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UTILIZATION OF THE METHOD OF CHARACTERISTICS TO SOLVE ACCURATELY TWO-DIMENSIONAL TRANSPORT PROBLEMS BY FINITE ELEMENTS

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SUMMARY

A new finite element method is presented for the solution of two-dimensional transport problems. The method is based on a weighted residual formulation in which the method of characteristics is combined with the finite element method. This is achieved by orienting sides of the space-time elements joining the nodes at subsequent time levels along the characteristics of the pure advection equation associated with the transport problem. The method is capable of solving numerically the advection–diffusion equation without generating oscillations or numerical diffusion for the whole spectrum of dispersion from diffusion only through mixed dispersion to pure convection.

The utility and accuracy of the method are demonstrated by a number of examples in two space dimensions and a comparison of the numerical results with the exact solution is presented in one case. A very favourable feature of the method is the capability of solving accurately advection dominated transport problems with very large time steps for which the Courant number is well over one.

KEY WORDS Advection–diffusion Characteristics Space-time Finite Elements Water Resources

INTRODUCTION

Environmental impact studies require accurate predictions of dispersion of pollutants in the atmosphere, bodies of water or in the ground by seepage. The dispersion of pollutants occurs by both advection and turbulent diffusion. Owing to the complex variations in the environmental conditions in time and space, the analyst is generally limited to numerical model studies in predicting transport of pollutants.

A group of papers presented[1–5] at the First International Conference on Finite Elements in Water Resources gave a review and comparison of several numerical methods for the solution of the advection–diffusion equation. From these studies it can be concluded that most of the numerical methods give accurate results for diffusion-dominated transport problems. However, when the transport is dominated by advection, numerical solutions exhibit oscillations and overshooting or numerical diffusion and clipping errors in the neighbourhood of sharp fronts. Reduction of time step or reduction of space increment to practically meaningful levels is not sufficient for eliminating numerical difficulties encountered in some advection–dominated transport problems. Neither higher order finite elements[3] nor higher order integration schemes in time[5] eliminate oscillations even in some one-dimensional transport problems.

The authors[6,7] utilized the method of characteristics in a space-time finite element

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framework to solve accurately the advection–diffusion equation in one space dimension. The method degenerates into the method of characteristics for pure advection problems and into a conventional space-time finite element method[8] for pure diffusion problems.

The derivation of the method will be given here for transport problems in two space dimensions. The transport problem is solved step by step in time. The spatial mesh at the end of each time step is obtained by moving the nodes of the spatial mesh at the beginning of the time step along the characteristics of the associated pure advection problem. Discretization of the problem is achieved in the framework of an unconventional isoparametric finite element method in space-time. A detailed study of isoparametric elements is given by Oden[9] and Zienkiewicz.[10] Isoparametric space-time elements are employed to solve free boundary problems associated with the heat equation[11–12] and to solve the systems of equations representing conservation laws.[13]

The utility and accuracy of the method are illustrated by three two-dimensional test problems. The numerical results for the first test problem are compared with the exact solution. In contrast to several numerical methods[14–16] numerical results for two-dimensional problems given here and elsewhere,[17] demonstrate that very accurate results are obtained for very large time steps for which the Courant number is well over one. Previously, this property of the method was also demonstrated for linear and non-linear transport problems in one dimension.[7,18]

STATEMENT OF THE PROBLEM

The horizontal scales of motions in the lakes and oceans are much greater than the vertical scales and therefore, in many cases, the horizontal and vertical dispersions may be considered separately.[19] The partial differential equation governing the horizontal dispersion of an effluent patch in an incompressible flow in two space dimensions x and y can be written as

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right)-\frac{\partial}{\partial x}(uC)-\frac{\partial}{\partial y}(vC) \quad \text{in } \Omega, \qquad t>0 \tag{1}$$

Here, the x-axis is chosen in the direction of the mean current. The eddy diffusion coefficients D_x, D_y and the velocity components u, v are given. The solute concentration $C(x, y, t)$ is sought. The flow region of interest and time are denoted by Ω and t, respectively. The development of the method will be given for a concrete example in which the boundary condition and the initial condition are prescribed respectively as

$$D_x\frac{\partial C}{\partial x}n_x+D_y\frac{\partial C}{\partial y}n_y=0 \quad \text{on } \partial\Omega, \qquad t>0 \tag{2}$$

$$C(x, y, 0)=f(x, y) \qquad \text{in } \Omega. \tag{3}$$

Here, $\mathbf{n}(n_x, n_y)$ denotes the outer normal unit vector at a point on the boundary $\partial\Omega$.

THE METHOD OF WEIGHTED RESIDUALS

Let $c(x, y, t)$ be a weighted residual approximation to the solution of equation (1) which satisfies the boundary condition and the initial condition (equations (2)–(3)). The vanishing of the weighted residual of equation (1) with respect to a continuous weighting function

$w(x, y, t)$ defined in Ω, for $0 \le t^n \le t \le t^{n+1}$ can be expressed as

$$\int_{t^n}^{t^{n+1}} \iint_{\Omega} \left[-c\frac{\partial w}{\partial t} + D_x \frac{\partial c}{\partial x}\frac{\partial w}{\partial x} + D_y \frac{\partial c}{\partial y}\frac{\partial w}{\partial y} - uc\frac{\partial w}{\partial x} - vc\frac{\partial w}{\partial y} \right] \mathrm{d}\Omega\, \mathrm{d}t$$

$$+ \iint_{\Omega} [c(x, y, t^{n+1})w(x, y, t^{n+1}) - c(x, y, t^n)w(x, y, t^n)]\, \mathrm{d}\Omega$$

$$+ \int_{t^n}^{t^{n+1}} \int_{\partial\Omega} cw(un_x + vn_y)\, \mathrm{d}s\, \mathrm{d}t = 0 \tag{4}$$

Here, $\mathrm{d}s$ denotes the arc length along the boundary $\partial\Omega$. The line integral on $\partial\Omega$ will be evaluated on the counterclockwise direction.

DISCRETIZATION BASED ON CHARACTERISTICS

Let t^n and t^{n+1} denote the beginning and the end of a typical time step. The problem will be solved step by step in time employing finite elements in space and time.

Consider a discretization of the region of interest Ω at $t = t^n$ by triangular area elements. Let $P_i^n(x_i^n, y_i^n, t_i^n)$ denote a typical node at time $t = t^n$ in the region Ω or on the boundary $\partial\Omega$.

In order to discretize the domain of integration (equation (4)), $(x, y) \in \Omega$ and $t^n < t < t^{n+1}$, by spatial-temporal volume elements, a node $P_i^{n+1}(x_i^{n+1}, y_i^{n+1}, t_i^{n+1})$ at $t = t^{n+1}$ is associated with each typical node P_i^n. To a typical triangular area element K_{ijk}^n with nodes $P_i^n P_j^n P_k^n$ in Ω at $t = t^n$, there corresponds a typical prism volume element V_{ijk} in the $x-y-t$ space which is obtained by joining the associated nodes of the triangular bases ($P_i^n P_j^n P_k^n$ and $P_i^{n+1} P_j^{n+1} P_k^{n+1}$) as subsequent time levels t^n and t^{n+1} as shown in Figure 1.

Typical line segments $P_i^n P_i^{n+1}$ joining the associated nodes at subsequent time levels are oriented along the linearized characteristics of the hyperbolic equation which is obtained by substituting $D_x = 0$ and $D_y = 0$ into equation (1), thus

$$x_i^{n+1} = x_i^n + (t^{n+1} - t^n)u(P_i^n), \qquad y_i^{n+1} = y_i^n + (t^{n+1} - t^n)v(P_i^n) \tag{5}$$

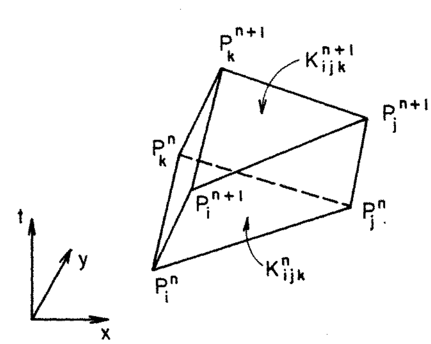

Figure 1. A typical prism volume element

In the following formulation, we are interested in investigating dispersion of an effluent patch in an infinite region. For this model, the concentration distribution at infinity should vanish. In order to solve a problem in an infinite region numerically, the finite region Ω is taken large enough initially and the nodes on $\partial\Omega$ are allowed to move along the characteristics (equation (5)) at each time step so that the boundary is sufficiently far away from the patch at all times. The flow region at $t=t^n$ and $t=t^{n+1}$ is illustrated in Figure 2.

Finite element approximation

In order to derive a finite element approximation to equation (4), the prism volume elements are transformed from the $x-y-t$ global co-ordinate system to the $\eta-\xi-\zeta$ local co-ordinate system such that the transformed volume element is a unit right triangular prism. In the local co-ordinates, the approximate solution over a typical right unit triangular prism will be taken as a polynomial of the form

$$c(\eta,\xi,\zeta)=\eta[(1-\zeta)c_i^n+\zeta c_i^{n+1}]+\xi[(1-\zeta)c_j^n+\zeta c_j^{n+1}]\\ +(1-\eta-\xi)[(1-\zeta)c_k^n+\zeta c_k^{n+1}] \quad (6)$$

in which $c_q^m(q=i,j,k;\ m=n,n+1)$ denote the nodal values of the approximating function, $c(P_q^m)$. It can be easily verified that the co-ordinate transformation is also achieved employing the shape functions used in equation (6). Therefore, the finite elements are isoparametric.

At a typical time step n, the nodal values c_i^n of the approximating function are prescribed for $n=0$ or are evaluated at the previous step for $n>0$. Therefore, there is one unknown c_i^{n+1} for each node P_i^{n+1} in Ω or on the boundary $\partial\Omega$.

Let V denote the space of all continuous functions defined on triangular prisms by equation (6). A function w in V is uniquely determined by its values at all the nodes. The weighting function $w^m(x,y,t)$ for each node will be defined as a function of the space V as follows:[13]

$$w^m(P_i^n)=w^m(P_i^{n+1})=\begin{cases}1 & \text{if} \quad m=i\\ 0 & \text{if} \quad m\neq i\end{cases} \quad (7)$$

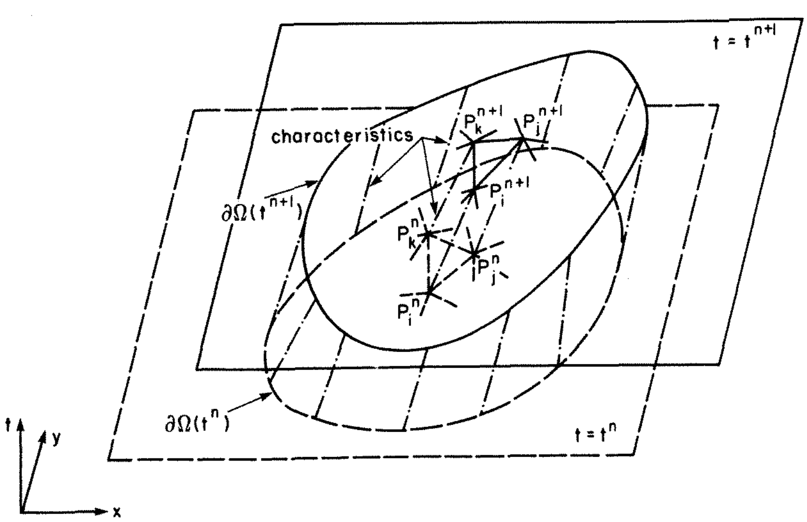

Figure 2. Transformation of the flow region Ω at a typical time step

This definition of the weighting function w^m ensures that

$$\sum_m w^m(x, y, t) = 1, \qquad (x, y) \in \Omega(t), \qquad t^n < t < t^{n+1} \tag{8}$$

Therefore, the conservation relation is satisfied in integral form at each time step.

For brevity, we define I_{ijk} and S_{ijk} as

$$I_{ijk}(\psi) = \iiint_{V_{ijk}} \psi(x, y, t)\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}t \tag{9}$$

$$S_{ijk}(\psi) = \iint_{K_{ijk}^{n+1}} \psi(x, y, t^{n+1})\, \mathrm{d}x\, \mathrm{d}y - \iint_{K_{ijk}^{n}} \psi(x, y, t^n)\, \mathrm{d}x\, \mathrm{d}y \tag{10}$$

for an arbitrary continuous function ψ defined on the domain of integration of each integral. Replacing $w(x, y, t)$ by w^m in equation (4), a system of linear equations

$$\sum_{ijk} \left\{ -I_{ijk}\left[c\frac{\partial w^m}{\partial t} + uc\frac{\partial w^m}{\partial x} + vc\frac{\partial w^m}{\partial y} \right] + I_{ijk}\left[D_x \frac{\partial w^m}{\partial x}\frac{\partial c}{\partial x} + D_y \frac{\partial w^m}{\partial y}\frac{\partial c}{\partial y} \right] + S_{ijk}(cw^m) \right\} = 0, \qquad m = 1, 2, \ldots, N \tag{11}$$

in the unknowns c_i^{n+1} at nodes P_i^{n+1} $(i = 1, 2, \ldots, N)$ is obtained. The summation is performed over all the triangular area elements in Ω at $t = t^n$. In obtaining equation (11), the boundary contribution given by the last integral in equation (4) is neglected. This approximation is believed to be appropriate for the dispersion analysis of an effluent patch in an infinite region, although the non-vanishing contributions from the boundary $\partial\Omega$ can be easily incorporated in the formulation if the effect of the boundary is thought to be important. Here, it should be noted that the concentration distribution on $\partial\Omega$ is not taken as zero. But, the concentration distribution on the boundary $\partial\Omega$ far away from the patch is assumed not to affect the concentration distribution inside the patch as in the case of an infinite region.

The system of linear equations can be constructed by evaluating element contributions in equation (11) by numerical integration. The explicit form of the system of linear equation will be given for the case u = constant, v = constant, D_x = constant, D_y = constant. The resulting equations in this case are

$$(\mathbf{Q} + \mathbf{Z})\mathbf{c}^{n+1} = (\mathbf{Q} - \mathbf{z})\mathbf{c}^n \tag{12}$$

where

$$\mathbf{c}^{n+\zeta} = \{c_1^{n+\zeta}, c_2^{n+\zeta}, \ldots, c_N^{n+\zeta}\}^{\mathrm{T}}, \qquad \zeta = 0, 1 \tag{13}$$

and, $\mathbf{Q}$ and $\mathbf{Z}$ are a diagonal and a banded symmetric matrix, respectively. The elements of the matrices $\mathbf{Q}$ and $\mathbf{Z}$ are obtained by summing up the volume and area element contributions associated with all the triangular elements in Ω at $t = t^n$ as

$$Q_{mm} = \sum_{ijk} q_{mm}^{ijk}, \qquad Z_{ml} = \sum_{ijk} z_{ml}^{ijk} \tag{14}$$

Table I. Definition of symbols

Symbols	Indices i	j	k
X^n	$x_k^n - x_j^n$	$x_i^n - x_k^n$	$x_j^n - x_i^n$
Y^n	$y_j^n - y_k^n$	$y_k^n - y_i^n$	$y_i^n - y_j^n$
A_{xy}^n		$\frac{1}{2}(x_i^n y_i^n + x_j^n Y_j^n + x_k^n Y_k^n)$	

Total contributions associated with a typical triangular element K_{ijk}^n $(P_i^n P_j^n P_k^n)$ are given by

$$q_{mm}^{ijk} = \begin{cases} \dfrac{A_{xy}^n}{3}, & m = i, j, k \\ 0, & m \neq i, j, k \end{cases} \tag{15}$$

$$Z_{ml} = \begin{cases} \dfrac{t^{n+1} - t^n}{8A_{xy}^n}(D_x Y_m^n Y_l^n + D_y X_m^n X_l^n), & m = i, j, k \text{ and } l = i, j, k \\ 0, & m \neq i, j, k \text{ or } l \neq i, j, k \end{cases} \tag{16}$$

The definitions of symbols appearing in equations (15)–(16) are given in Table I.

It is a well known fact that most of the numerical solution methods of the advection–diffusion equation encounter severe numerical difficulties when employed to solve a pure convection problem. In the case of pure convection, $D_x = D_y = 0$ and the advection–diffusion equation (equation (1)) reduces to a hyperbolic equation. In the proposed method, the nodes P_i^n and P_i^{n+1}, $i = 1, 2, \ldots, N$ are on the same characteristic line of this hyperbolic equation. Therefore, the exact solution of the pure convection problem at nodes is given by

$$c_i^{n+1} = c_i^n, \qquad i = 1, 2, \ldots, N \tag{17}$$

Here, we want to study the numerical solution to be obtained in this case. For $D_x = D_y = 0$, the matrix $\mathbf{Z}$ (equation (16)) becomes a null matrix and, therefore, in view of equation (12) the proposed method also gives the exact solution at nodes

$$\mathbf{c}^{n+1} = \mathbf{c}^n \tag{18}$$

in the case of the pure convection problem.

APPLICATIONS

The numerical solution of the horizontal dipersion of a cone-shaped initial concentration distribution will be presented. The initial condition is taken as

$$C(r, 0) = \begin{cases} c_0\left(1 - \dfrac{r}{r_0}\right), & 0 \leq r \leq r_0 \\ 0, & r > r_0 \end{cases} \tag{19}$$

Here, r denotes the distance from the centre of the circular base of the cone, and c_0 is the maximum value of the concentration. The centre of the circular base is located at the origin of the $x - y$ plane and the radius is chosen as $r_0 = 800$ m.

Table II. Parameters used in the test problems

Problem No.	Velocity (m/s) u	v	Eddy coefficients (m^2/s) D_x	D_y
1	0·25	0	2	2
2	0·25	0	0	2
3	0·25	0	$10^{-4}t+1$	$10^{-4}t+1$

Three test problems are analysed. The velocity field and the eddy coefficients used in each problem are summarized in Table II. The initial spatial mesh is chosen to be symmetric with respect to $x=0$, $y=0$ and $x=y$ lines. The part of the initial mesh in the first quadrant of the $x-y$ plane is illustrated in Figure 3. The same initial mesh is employed for all the test problems.

For the first test problem, the constant concentration lines at $t=0$, $t=2500$ s and $t=50{,}000$ s are illustrated in Figure 4. The numerical solution gives the correct location of the centre of concentrations at $t=2500$ s and $t=50{,}000$ s as $x=625$ m and $x=12{,}500$ m on the $y=0$ axis, respectively. The concentration distribution calculated numerically are axi-symmetric with respect to the concentration centres with maximum concentrations $c/c_0=0{\cdot}86$ at $t=2500$ s and $c/c_0=0{\cdot}36$ at $t=50{,}000$ s.

The total number of unknowns for the mesh employed is 65 and is independent of the final time in which the solution is sought, owing to the fact that the initial mesh moves in time with the concentration distribution. However, in order to solve the same problem from $t=0$ to $t=50{,}000$ s by conventional finite element methods at least a rectangular area of dimensions $-1000\leq x\leq 14{,}000$ and $-1600\leq y\leq 1600$ must be discretized by a rectangular mesh of reasonable increments $\Delta x=\Delta y=200$ m, which yields more than 650 unknowns even when the symmetry of the solution with respect to the x-axis is taken into consideration.

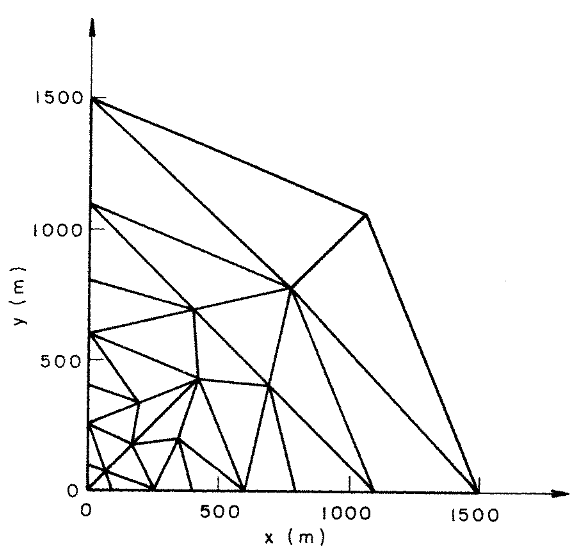

Figure 3. A quarter of the initial mesh

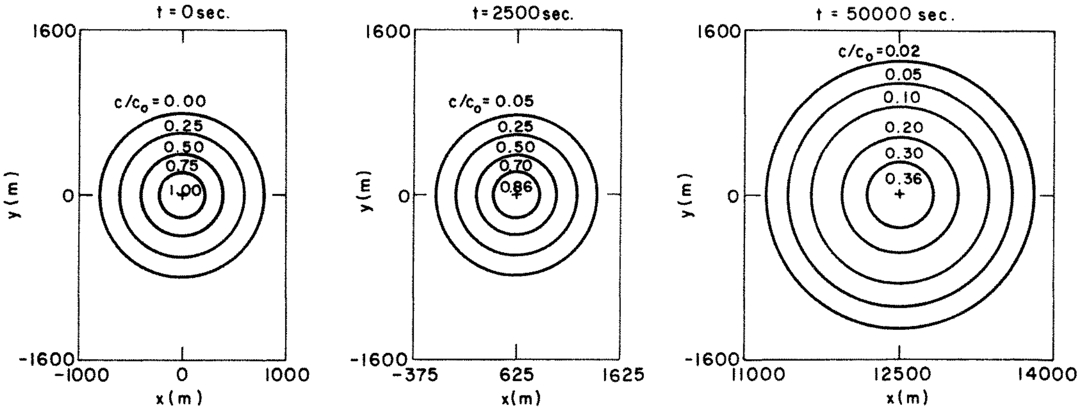

Figure 4. Constant concentration lines at various times, problem 1

The concentration distributions evaluated numerically at various times are compared with exact solutions in Figure 5. The comparison is very favourable to the method. The time step $\Delta t = 500$ s is employed in obtaining the numerical results presented in Figures 4 and 5. By choosing a finer mesh in the radial direction the accuracy of the results presented in Figure 5 can be improved if desired. However, the numerical results appear to be independent of the time step size for all practical purposes. For instance, the solutions obtained for $\Delta t =$ 250, 500, 2500 and 5000 s cannot be distinguished up to the scale of Figure 5.

Since the loss of accuracy due to the use of large time steps is negligible, accurate long time solutions can be obtained by marching in time by large but few time steps. This is a very favourable feature of this numerical method. The results obtained from the numerical

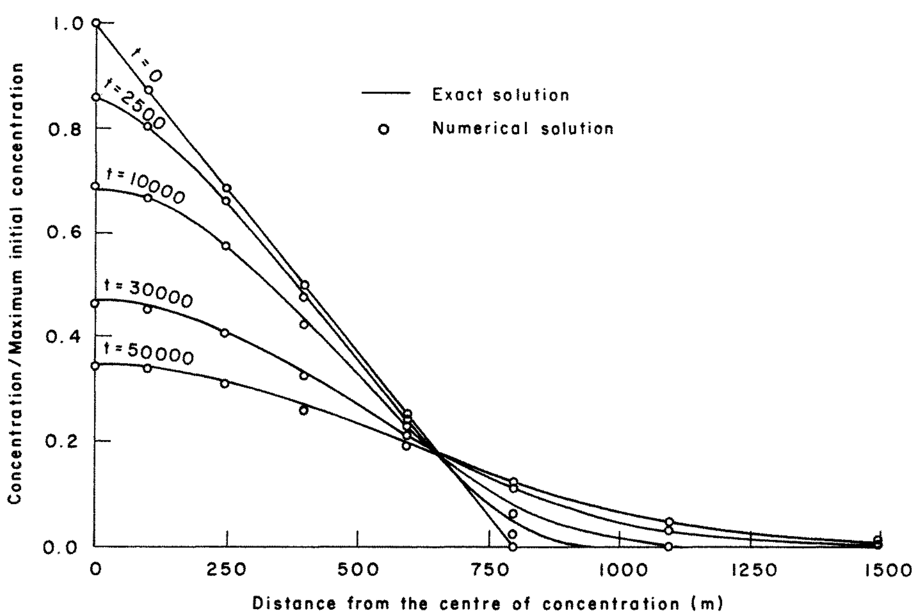

Figure 5. A comparison of numerical and exact solutions, problem 1

analysis neither exhibit any oscillation nor produce negative concentrations. The numerical solutions of test problem 1, by using the conventional finite element method[20] and the finite difference method,[1] are available. At early times ($t = 2500$ s) the axisymmetry of the concentration distribution is lost in finite element and finite difference solutions. The conventional finite element solutions exhibit oscillation with some negative concentrations. The upstream differencing scheme introduces large numerical diffusion. The one-sided flux corrected upstream differencing scheme is not oscillatory but produces clipping errors.

In the second test problem, eddy diffusion coefficients in the flow direction and the cross-flow direction are taken as $D_y = 2\text{m}^2/\text{s}$ and $D_x = 0$, respectively. The constant concentration lines at $t = 0$ and $t = 50{,}000$ s are illustrated in Figure 6. The concentration distributions calculated numerically are symmetric with respect to the axes passing through the concentration centre which are parallel to the flow and cross-flow directions. The concentration distributions along the two symmetry axes $\Theta = 0$, $\Theta = \pi/2$ and $\Theta = \pi/4$ at $t = 2500$ and $t = 50{,}000$ s are illustrated in Figure 7. The angle between the line passing through the concentration centre and the flow direction is denoted by Θ. The results presented in Figures 6 and 7 are obtained by using $\Delta t = 2500$ s.

In the Fickian diffusion model, the eddy diffusivity is assumed to be constant in time as in test problems 1 and 2. There are several turbulent diffusion models[21,22] in which the effect of the growth of the eddy size as the concentrations spread to a larger area with time is taken into consideration by choosing eddy diffusivity dependent on the mean concentration. The diffusion characteristics of 'dye patch tests' are available as the variance of the concentration distribution versus the diffusion time or the eddy diffusivity versus the length scale of diffusion.[19,23] The diffusion time is defined as the time elapsed since dye release.

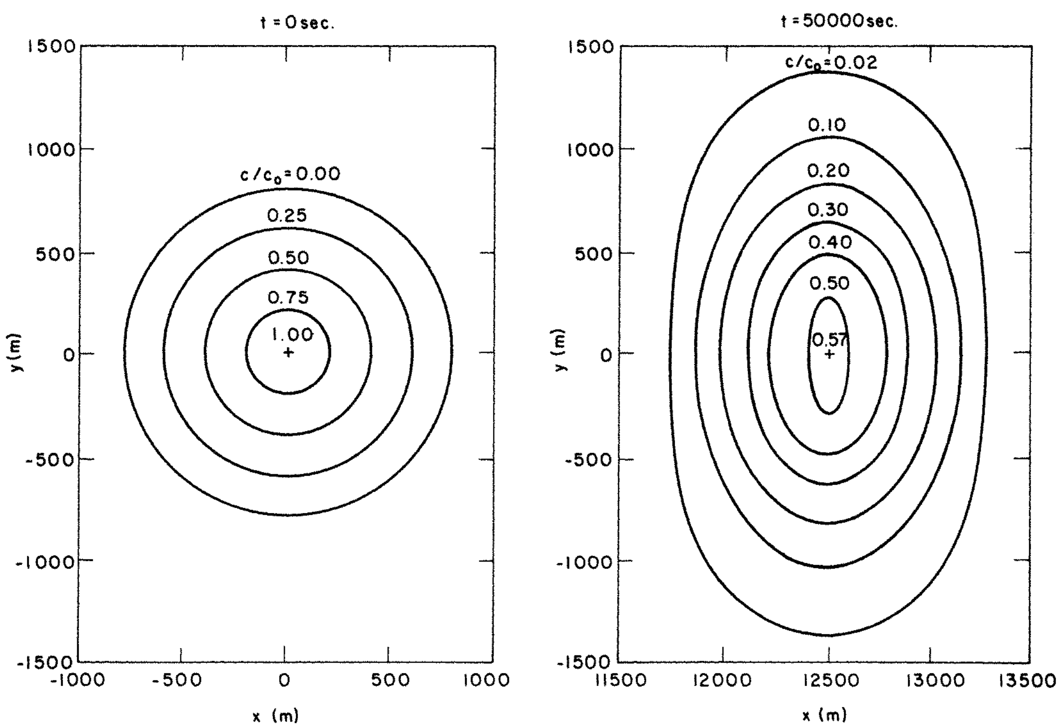

Figure 6. Constant concentration lines, problem 2

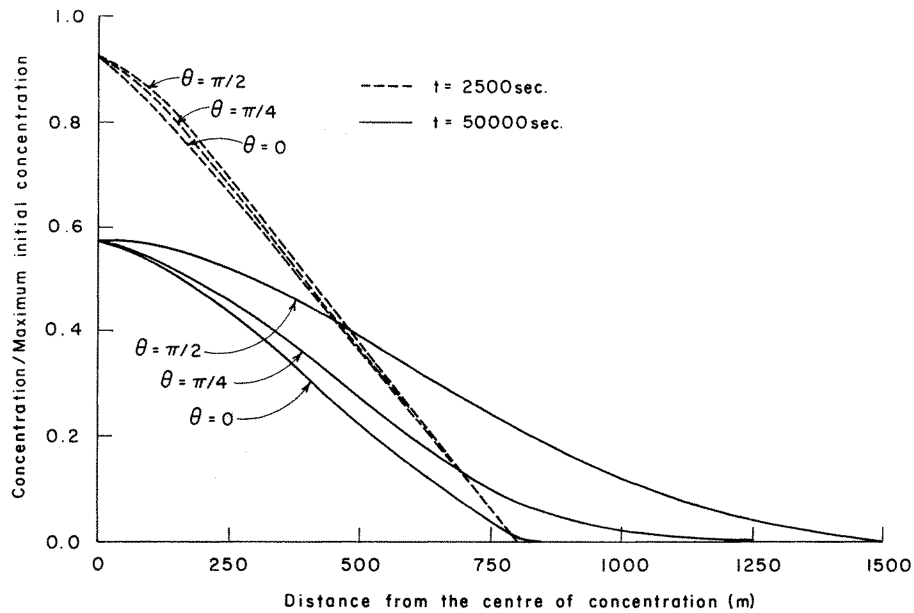

Figure 7. Concentrations at $t = 2500$ s and $t = 50{,}000$ s, problem 2

The third test problem is chosen to demonstrate the utility of the numerical method in the case of eddy diffusivities varying with time. A linear time dependence of the eddy diffusivities is chosen as shown in Figure 8. This choice gives $D_x = D_y = 1\ \mathrm{m^2/s}$ at $t = 0$ and $D_x = D_y = 6\ \mathrm{m^2/s}$ at $t = 50{,}000$ s. Thus, the eddy diffusivity used in this problem and test problem 1 are of the same order of magnitude. The concentration distribution versus the distance from the centre of concentrations for several times is illustrated in Figure 9. The

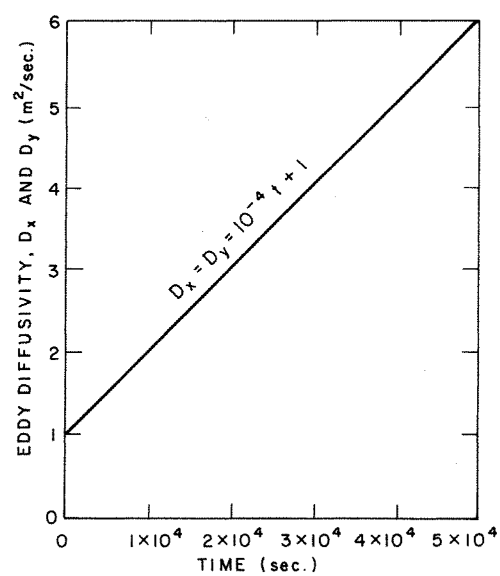

Figure 8. Time dependent eddy coefficients, problem 3

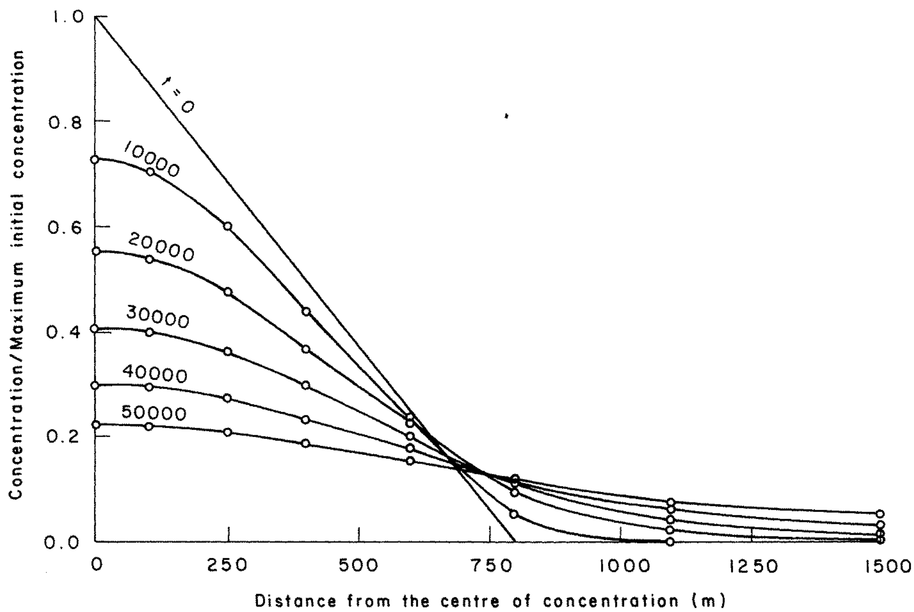

Figure 9. Concentrations at various times, problem 3

numerical results are obtained by using a time step $\Delta t = 500$ s. For all practical purposes, results are axisymmetric with respect to the centre of concentration. Neither oscillations nor negative concentrations are produced.

The numerical results presented are obtained on an AMDAHL 470 V/8 computer. The total processing time used at each time step is less than 0.2 s.

CONCLUSIONS

A new numerical method for the solution of the transport problem in two space dimensions is presented. The novel feature of the method is the utilization of the characteristics of the pure advection problem in a space-time finite element framework. The method is employed to solve the horizontal dispersion of an effluent patch in an infinite domain. Some of the numerical results are compared with exact solutions. The numerical results presented here and elsewhere[6,7,17,18] demonstrate that numerical solutions involving movements of steep fronts in flow fields with constant or variable velocities and eddy coefficients do not exhibit any oscillation or numerical diffusion. A very favourable feature of the method is the capability of accurately solving advection dominated transport problems large time steps for which the Courant number is well over one.

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