAX(5,2),FACTORY(5,2),RATIO(5,3,51)
      NT1=NTS+1
      DO 200 L=1,5
      DO 200 J=1,NT1
      RATIO(L,1,J)=(PHIPLOT(L,1,J)+1.0E-10)/(PHIPLOT(L,1,J)+1.0E-10)
      RATIO(L,2,J)=(PHIPLOT(L,2,J)+1.0E-10)/(PHIPLOT(L,1,J)+1.0E-10)
      RATIO(L,3,J)=(PHIPLOT(L,3,J)+1.0E-10)/(PHIPLOT(L,1,J)+1.0E-10)
200   CONTINUE
      XMAX=FLOAT(NTS)*DT
      XMIN=0.
      RNX=RNY=5.0
      NXNY=IFIX(RNX+1.0)
      DO 2 IG=1,2
      DO 2 L=1,5
      FACTORY(L,IG)=1.0E+100
      YMAX(L,IG)=-1.0E+100
      YMIN(L,IG)=1.0E+100
      DO 4 K=1,3
      DO 6 J=1,NT1
      GOTO (204,206) , IG
204   CONTINUE
      IF(PHIPLOT(L,K,J).GT.YMAX(L,IG)) YMAX(L,IG)=PHIPLOT(L,K,J)
      IF(PHIPLOT(L,K,J).LT.YMIN(L,IG)) YMIN(L,IG)=PHIPLOT(L,K,J)
      GOTO 6
206   CONTINUE
      IF(RATIO(L,K,J).GT.YMAX(L,IG)) YMAX(L,IG)=RATIO(L,K,J)
      IF(RATIO(L,K,J).LT.YMIN(L,IG)) YMIN(L,IG)=RATIO(L,K,J)
6     CONTINUE
      SIZEY=3.00
```

```
      DUMMY=(SIZEY+1.0E-20)/((YMAX(L,IG)-YMIN(L,IG))+1.0E-20)
      IF(FACTORY(L,IG).GT.DUMMY) FACTORY(L,IG)=DUMMY
4     CONTINUE
2     CONTINUE
      SIZEX=4.75
      FACTORX=SIZEX/TIME
      CALL PLOT(100.,10.5,60)
      DO 10 I=1,5
      DO 210 IG=1,2
      XIG=-(0.75+4.7*(FLOAT(IG)-1.0))
      CALL PLOT(XIG,0.0,40)
      CALL PLOT(0.5,5.25,3)
      CALL PLOT(3.5,5.25,2)
      CALL PLOT(3.5,10.0,2)
      CALL PLOT(0.5,10.0,2)
      CALL PLOT(0.5,5.25,2)
      CALL LETTER(16,.10,90.,4.10,6.7,16HT I M E  (SECS.))
      IT1=ISOL+1
      IT2=2*I+IG-2
      ENCODE(10,600,TITLE1) IT1
600   FORMAT(9HFIGURE 4.,I1)
      IF(IT2.EQ.10) GOTO 604
      ENCODE(3,605,TITLE2) IT2
605   FORMAT(1H.,I1,1H )
      GOTO 606
604   ENCODE(3,608,TITLE2) IT2
608   FORMAT(1H.,I2)
606   CONTINUE
      RRR=7.6-1.8*(FLOAT(IG)-1.0)
      CALL LETTER(10,.15,90.0,0.8,RRR,TITLE1)
      RRR=RRR+1.5
      CALL LETTER( 3,.15,90.0,0.8,RRR,TITLE2)
      IN=2*I
      X=7.5-2.0*(FLOAT(IG)-1.0)
      GOTO(250,260) , IG
```

```
250   CONTINUE
      CALL GREEK(2.0,3.70,0.50,90.0,21)
      ENCODE(35,700,SUBT1) IN
700   FORMAT(23HCONCENTRATION AT NODE  ,I2,10H  VS. TIME)
      CALL LETTER(35,0.05,90.0,1.0,X,SUBT1)
      GOTO 270
260   CONTINUE
      CALL LETTER(28,0.10,180.0,3.4,4.10,28HRATIO TO ANALYTICAL SOLUTION
     2)
      ENCODE(39,710,SUBT2) IN
710   FORMAT(27HRATIO OF SOLUTIONS AT NODE ,I2,10H  VS. TIME)
      CALL LETTER(39,0.05,90.0,1.0,X,SUBT2)
270   CONTINUE
      RRR=5.8+2.75*(FLOAT(IG)-1.0)
      CALL LETTER(19,.05,90.0,3.0,RRR,19HANALYTICAL SOLUTION )
      CALL LETTER(20,.05,90.0,3.1,RRR,20HONE SIDED DIFFERENCE)
      CALL LETTER( 9,.05,90.0,3.2,RRR, 9HTHIS WORK)
      RRR=5.5+2.75*(FLOAT(IG)-1.0)
      CALL GRAF(2.95,RRR,0.1,1)
      CALL GRAF(3.05,RRR,0.1,2)
      CALL GRAF(3.15,RRR,0.1,3)
      RRR=7.6-2.0*(FLOAT(IG)-1.0)
      GOTO (1100,1200,1300) , ISOL
1100  CALL LETTER(32,.05,90.0,1.2,RRR,32H(VELOCITY FUNCTION OF TIME ONLY
     2))
      GOTO 1400
1200  CALL LETTER(30,.05,90.0,1.2,RRR,30H (VELOCITY FUNCTION OF X ONLY))
      GOTO 1400
1300  CALL LETTER(30,.05,90.0,1.2,RRR,30H  (FULLY  VARIABLE  VELOCITY) )
1400  CONTINUE
      DXL=SIZEX/RNX
      DYL=SIZEY/RNY
      DXN=(XMAX-XMIN)/RNX
      DYN=(YMAX(I,IG)-YMIN(I,IG))/RNY
      XL=5.25-DXL
```

```
      XN=-DXN
      YL=3.575+DYL
      YN=YMIN(I,IG)-DYN
      DO 15 M=1,NXNY
      XN=XN+DXN
      XL=XL+DXL
      YN=YN+DYN
      YL=YL-DYL
      ENCODE(9,490,Y) YN
490   FORMAT(E9.3)
      IF(IG.EQ.2) ENCODE(9,495,Y) YN
495   FORMAT(F9.5)
      ENCODE( 9,500,X) XN
500   FORMAT(E9.2)
      XX=XL-0.525
      IF(M.EQ.1) XX=XL-0.2
      CALL LETTER(9,.100,90.0,3.75,XX,X)
      CALL LETTER( 9,.075,90.0,YL,4.40,Y)
      IF(M.EQ.1.OR.M.EQ.NXNY) GOTO 15
      CALL PLOT(YL,5.20 ,3)
      CALL PLOT(YL,5.30 ,2)
      CALL PLOT(YL,9.95 ,3)
      CALL PLOT(YL,10.05 ,2)
      CALL PLOT(3.45 ,XL,3)
      CALL PLOT(3.55 ,XL,2)
15    CONTINUE
      DO 20 K=1,3
      CALL PLOT(SIZEY+0.5,5.25,3)
      DO 30 N=1,NT1
      X1=FLOAT(N-1)*DT*FACTORX
      Y1=(PHIPLOT(I,K,N)-YMIN(I,IG))*FACTORY(I,IG)
      IF(IG.EQ.2) Y1=(RATIO(I,K,N)-YMIN(I,IG))*FACTORY(I,IG)
      X1=X1+5.25
      Y1=3.5-Y1
      CALL PLOT(Y1,X1,2)
```

```
30      CONTINUE
20      CONTINUE
        DO 120 K=1,3
        NN2=NTS/5
        DO 130 N=1,NT1,NN2
        X1=FLOAT(N-1)*DT*FACTORX
        Y1=(PHIPLOT(I,K,N)-YMIN(I,IG))*FACTORY(I,IG)
        IF(IG.EQ.2) Y1=(RATIO(I,K,N)-YMIN(I,IG))*FACTORY(I,IG)
        X1=X1+5.25
        Y1=SIZEY+0.5-Y1
        CALL GRAF(Y1,X1,0.100,K  )
130     CONTINUE
120     CONTINUE
210     CONTINUE
        CALL PLOT(12.0,5.25,-3)
10      CONTINUE
        RETURN
        END
        END
```