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A FRACTIONAL STEP METHOD FOR MASS TRANSPORT IN GROUNDWATER

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ABSTRACT

A computer model based on the fractional step method is presented for modelling density coupled mass transport in groundwater. Although several models utilising the fractional step method had been developed previously, all were based on the Eulerian solution approach. The model developed by the authors uses the Langrangian approach which has some inherent advantages and disadvantages. The problems associated with the implementation of the fractional step method and techniques by which they were overcome are discussed. The performance of the model is examined and results obtained for standard problems are compared with those from other computer packages.

KEY WORDS Fractional step method Operator splitting Advection-diffusion equation Fluid flow/transport in porous media Groundwater pollution

INTRODUCTION

In general there are two alternative approaches for solving flow problems, the Eulerian and the Lagrangian approaches. In the Eulerian approach a fixed reference system is used, while in the Lagrangian approach the system of reference moves with the flow. Each approach has its advantages and disadvantages.

For mass transport problems, the Eulerian approach is easier to implement but, as is well known, is prone to solution oscillations and numerical dispersion[8,10]. On the other hand, the Lagrangian approach has the advantage that it follows the movement of the fluid and thus the conservation equations take their simplest form, hypothetically at least, eliminating numerical dispersion. The Lagrangian approach has a fundamental difficulty associated with large deformations generated by fluid motions although this difficulty can be overcome by having the mesh re-generated after each timestep.

The Lagrangian approach, with mesh regeneration after each timestep, is adopted here to develop a fractional step method (FSM)[21] for solving the advection-diffusion equation. The idea of the fractional step method originated in the early seventies[29] but did not become popular until a decade later. The term fractional step, which also is known as operator splitting, is used in the literature to cover various numerical procedures. Terminology associated with these procedures is inconsistent and neither the theoretical background nor advantages and limitations of the various splitting techniques are clearly established.

Various operator splitting criteria can be used; space splitting, time splitting and process splitting. Space splitting is customary when multidimensional modelling based on finite differences is involved. Time splitting is adopted when a complete system of equations is solved using different discretisation techniques. The well known Alternating Direction Implicit (ADI) scheme

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falls into the time splitting category. In process splitting (which is the method adopted in this paper) the governing equations are split up into fractional steps corresponding to the basic physical processes involved.

In this study the development of the method based on the Lagrangian approach for two-dimensional flow and mass transport in groundwater[3,7] is presented together with the results obtained.

THE FRACTIONAL STEP METHOD

Characteristics of the fractional step method

The fractional step method can be applied in the numerical solution of initial value problems involving a number of transport directions and interacting influences[21]. Consider an initial value problem, with dependent variable ε, of the form,

$$\frac{\partial \varepsilon}{\partial t} = L[\varepsilon] \tag{1}$$

where L is some operator. While L is not necessarily linear, suppose that it can be written as a linear sum of m individual differential operators, which act additively on ε,

$$L\varepsilon = L_1\varepsilon + L_2\varepsilon + L_3\varepsilon + \ldots + L_m\varepsilon \tag{2}$$

The numerical solution of (1) over a time step Δt is achieved in m fractional steps, each of duration $\Delta t/m$ because each partial operation acts with all the terms of the original operator. Each of the fractional steps involves the numerical solution of one of the consecutive initial value problems:

$$\frac{\partial \varepsilon}{\partial t} = mL_i[\varepsilon] \qquad \mathrm{i} = 1, 2, \ldots, \mathrm{m} \tag{3}$$

The major advantage of the fractional step method is that separate consideration can be given to each step, providing the freedom of employing the most appropriate numerical algorithm for each separate equation (process) and not forcing the adoption of a single algorithm for the complete process.

To demonstrate the fractional step method, consider the two-dimensional advection-diffusion equation, with no chemical reaction terms:

$$\frac{\partial C}{\partial t} = -u_i \frac{\partial C}{\partial x_i} + D_{ij} \frac{\partial^2 C}{\partial x_i^2} \tag{4}$$

where x_i (with $i = 1, 2, 3$) are the components of the Cartesian coordinate system, t is time, C is concentration of the dissolved constituent, u_i is local pore velocity in the ith direction and D_{ij} is the coefficient of hydrodynamic dispersion[2].

In the context of the fractional step method, (4) becomes:

$$\frac{\partial C}{\partial t} = (L_1 + L_2)[\mathrm{C}] \tag{5}$$

where,

$$L_1[\mathrm{C}] = -\mathrm{u}_i \frac{\partial C}{\partial x_i} \tag{6a}$$

$$L_2[\mathrm{C}] = \mathrm{D}_{ij} \frac{\partial^2 C}{\partial x_i^2} \tag{6b}$$

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An explicit scheme can be used for the advection term, (6a), with an implicit scheme for the diffusion term, (6b). The inclusion of chemical reactions involves a relatively minor extension. Finally, it should be noted that by employing the fractional step method, special attention can be given to the advection terms which are the main cause of numerical dispersion. Numerical dispersion is pronounced in the cases where density coupling of the fluid flow and the advection-diffusion equations is required.

The solution of the flow and advection-diffusion equations using the fractional step method

The flow equation as well as the advection-diffusion equation, the appropriate boundary conditions, and also the method of their solution using stationary finite elements are well documented[7,13]. The method of solution based on the fractional step method utilising moving coordinates, can be summarised as follows:

The flow equation (6a) is solved for the hydraulic heads at the nodes and then the corresponding velocities at the nodes are calculated. The first fractional step is the advection step in which, knowing the velocities at the nodes and the timestep Δt, the nodes are moved to new positions determined from a fourth-order Runge-Kutta method. Nodes passing the outflow boundary are taken out of the system and new nodes are introduced on the inflow boundary. The nodes are then located ready for the diffusion part of the fractional step algorithm. For the second part of the fractional step (6b) the concentrations of all the nodes are estimated by solution of the diffusion equation.

PREVIOUS WORK WITH THE FRACTIONAL STEP METHOD

Numerical experiments in only one dimension were carried out by Sobey[21] in order to determine the performance of the FSM. The Fourier response and the integrated square error characteristics were computed[22,23]. Sobey's[21] approach has been extended to two dimensional flow in this paper, and applied to the solution of the advection-diffusion equation[3] utilising moving coordinates. In recent years, the fractional step method has been widely utilised in Eulerian based models, such as models for industrial codes[25], three-dimensional finite element code for modelling seawater intrusion[4], and a three-dimensional model simulating coupled groundwater flow and transport within saturated and unsaturated zones[26]. The fractional step method was also utilised in the solution of advection-dispersion-reaction problems[27]. The solution was achieved in two steps. The first half of the timestep involves the solution of the advection-dispersion step, while the second half involves the solution of the reaction step[27].

A problem commonly used for evaluating numerical schemes for the advection-diffusion equation is the rotating cone problem[18]. An initially conical distribution with peak concentration $C=1.0$, is given a solid body rotation with an angular velocity of unity. The diffusion coefficient D_{ij} is assumed to be constant and is denoted by D. At time $t=0.0$ the cone with initial radius at the base r_0 is placed on a plane of extent $-1 \leqslant (x, y) \leqslant 1$ with the centre of the cone at position (x_0, y_0). The concentration C at any position on the plane is given by:

$$C(x, y, 0)=C_0(x, y)=\begin{cases}1-r/r_0 & r<r_0\\ 0 & r\geqslant r_0\end{cases} \tag{7}$$

where,

$$r=\sqrt{x-x_0)^2+(y-y_0)^2}$$

The velocity field is given by,

$$u=-\omega y, \qquad v=+\omega x \tag{8}$$

where,

ω = angular velocity of the cone (anti-clockwise direction positive).

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The parameters used in this paper are $r_0=0.25$ m and $(x_0, y_0)=(-0.5, 0.0)$ (see *Figure 1*).

In the case where the diffusion coefficient is zero ($D=0.0$ m) the cone which rotates about the origin should return undistorted to its original position after any integral number of periods $\tau=2\pi/\omega$ (provided there are no numerical errors) since the elements of the cone describe concentric circles about the origin of the axes.

It is widely recognized that numerically it is much more difficult to obtain accurate solutions for an advectively dominated flow problem than for a diffusion dominated problem. The ratio of advection to diffusion can be represented by the Peclet number, $Pe=uL/D$ where u is the velocity, L is a characteristic length, and D is the diffusion coefficient. A difficult case for numerical solution would be an advectively dominated flow in which $Pe\gg 1$ with finite diffusion ($D\neq 0$), for which the solution will be a slowly diffusing cone. The analytical solution for the amplitude of a purely diffusing cone is known[5]. With a slight adaptation of case VII in §10.3 of Carslaw and Jaeger[5], the value of concentration C for a cone with initial radius r_0 and amplitude unity, centred at the origin of an unbounded region can be expressed as[3]:

$$C(t)=1-\frac{\sqrt{\pi Dt}}{r_0}\,erf\left(\frac{r_0}{\sqrt{4Dt}}\right) \tag{9}$$

where *erf* is the tabulated error function. Equation (9) can be used for checking the accuracy of the numerical solution as long as $\sqrt{Dt}$ is very small and therefore the answer is not affected by the presence of the boundaries.

An investigation was carried out[3] on a 17×17 grid with $D=0.001$ for a single time step of $\Delta t=0.25$ s, and hence diffusion parameter ($D'=D\,\Delta t/\Delta s^2$) of 0.1 The result for the peak concentration ($r/r_0=0.0$) after this quarter revolution was 0.721 which compares favourably with the value of 0.719 obtained from the analytical solution.

DETAILS OF THE IMPLEMENTATION OF THE FRACTIONAL STEP METHOD IN A COMPUTER PROGRAM

Grid generation

In the solution based on the fractional step method, the solution domain is covered by grid points, each with known concentration. *Figure 2* shows a small area within the boundaries with nodes and a superimposed grid at the commencement of the timestep. After the diffusion step, the new concentrations are known and also their velocities. Thus the new position of the nodes can be determined (empty circles in *Figure 2*). For the first step of the fractional step method adopted, advection takes place while for the second, diffusion takes place. Thus due to the actual

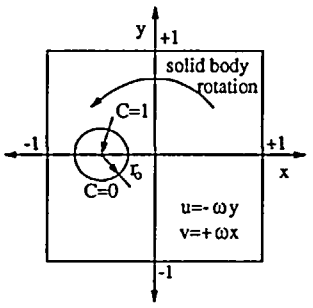

Figure 1 Plan view of the cone problem

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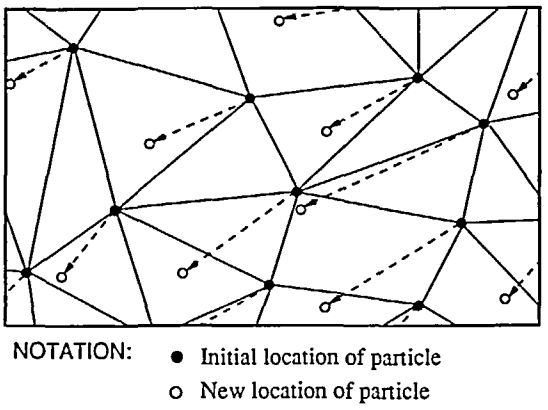

Figure 2 Movement of nodes (Advection step)

Table 1 Comparison of non-dimensional concentration obtained from different element arrangements with a 17 by 17 grid for a 2-D cone problem

		Computer results		
		Arrangement (a)	Arrangement (b)	
r/r_0	Analytical	6 element nodes	8 element nodes	4 element nodes
0.0	0.7190	0.7201	0.7821	0.6324
0.5	0.4476	0.4521	0.4331	0.4653
1.0	0.0761	0.0767	0.0498	0.0720
1.5	0.0008	−0.0076	−0.0028	−0.0130
2.0	0.0000	0.0004	0.0016	0.0004

movement of nodes during the advection part, a loss of grid points on the outflow boundary of the computational region and a gain of points on the inflow boundary occurs. These complications require careful bookkeeping operations. In every timestep a new mesh is required to take into account the new position of the nodes after advection.

Many grid generation algorithms are available in the literature[6,15,24]. These algorithms can be divided into two major groups, automatic and semi-automatic. In this project, since a new mesh is required in every iteration, an automatic and computationally efficient algorithm was used.

A triangular mesh is the most convenient to fit to what becomes an arbitrary arrangement of points because the nodes move in a random way, and also the triangular mesh gives a better representation of the boundaries than one using elements with larger numbers of straight sides.

Effects due to orientation of the elements

The accuracy of the results obtained for the diffusing cone problem can be estimated by comparing them with the corresponding ones from the analytical solution[3]. For nodes uniformly spaced in two directions at right angles, as illustrated in *Figure 3* in arrangements (a) and (b), it will now be shown that different triangular mesh arrangements give significantly different results. This has been also noted by other researchers[30].

A summary of the results is presented in *Table 1*. After a quarter of a revolution ($\Delta t = 0.25$ s) and with the diffusion coefficient D set to 0.001 $m^2 s^{-1}$, the peak concentrations calculated using

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different mesh arrangements varied by more than ten percent from those obtained from the analytical equation. For this problem, comparison with the analytical solution shows that the mesh arrangement which connects each internal node to six elements (*Figure 3a*) gives better results than a mesh arrangement which has some nodes connected to four elements while others are connected to eight elements (*Figure 3b*).

Table 1 presents concentrations at different positions defined by the ratio of the distance r of the point under consideration from the centre of the cone to the original radius of the cone r_0. The results are presented for r/r_0 ranging from zero (the centre of the cone), to two (twice the initial radius of the cone) for the two mesh arrangements presented in *Figure 3*. The simulation was performed by a 17 by 17 grid. Results from other grid densities are compared later.

Table 2 presents non-dimensional concentration results obtained from different element arrangements for three different grid sizes (9 by 9, 17 by 17 and 33 by 33). For each of these grid sizes the concentrations at r/r_0 equal to 0.0 and 0.5 are presented. The first row of *Table 2* presents results for the case where the centre of the cone is located on a node which is connected to six elements [arrangement (a_1)] in which all elements lean towards the lower left corner. The second row presents results for a case similar to the first except that the elements follow arrangement (a_2) in which all elements lean towards the lower right corner. The results presented on the third row are from the case where the mesh arrangement is such that the centre of the cone can be placed on a node which is connected either to four or to eight elements.

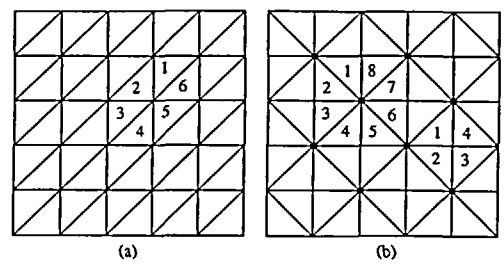

Figure 3 Alternative mesh arrangements

Table 2 Comparison of non-dimensional concentration results for a 2-D cone for different node connections

Element configuration	r/r_0	9 by 9	17 by 17	17 by 17	33 by 33
arrangement (a_1)					
	0.0	0.72005	0.72005	not	0.7139
	0.5	0.45211	0.45211	applicable	0.4413
arrangement (a_2)					
	0.0	0.72005	0.72005	not	0.7139
	0.5	0.45211	0.45211	applicable	0.4413
rhombic		4 elements	4 elements	8 elements	8 elements
	0.0	0.63243	0.63243	0.78209	0.6916
	0.5	0.46526	0.46527	0.43310	0.4472
Analytical values		$r/r_0=0.0$, $C=0.7190$; $r/r_0=0.5$, $C=0.4476$			

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Since advection moves nodes in a non-regular pattern, it is necessary to fit a mesh to randomly placed nodes. Further solutions have been obtained with arbitrarily arranged meshes for comparison with the analytical solution as shown in *Table 3*, where the centre of the cone is placed on a node connected either to five, six, or eight elements. The results show that for this case of randomly connected nodes, errors of up to eight percent can occur in the numerical solution of the diffusion equation.

The same test (for the diffusion part only) was applied to the finite difference method alternating direction implicit scheme (ADI). A cone with radius $r_0=0.25$ and initial peak concentration C of 1.0, is placed on a plane region with x and y dimensions ranging from -1.0 to $+1.0$ and is left to diffuse for a timestep Δt of $\pi/4$. As can be observed from *Table 4*, except for the 65 by 65 grid, the results for the more demanding case of $r/r_0=0.0$ are not very encouraging when compared with those obtained from the analytical solution and from the finite element method for the same grid size.

It should be recognized, however, that the initial conical distribution provides a reasonably severe test of the accuracy of numerical methods. From the above it was concluded that the triangulation algorithm (FPMESH[16]) which has the tendency to connect six elements to each node where all the elements are leaning in the same direction (arrangements a_1 and a_2) would be preferable since it produces more accurate results than a triangulation algorithm (TRMESH[20]) which connects the nodes at random in any direction.

The algorithm on which FPMESH is based, initially specifies the boundary points in an anti-clockwise direction and then it generates starting from the boundaries, moving inwards in an anti-clockwise spiral direction.

Table 3 Comparison of non-dimensional concentration results for a 2-D cone for elements with random node connections

Element configuration	r/r_0	5 elements	6 elements	8 elements
random	0.0	0.68378	0.72205	0.77828
	0.5	0.46513	0.45127	0.43478
Analytical values	$r/r_0=0.0$, $C=0.7190$; $r/r_0=0.5$, $C=0.4476$			

Table 4 Comparison of non-dimensional concentrations obtained using finite difference (ADI) and finite element methods for the 2-C cone case

Grid size	Concentration at			
	$r/r_0=0.5$		$r/r_0=0.0$	
	finite difference	finite element	finite difference	finite element
17 by 17	0.4583	0.4521	0.8265	0.7200
33 by 33	0.4499	0.4413	0.7431	0.7139
65 by 65	0.4502	not run	0.7191	not run
Analytical values	0.4476		0.7190	

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In the algorithm on which TRMESH is based, the nodes have initially to be sorted since this helps the algorithm to operate more efficiently. Two nodes are considered and a line is drawn between them. The position of a third node with respect to the line is estimated. The mesh is generated so that the maximum number of equilateral triangles are created. Mesh generation commences on one boundary and finishes on the opposite boundary.

The second algorithm was adopted because firstly it has a tendency to generate elements leaning in one direction and secondly, it is about 2.5 times faster than FPMESH. Speed is a very important criterion in the selection of a triangulation algorithm because in every timestep a new triangulation is required and the triangulation component of the computer model consumes most of the central processing unit (CPU) time in each timestep.

Boundary conditions

Another problem associated with the implementation of the fractional step algorithm is the imposition of the boundary conditions. Process splitting within the solution domain requires a corresponding splitting of the boundary conditions. The major criticism of splitting techniques[19] has been related to the treatment of the boundary conditions. The known boundary conditions correspond to the complete differential equation and not to the split equations. There is no doubt that this is a relevant criticism, given that most applications of the advection-diffusion equations are sensitive to the boundary conditions. An investigation[1] showed that for the parameters used in the present study, the boundary condition for the complete advection-diffusion equation provides a satisfactory estimate of the intermediate level boundary value which has to be specified at the end of the advection step and at the beginning of the diffusion step.

In the above investigation[1], different methods for implementing the boundary conditions are proposed, and the normalised mean square error for the different one-dimensional cases is presented in the form of contour plots. The normalised mean square error is dependent on the dimensionless flow parameter which is defined as $u_* = u\,\Delta t/\Delta x$ and the logarithm of the dimensionless dispersion parameter $D_* = D\,\Delta t/\Delta x^2$.

For the present study the flow parameter u_* and the logarithm of the dispersion parameter $\log_{10} D_*$ are estimated to be less than 1.0×10^{-3} and -5.0 respectively. Based on the above estimated parameters, for the method where the initial boundary conditions for the *complete* one-dimensional advection-diffusion equation are implemented, the normalized mean square error was less than 0.005 (according to Reference 1). Although a two-dimensional problem is solved in the present study, an error of the same order as for the one-dimensional case would be expected. Errors of that magnitude indicate that, the given boundary condition for the complete advection-diffusion equation provides a satisfactory estimate of the intermediate level boundary value. Another indication is the good agreement between results obtained from the model and from known solutions for specific problems which will be presented in the following section.

Accounting for moving nodes—the bookkeeping procedure

Since the nodes move after every timestep, bookkeeping of the nodes proved to be a crucial part of the implementation of the fractional step method. After each time step the nodes which moved across the outflow boundary had to be taken from the system and new nodes introduced on the recharge boundary. Nodes that tended to cross the impermeable boundaries were relocated on the boundary (refer to *Figure 4*). Theoretically, nodes should not cross the impermeable boundaries and the tendency to do so results from too large a timestep being employed. For the new nodes introduced on the recharge and constant head boundaries, associated boundary conditions (known fluxes and known heads) had to be implemented. In the case of an unconfined aquifer the position of the free surface also had to be estimated at every time step. For recharge from the top, the new nodes had to be introduced along the free surface as well.

Another complication which arose in the implementation of the fractional step method was a tendency towards local overcrowding of nodes. This should be avoided because it creates

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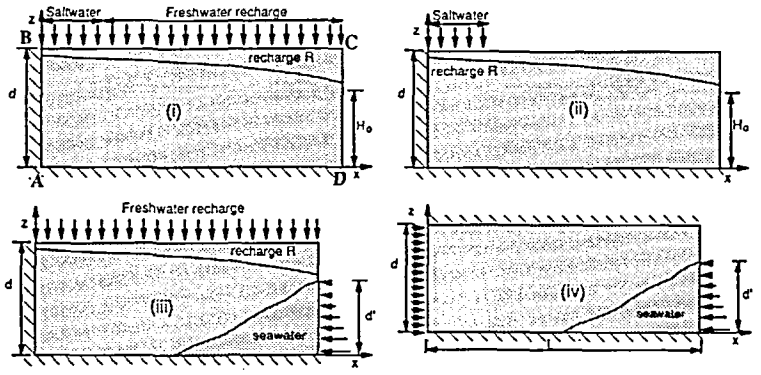

Figure 4 Cases to which the computer model was applied

triangles with large differences between the obtuse and acute angles which, as is well known in the application of the FEM[30], causes numerical errors. For the case of two nodes too close together, both were deleted and a new node with average x and z coordinates was introduced. The concentration of the new node was estimated by ensuring the mass of contaminant in the region of all the elements affected by those nodes was conserved.

Problems also arose when nodes were too far apart. This also should be avoided because the accuracy of the solutions in this region is reduced due to coarseness of the mesh. An additional node with average x and z coordinates was introduced with a concentration so that the mass in the region was conserved.

Choice of timestep

The computer program based on the fractional step method was used to simulate several different cases. These are shown in *Figure 4* and include (i) an unconfined aquifer with recharge over its whole length, part of which is recharged by contaminated water which may have a density different from that of freshwater; (ii) an unconfined aquifer with localised contaminated surface recharge which may have a density different from that of freshwater; (iii) seawater intrusion in a coastal unconfined aquifer which is replenished from the surface and; (iv) seawater intrusion in a confined aquifer.

It should be noted that the pollutant, which is simulated with saltwater, could have densities different from that of the groundwater. It should also be noted that the seepage surface at the downstream boundary is not taken into account by the computer model because this would significantly increase the complexity of the computer code without any appreciable improvement in accuracy of the model.

The main program which calls all the other subroutines is called DRIVER, a flowchart of which is given in Demetriou[7] and is reproduced in *Figure 5* for convenience.

Because the velocities of the nodes vary and this variation becomes more pronounced when there is an appreciable density difference, the choice of the timestep is critical to the successful execution of the computer program. For the computer runs performed for an unconfined aquifer with recharge over its whole length as shown in *Figure 4*(i), it was observed that the largest nodal velocities are of the order of one hundred times the smallest ones.

By choosing a large timestep the nodes move longer distances, less nodes are involved in the calculations, and larger elements are generated, all of which reduces the accuracy of the computer model. By choosing a small timestep some of the nodes hardly move, too many nodes are accumulated in the working area and this increases the CPU (central processing unit) time. Of course the optimum condition is to choose a large enough timestep so that the CPU time is

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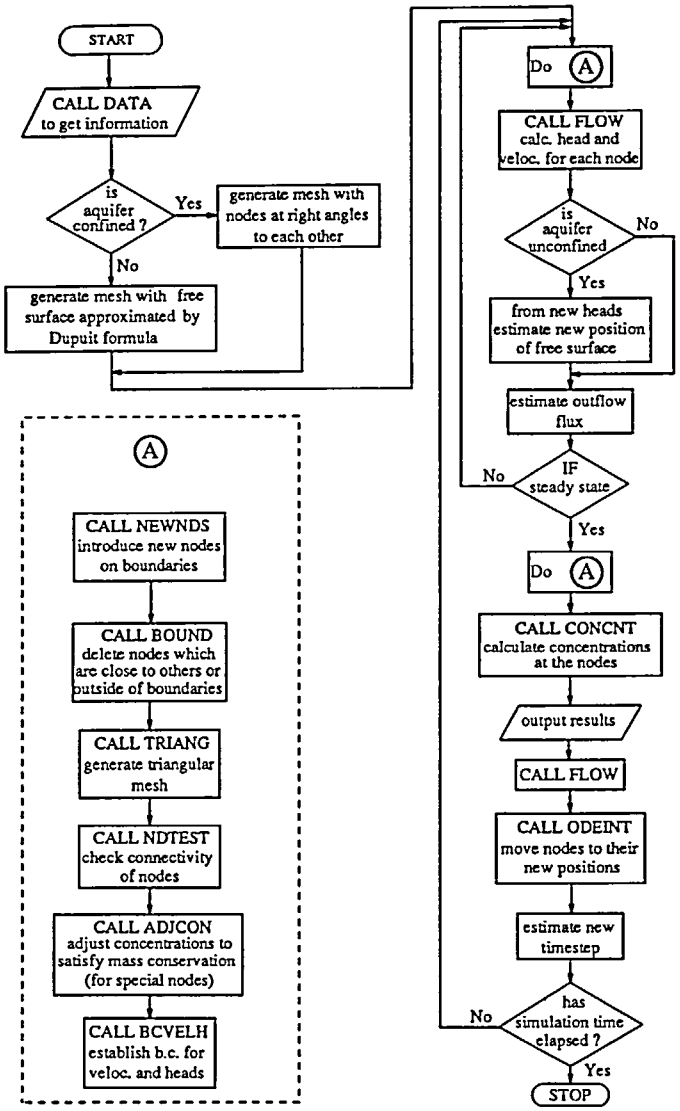

Figure 5 Flowchart of the computer program DRIVER

kept to acceptable limits while maintaining the required accuracy in the calculations.

Criteria established for determining the duration of each timestep for case (i) in *Figure 4* include: (a) determine the node with the highest velocity; (b) estimate the time required to move the node a distance equivalent to the depth of the aquifer; (c) determine the smallest non-zero velocity from the nodes which lie underneath the contaminant (saltwater) recharge area; (d) estimate the time required to move the node with the smallest non-zero velocity a distance equivalent to $dz/10$, where dz is the original vertical distance between the nodes at the outflow bounday CD in *Figure 4*(i). The timestep is then determined as the maximum of (b) and (d). Normally criterion (d) dominates and the difference between the values of (b) and (d) is usually not more than 500 s.

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It was observed that for a timestep larger than 2000 s, the error in mass conservation was high, and thus the timestep was not allowed to exceed this value.

The limits chosen, such as $dz/10$, depth of the aquifer and 2000 s, were determined by trial and error and are therefore valid only for the case of an unconfined aquifer with recharge over its entire length. For other cases such as seawater intrusion in both an unconfined aquifer and a confined aquifer (as shown in *Figures 4*(iii) and (iv)), a constant timestep also determined by trial and error was employed. More work would be required to establish a rigorous methodology for determining the timestep for general groundwater contamination problems.

Mass conservation

Mass conservation is one of the most important conditions to be satisfied by the results from any computer model of mass transport. A number of previous computer models have been developed with mass or momentum conservation specifically in mind, by implementing complex differencing schemes, which usually are very expensive in CPU time. In the computer runs performed in this study, it was found that the accuracy with which mass is conserved depends on the case to be simulated (generally high density differences result in difficulties), and the length of the timestep employed.

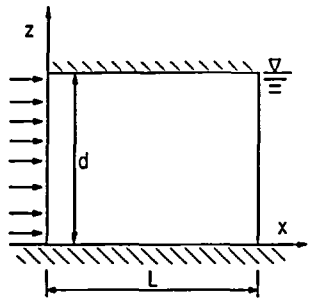
As mentioned above, the optimum timestep is one which is long enough to maintain the computing time within acceptable limits while restricting the error in mass conservation. In order to obtain a high degree of accuracy, the timestep has to be reduced causing the computing time to increase dramatically since not only are more timesteps required to cover the specified simulation period but also more nodes are introduced into the system making the computer simulation more expensive for each of those timesteps.

NUMERICAL RESULTS

Numerical results obtained for well known standard problems are compared with those from other computer packages and from theoretical solutions. Results from the model are also compared with those from an instrumented sandbox simulating contamination of an unconfined aquifer recharged from the surface.

Uniform flow in a confined aquifer

A simple test of the performance of the fractional step method (and other computer models) is the problem involving constant velocity horizontal flow through a confined aquifer with constant concentration ($C=1$) on the inflow boundary. This case is depicted in *Figure 6* where



$t<0, \quad 0<x<L, \quad 0<z<D, \quad C=0$

$t\geq 0, \quad x=0, \quad 0<z<D, \quad C=1$

$-\infty<t<+\infty \quad 0<x<L, \quad 0<z<D \quad u=\text{const}$

$0<x<L, \quad z=0, z=D \quad w=0$

Figure 6 Horizontal flow in a confined aquifer

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the initial and boundary conditions are also given. In *Figure 6*, u and w are velocity components in the x and z directions respectively. Results are obtained using the fractional step method and compared with results from an alternative computer package called SUTRA[28] and from the theoretical equations given by Ogata and Banks[17]. The position and width of the front between fresh ($C=0$) and contaminated ($C=1$) water was determined by the three methods. The diffusion coefficient is specified as $D=1.0\times10^{-9}\,m^2\,s^{-1}$ and the timestep as $\Delta t=500$ s. *Figure 7* shows the results obtained in a section of the solution area for the three methods after a certain time.

As can be observed from *Figure 7*, the width of the front W_2 predicted by the FSM agrees reasonably well with the analytical solution W_1 whereas the width from SUTRA (W_3) is relatively large, due presumably to numerical dispersion for the particular mesh used. It should be emphasised that no attempt has been made to optimize the number of grid points for either of the numerical solutions and it is clear that the mesh required to give a reasonable solution from SUTRA would be much finer than the one employed. Nevertheless, the number of nodes used in the FSM mesh (7 by 21) was the same as for SUTRA. These results indicate the ability of the FSM to give acceptable results with relatively few nodal points compared with methods which simultaneously solve the advective and dispersive parts of the equation.

Seawater intrusion in a confined aquifer (Henry's solution)

A solution often used to test the accuracy of a groundwater mass transport computer model is that of Henry[12] for the seawater intrusion problem.

As described in the documentation for SUTRA[28], the problem involves seawater intrusion into a confined aquifer in two dimensions under steady conditions. Freshwater recharge originating from inland, passes over saltwater and discharges at a vertical sea boundary. This case is shown in *Figure 4*(iv).

The intrusion problem is non-linear and may be solved by approaching the steady-state gradually through a series of timesteps. Initially there is no saltwater in the aquifer and, at time zero, saltwater begins to intrude from the seaward boundary under the freshwater. The intrusion is promoted by the greater density of the saltwater.

The dimensions of the problem were selected to facilitate comparison with the steady-state dimensionless solution[12] and with results from a number of other published simulation models, such as SUTRA[28] and INTERA[14].

A total simulation time of $t=6000$ s, was selected by Voss[28] and was considered to be sufficient to reach essentially steady-state conditions at the scale simulated.

Simulation steup

For the SUTRA computer model, the mesh consists of twenty by ten square elements each of size 0.1 m by 0.1 m. The mesh has 231 nodes and 200 square elements. The length of the

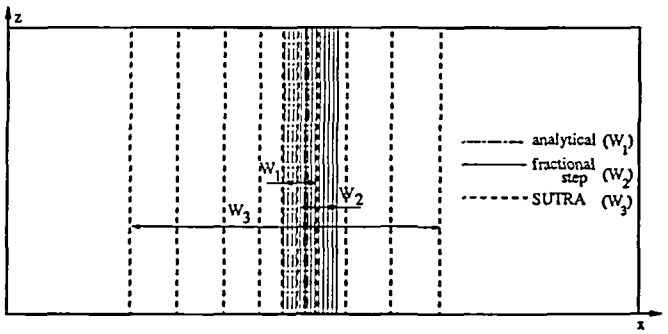

Figure 7 Front widths and positions from three solution techniques

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timestep is 60 s, and 100 timesteps are required. At every timestep both pressure and concentration are calculated.

The freshwater inflow is represented by employing source nodes at the left-hand vertical boundary (in *Figure 4*(iv)) with inflow rate of 6.6×10^{-2} kg s^{-1} (divided among 11 nodes) and relative concentration of 1.0. The porosity of the medium is equal to 0.35 and the hydraulic conductivity $K = 1.0 \times 10^{-2}$ m s^{-1}.

The following boundary conditions are implemented. There is no flow across the top and bottom boundaries. The freshwater source is set along the vertical boundary at $x = 0$. The vertical boundary at $x = L$ in *Figure 4*(iv) is held at the hydrostatic pressure due to sea water through the use of specified pressure nodes. Any water entering through these nodes has the concentration of seawater.

The initial conditions are constant pressures based on the freshwater inflow set everywhere in the aquifer, zero concentration everywhere, and specified pressures at the sea boundary.

Henry's solution assumes that the dispersion is represented by a constant coefficient of diffusion, rather than by velocity dependent dispersion coefficient. In order to match Henry's parameter a dispersion coefficient of $D = 6.6 \times 10^{-6}$ m^2 s^{-1} was used.

For the INTERA[14] finite difference code (with centered-in-space and centered-in-time approximations) and using a dispersion coefficient of $D = 6.6 \times 10^{-6}$ m^2 s^{-1}, results were obtained at $t = 6000$ s. The results from INTERA[14] were obtained from Voss[28].

For the computer model based on the FSM, the same boundary conditions as for SUTRA were implemented, and the elements used were triangular instead of squares. The initial number of nodes was the same (231) but in the FSM since the nodes move, new nodes are added and others are taken out from the working space and therefore the number of nodes varies (and usually increases) during the simulation time. Two simulation runs were performed. The total simulation time was 6000 s as for SUTRA and INTERA but the timestep chose was 100 s for the first run and 300 s for the second.

Results

Both computer models were run on a VAX station 3100 Model 38 and for Henry's problem the corresponding CPU times for compiling and executing are as follows:

- SUTRA 299 s
- FSM with timestep of 100 s (max. mumber of nodes = 700) 980 s
- FSM with timestep of 300 s (max. number of nodes = 308) 157 s

It should be noted that SUTRA produces various output files, the preparation of which consumes a significant part of the the CPU time.

Figure 8 presents the results for SUTRA, INTERA, FSM and Henry's solution for the 0.5 isochlor (line of constant level of salt concentration). As can be observed, both results from the

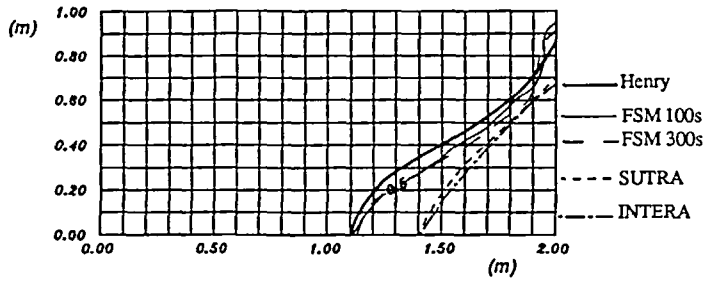

Figure 8 Comparison of results of seawater intrusion in a confined aquifer (Henry's solution)

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FSM match relatively well with Henry's solution but, while SUTRA agrees very well with INTERA, neither compares favourably with Henry's solution nor with FSM. It should be noted that Henry's solution, although analytic is still approximate and many researchers have their reservations about using this solution for comparison purposes. Better correspondence of the FSM result with Henry's 0.5 isochlor therefore, does not necessarily represent superiority of a model.

The results of the two runs performed by the computer model based on the FSM agree very well though the timesteps were different. This demonstrates the importance of optimizing the timestep in a model based on the FSM so that the number of nodes involved in the simulation is kept small (and hence the execution time remains acceptably short), while at the same time the accuracy is preserved.

Unconfined aquifer with uniform recharge over its whole length

For this case the unconfined aquifer is uniformly recharged over its whole length, but part of the recharge is contaminated by saltwater which simulates the pollutant. This case is depicted in *Figure 4*(i) in which boundaries AB and AD are impermeable while on the outflow boundary CD the pressure is hydrostatic. Experimental runs were performed on an instrumented $6.0\,m \times 0.6\,m \times 0.14\,m$ sandbox[7] to simulate the above case.

The values of the different parameters used in the computer runs such as hydraulic conductivity and porosity of the porous medium, were measured in situ in the sandbox. The hydraulic conductivity K is $9.60 \times 10^{-3}\,m\,s^{-1}$, the fillable porosity θ_f is 0.34, and Darcy porosity θ_D is taken as 0.40. The values for the dispersivities were obtained from Guvanasen and Volker[11] who used the same experimental setup. The longitudinal dispersivity a_L is 5.5×10^{-3} m and the transverse dispersivy a_T is 6.76×10^{-5} m. The density of freshwater is taken as that of water at 23°C, which is $998.0\,kg\,m^{-3}$ and the gravitational acceleration as $9.81\,m\,s^{-2}$. The molecular diffusion coefficient D_m for homogeneous sand[9] can be taken as $1.0 \times 10^{-9}\,m^2\,s^{-1}$. A detailed definition of the above mentioned parameters can be found in Bear[2].

The length of the aquifer was 6.0 m with a constant head H_0 of 0.53 m at the outflow end. For a length of 0.5 m adjacent to the vertical impermeable boundary, the water density at the free surface nodes was equal to that of saltwater while the concentration was equal to 1.0 and the vertical recharge rate R, expressed in a non-dimensional form as R/K, was 2.36×10^{-3} (recharge of $8.15\,mm\,h^{-1}$). The remainder of the free surface nodes had R/K equal to 2.36×10^{-3} but with relative concentration of 0.0 (freshwater).

Mass conservation

Mass conservation checks[7] for these runs showed that, in general, there is a better mass conservation for the neutrally buoyant cases than for the simulation runs with density difference $\Delta\rho_r > 0.000$. $\Delta\rho_r$ is the density difference ratio and is expressed as $(\rho_s - \rho_o)/\rho_o$ in which ρ_s is the density at the maximum value of concentration C_s, and ρ_o is the freshwater reference density. The reasons for the increased difficulty in handling cases with density differences will now be given. It was observed that for the cases with density difference above 0.000 the timestep ranges from about 750 s to 1500 s while for the neutrally buoyant case it ranges from 1100 s to 1900 s. This was expected because, for cases with density difference $\Delta\rho_r > 0.000$, more nodes are required to achieve the desired accuracy.

From the computer runs it was noted that, during early timesteps, the error in mass conservation is higher than that at later stages. This feature can be attributed to the fact that the saltwater plume is defined by a very small number of nodes in an area where there is a very high concentration gradient (underneath the saltwater recharge basin). It should be noted that all computer models generally suffer from high errors in the early stages of simulation, because the initial condition assumed in simulation is an infintely large concentration gradient at the source.

During the trial runs performed to establish a procedure for determining the optimum magnitude of the timestep, it was observed that by decreasing the timestep below a certain value,

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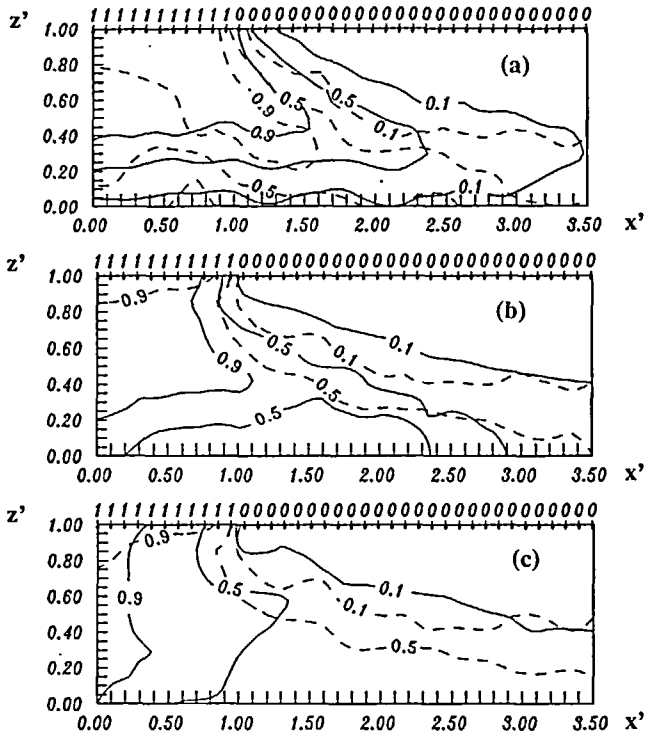

Figure 9 Dimensionless contours from experiment (broken lines) and computation (solid lines) at t' of 2.0 ($\approx$18,600 s since start) (a) $\Delta\rho_r$ of 0.000, (b) $\Delta\rho_r$ of 0.010, (c) $\Delta\rho_r$ of 0.022

the error in mass conservation increased rather than decreased. By studying the positions, velocities and concentrations of the nodes in the working region of the model, the cause of this was shown to be the fact that high concentration nodes from underneath the saltwater recharge source, because of their higher velocities, moved to within groups of nodes with small concentrations (i.e. freshwater nodes) and this caused numerical instabilities.

Comparison with experimental results

The model was run for different density difference situations and the results obtained at set dimensionless times t' ($t'=tR/\theta_D H_o$) were used to produce contour plots. *Figure 9* presents contour plots for density differences of 0.000, 0.010 and 0.022, at a dimensionless time of 2.0. Solid line contours are computational results and broken lines are experimental results. In both cases the 0.1, 0.5 and 0.9 dimensionless contours are shown. The concentrations are made dimensionless by dividing them by the initial concentration C_s, and the length parameters by dividing them by the constant head H_o at the outflow boundary.

As can be observed from *Figures 9*(a), (b) and (c), the general shapes of the contaminant plume from experimental and computational results agreed reasonably well and the differences can be attributed to the following reasons:

- the contours obtained from the experimental results were based on only fifty-six readings and the accuracy of the interpolated contours is limited;
- in spite of the great care taken in placing the sand some heterogeneities in the porous matrix will remain and in certain situations may cause the saltwater plume to disperse further than it would in homogeneous conditions.

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CONCLUSIONS

A comparison of the results obtained for some standard hydraulic problems shows that the FSM based computer model presented here performs better than some well known computer models when simulating variable density fluid flow in aquifers.

The FSM gave acceptable results with relatively few nodal points compared with methods which simultaneously solve the advective and dispersive parts of the equation. It has also been established that the computer model based on the FSM was relatively free from numerical diffusion and the oscillatory solution behaviour to which fixed grid numerical methods are prone under certain conditions.

The model was also used to simulate laboratory experiments of variable density flow in unconfined aquifers. Generally there was good agreement between experimental and numerical results.

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