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NUMERICAL MODELLING OF MASS TRANSPORT PROBLEMS IN POROUS MEDIA: A REVIEW

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Abstract—To seek the numerical solution to the contaminant transport problem in a porous medium, numerous publications on this aspect have emerged during the last three decades. Among them the finite difference method and finite element method have been widely used in this process of solution. Thus, the finite difference method for dealing with contaminant transport problems in porous media is briefly outlined in this paper. Considering the certain advantages of the finite element method over the finite difference method, the finite element method and its formulation for modelling contaminant transport problems are discussed in great detail. Finally, a numerical example has been given to show how the finite element method is applied to solve contaminant transport problems in engineering practice.

1. INTRODUCTION

The most common approach used for modelling contaminant transport in porous media is the advection–dispersion equation. The advection–dispersion equation includes terms which describe the physical processes governing the movement, dispersion and transformation of a solute. Generally, the advection is due to bulk movement of water, either caused by differences in density (natural convection), by regional movement in the aquifer (advection), or by some artificial disturbance (forced convection). The dispersion is due to the irregular movement of water. On the pore scale, these irregularities are due to the tortuosity of the flow paths and on a large scale they are due to the presence of zones of different permeabilities.

In the case of constant transport parameters with respect to time and position, the advection–dispersion equation is linear and the corresponding closed-form solutions can generally be derived. Many analytical solutions for the advection–dispersion equation are now available for a large number of initial and boundary conditions for one-dimensional transport problems [1] and a smaller number of conditions for two- and three-dimensional transport problems [2–4]. Because of the large variability of flow and mass transport properties in the field, the often transient nature of the flow regime, and the non-ideal nature of the applicable initial and boundary conditions, the usefulness of analytical solutions is often limited and numerical methods such as finite difference methods and finite element methods are needed to solve such problems.

In terms of numerical methods, a number of finite difference models [5–7] and finite element models [8–16] have been developed to deal with water and contaminant transport problems in porous media. Also, a number of finite difference models [17–25] and a finite element model [26] were presented to model unsaturated flow in porous media in which the hydraulic parameters are considered hysteretic. Considering the fact that numerical models have become the favoured type of model for studying contaminant transport problems in engineering practice, the subject of this paper is the use of numerical methods to simulate mass transport problems in porous media. Thus, a fundamental and practical introduction to finite difference methods and finite element methods is provided in great detail.

The arrangement of the main contents of this paper is as follows. In the second section, the governing equation of mass transport in porous media is derived from some physical principles. In the third section, the finite difference method for dealing with mass transport problems is outlined and the related formulae are given. In the fourth section, the finite element formulation for dealing with mass transport problems is derived and some problems associated with the method are also discussed. Finally, an example and discussion are given in Sec. 5 to illustrate how the finite element method is applied to solve the mass transport problems in porous media.

2. GOVERNING EQUATIONS OF MASS TRANSPORT PROBLEMS

Porous media and natural porous formation are very complex in reality because they display spatial variability of their geometric and hydraulic properties. Furthermore, this variability is of an irregular

and complex nature. It generally defies a precise description, either because of insufficiency of information or because of the lack of interest in knowing the very minute details of the structure and flow field. Indeed, in most circumstances we are only interested in the behaviour of a large portion of the formation, namely in averaging flow or transport variables over the space. This averaging process has a smoothing effect and filters out small scale variations associated with heterogeneity. Even in those cases in which this is not achieved, because of large scale variability, determining some gross features of the process may be quite satisfactory. Therefore, from the viewpoint of macroscopic mechanics, the porous media encountered in most engineering practice can be regarded as homogeneous, isotropic media.

For a homogeneous, isotropic and flow-saturated porous medium, the governing advection dispersion equation for mass transport processes can be derived from the law of conservation of mass under the following assumptions: (1) the porous medium is homogeneous and isotropic; (2) the medium is saturated by flow; (3) the flow in the medium is a steady-state one; (4) Darcy's law applies to the flow in the medium. Under the Darcy assumption, the flow is described by the average linear velocity, which carries the dissolved solute by advection and forms one of the mechanisms of mass transport processes in porous media. In reality, there is an additional mixing process, namely hydrodynamic dispersion, which is caused by variations in the microscopic velocity within each pore channel and from one channel to another. If the mass transport processes are described on a macroscopic scale using macroscopic parameters and taking into account the effect of microscopic mixing, it is necessary to introduce a second mechanism of mass transport, in addition to advection, to account for hydrodynamic dispersion.

As shown in Fig. 1, the solute flux into and out of an infinitesimal elemental volume in the porous medium is considered to derive the governing equations of the problem. It should be noted that these governing equations, as a matter of fact, are certain mathematical statements of the conservations of mass. In a three-dimensional rectangular coordinate system, the specific discharge (superficial flow velocity) v has three components, v_x, v_y and v_z, so that the average linear velocity $\bar{v} = v/n$ also has three components, $\bar{v}_x$, $\bar{v}_y$ and $\bar{v}_z$, where n is the porosity of the porous medium and is defined as the ratio of the volume of the voids V_v to that of the total volume of the representative element V_t. If the concentration of the solute C is defined as the mass of solute per unit volume of solution, the mass of solute per unit volume of porous media is nC. For a homogeneous medium, the porosity n is a constant. Thus, $\partial(nC)/\partial x = n(\partial C/\partial x)$. The mass of solute transported in the x direction by the two mechanisms of mass transport can be represented as

$$m_1 = \bar{v}_x nC \, dA$$

$$m_2 = nD_x \frac{\partial C}{\partial x} dA, \tag{1}$$

where m_1 is the mass transported by advection, m_2 is the mass transported by dispersion and is derived from Fick's first law, D_x is the dispersion coefficient in the x direction and dA is the elemental cross-sectional area of the cubic element. The dispersion

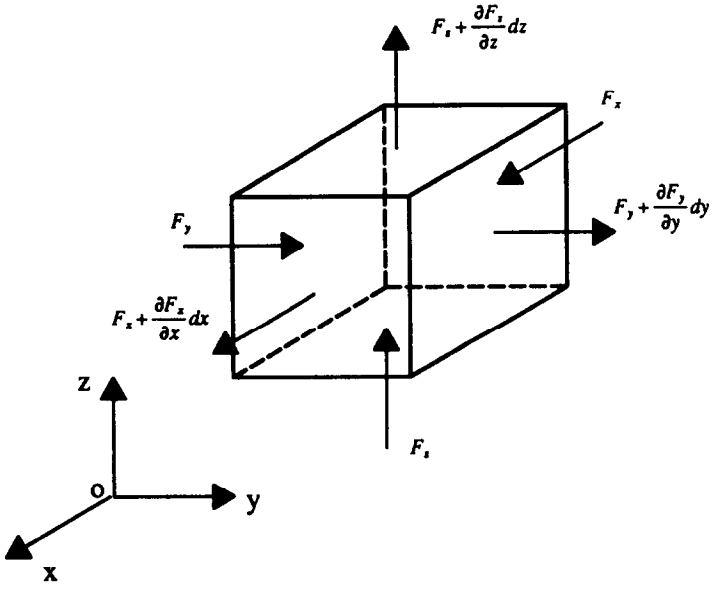


Fig. 1. Mass balance in an infinitesimal element.

coefficient D_x is related to the dispersivity α_x and the diffusion coefficient D^* as follows:

$$D_x = \alpha_x \bar{v}_x + D^*. \tag{2}$$

If F_x is defined to represent the total mass of solute per unit cross-sectional area transported in the x direction per unit time, then it can be written as

$$F_x = \bar{v}_x nC - nD_x \frac{\partial C}{\partial x}. \tag{3}$$

It is noted that the negative sign before the dispersive term indicates that the contaminant moves toward the zone of lower concentration. Similarly, expressions in the y and z directions can be written as

$$F_y = \bar{v}_y nC - nD_y \frac{\partial C}{\partial y}$$

$$F_z = \bar{v}_z nC - nD_z \frac{\partial C}{\partial z}, \tag{4}$$

where

$$D_y = \alpha_y \bar{v}_y + D^*$$

$$D_z = \alpha_z \bar{v}_z + D^*, \tag{5}$$

and α_y and α_z are dispersivity of the medium in the y and z directions respectively.

Therefore, the total amount of solute entering the cubic element in Fig. 1 is

$$m_{in} = F_x \, dz \, dy + F_y \, dz \, dx + F_z \, dx \, dy. \tag{6}$$

The total amount of solute leaving the cubic element is

$$m_{out} = \left(F_x + \frac{\partial F_x}{\partial x} dx\right) dz \, dy + \left(F_y + \frac{\partial F_y}{\partial y} dy\right) dz \, dx + \left(F_z + \frac{\partial F_z}{\partial z} dz\right) dx \, dy, \tag{7}$$

where the partial terms represent the spatial change of the solute mass in the corresponding direction. The difference in the amount entering and leaving the element can be expressed as

$$m_{out} - m_{in} = \left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right) dx \, dy \, dz. \tag{8}$$

If the dissolved substance is assumed to be nonreactive, the difference between the flux into the element and the flux out of the element equals the amount of dissolved substance accumulated in the element. The rate of mass change in the element is

$$m_{change} = -n \frac{\partial C}{\partial t} dx \, dy \, dz. \tag{9}$$

Using the law of conservation of mass, the governing equation of mass transport in the porous medium can be derived as

$$\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = -n \frac{\partial C}{\partial t}. \tag{10}$$

Substituting eqns (3) and (4) into eqn (10), the governing equation of mass transport in the three-dimensional porous medium can be written as

$$\left[\frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right)\right] - \left[\frac{\partial}{\partial x}(\bar{v}_x C) + \frac{\partial}{\partial y}(\bar{v}_y C) + \frac{\partial}{\partial z}(\bar{v}_z C)\right] = \frac{\partial C}{\partial t}. \tag{11}$$

For the homogeneous medium in which dispersion coefficients D_x, D_y and D_z are independent of the space variables and the velocity $\bar{v}$ is steady and uniform, eqn (11) can be further expressed as

$$\left[D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2}\right] - \left[\bar{v}_x \frac{\partial C}{\partial x} + \bar{v}_y \frac{\partial C}{\partial y} + \bar{v}_z \frac{\partial C}{\partial z}\right] = \frac{\partial C}{\partial t}. \tag{12}$$

It should be noted that eqn (12) is derived from a three-dimensional porous medium. The solution to this equation provides the solute concentration C as a function of space and time.

Using the same procedure as above, the governing equation of mass transport in a two-dimensional porous medium can be derived as

$$\left[D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2}\right] - \left[\bar{v}_x \frac{\partial C}{\partial x} + \bar{v}_y \frac{\partial C}{\partial y}\right] = \frac{\partial C}{\partial t}. \tag{13}$$

Similarly, the governing equation of mass transport in a one-dimensional porous medium is

$$D_x \frac{\partial^2 C}{\partial x^2} - \bar{v}_x \frac{\partial C}{\partial x} = \frac{\partial C}{\partial x}. \tag{14}$$

Moreover, it is possible to extend the governing equation of mass transport in a porous medium to include the effects of retardation of mass transport through adsorption, chemical reaction, biological transformation or radioactive decay. In this case, the mass balance carried out on the elemental volume must include a source–sink term. Taking retardation due to adsorption as an example, the governing equation of mass transport in a homogeneous medium in a one-dimensional system along the direction of flow can be written as

$$D_x \frac{\partial^2 C}{\partial x^2} - \bar{v}_x \frac{\partial C}{\partial x} + \frac{\rho_b}{n} \frac{\partial s}{\partial t} = \frac{\partial C}{\partial t}, \tag{15}$$

where ρ_b is the bulk mass density of the porous medium, s is the mass of chemical constituent absorbed on a unit mass of the solid part of the porous medium. The first term of eqn (15) is the dispersion term, the second is the advection term and the third is the reaction term.

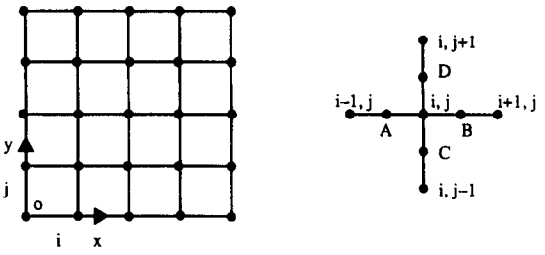
It should be pointed out that for certain simple boundary and initial conditions, there are some analytical solutions available for eqns (12), (13) and (14). However, in most field situations, the velocities are seldom uniform and the dispersivities are usually variable in space. For these situations, numerical methods such as the finite difference method and the finite element method must be used to obtain solutions.

3. FINITE DIFFERENCE METHODS FOR MASS TRANSPORT PROBLEMS

Finite difference and finite element methods are presently the most common numerical techniques for numerical modelling of mass transport problems in porous media. In these methods, not only the boundary conditions are approximated, but also the governing equation of the problem is discretized. One of the main characteristics for using both methods in their conventional forms is that the problem domain should be bounded. The advantages of both the finite difference and finite element methods lie in that: (1) hydraulic properties such as permeability and dispersivity can be easily varied throughout a system; (2) their formulations are suitable for modelling both steady-state and transient flow; and (3) they are comparatively simple and straightforward in implementation. Therefore, finite difference and finite element methods have found wide applications in engineering practice. In this section, the emphasis is on dealing with finite difference methods for mass transport problems in porous media in some detail. For the ease of brevity, a two-dimensional problem is considered to illustrate how the finite difference method is used to deal with such problems.

Finite difference methods are based on a discretization of the problem domain into a mesh that is usually rectangular, so that the contaminant concentration is computed at the grid points by solving the differential equation in a finite difference form throughout the mesh. There exist a variety of numerical techniques for solving the resulting linear equations of a system. Although the finite difference method may be applied with comparative ease to problems where the hydraulic properties vary from node to node, we will discuss the case where the hydraulic properties are constant, for the purpose of explaining the basic principles involved in the method for a square mesh. As mentioned in the last section, the governing equation of a two-dimensional mass transport problem in a porous medium is expressed as

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - \bar{v}_x \frac{\partial C}{\partial x} - \bar{v}_y \frac{\partial C}{\partial y} = \frac{\partial C}{\partial t}. \quad (16)$$



(A) An illustrative mesh (B) A typical node

Fig. 2. Finite difference mesh.

Using the finite difference method, the problem domain can be discretized by a square mesh as shown in Fig. 2(A). The nodes are identified as (i, j), where i and j are integers, such that the coordinates of node (i, j) are defined by

$$x = (i - 1)a$$

$$y = (j - 1)a, \quad (17)$$

where a is the distance between the grid points and can be expressed as

$$a = \Delta x = \Delta y. \quad (18)$$

The node (i, j) with its four surrounding grid points is shown in Fig. 2(B), where A, B, D and C are middle points between the corresponding nodes. The derivative $\partial C/\partial x$ may be approximately expressed at points A and B as

$$\left[\frac{\partial C}{\partial x}\right]_A = \frac{C_{i,j} - C_{i-1,j}}{a}$$

$$\left[\frac{\partial C}{\partial x}\right]_B = \frac{C_{i+1,j} - C_{i,j}}{a}. \quad (19)$$

Taking an average value of $[\partial C/\partial x]_A$ and $[\partial C/\partial x]_B$, the first derivative of C with respect to x at node (i, j) can be expressed as

$$\left[\frac{\partial C}{\partial x}\right]_{i,j} = \frac{C_{i+1,j} - C_{i-1,j}}{2a}. \quad (20)$$

The second derivative of C with respect to x at node (i, j) may be written in the finite difference form as

$$\left[\frac{\partial^2 C}{\partial x^2}\right]_{i,j} = \frac{C_{i-1,j} + C_{i+1,j} - 2C_{i,j}}{a^2}. \quad (21)$$

Similarly, the first and second derivatives of C with respect to y at node (i, j) can be derived as

$$\left[\frac{\partial C}{\partial y}\right]_{i,j} = \frac{C_{i,j+1} - C_{i,j-1}}{2a}$$

$$\left[\frac{\partial^2 C}{\partial y^2}\right]_{i,j} = \frac{C_{i,j-1} + C_{i,j+1} - 2C_{i,j}}{a^2}. \quad (22)$$

The first derivative of C with respect to t can be also expressed in the finite difference form as

$$\left[\frac{\partial C}{\partial t}\right]_{i,j} = \frac{C_{i,j}^{t+\Delta t} - C_{i,j}^{t}}{\Delta t}. \tag{23}$$

Substituting eqns (20)–(23) into eqn (16) and using the forward difference scheme for time, the finite difference equation of the system can be written as

$$\begin{aligned} C_{i,j}^{t+\Delta t} = C_{i,j}^{t} + \frac{\Delta t}{a^2}[&D_x(C_{i-1,j}^{t} + C_{i+1,j}^{t} - 2C_{i,j}^{t}) \\ &+ D_y(C_{i,j-1}^{t} + C_{i,j+1}^{t} - 2C_{i,j}^{t}) \\ &- \tfrac{1}{2}\bar{v}_x a(C_{i+1,j}^{t} - C_{i-1,j}^{t}) \\ &- \tfrac{1}{2}\bar{v}_y a(C_{i,j+1}^{t} - C_{i,j-1}^{t})], \end{aligned} \tag{24}$$

where the superscripts refer to the time level.

It is noted that the forward difference scheme for time has the advantages of flexibility and simplicity, but gives meaningful answers only if Δt is less than some critical value, Δt_{crit},

$$\Delta t < \Delta t_{\text{crit}}. \tag{25}$$

If Δt exceeds Δt_{crit}, the solution will become unstable, giving results that are clearly in error. The value of the critical time step may be found by numerical tests or estimated by analysing the simple problems.

Usually, there are three kinds of boundary conditions for mass transport problems in porous media. The first one is called the Dirichlet boundary condition in terms of C, where the contaminant concentration is known along the boundary, and therefore at each boundary node. The second is called the Neumann boundary condition in terms of $\partial C/\partial n$, where the first derivative of C with respect to the normal direction of the boundary n is specified along the related nodes. The third is called the mixed boundary condition, which is the combination of the Dirichlet and Neumann boundary conditions. In the finite difference method, the Dirichlet boundary condition can be directly applied to the boundary nodes, while the Neumann boundary condition needs to be considered using the following special technique. In order to approximate $\partial C/\partial n$ at boundary nodes, the mesh is extended one row of nodal points beyond the boundary as illustrated in Fig. 3. The values for either i and j are zero for nodes (i,j) outside the boundary, which are called imaginary nodes. For the case illustrated in Fig. 3, supposing $\partial C/\partial n$ is given along the boundary $x = 0$ $(i = 1)$, $\partial C/\partial n$ is approximated for node $(1, j)$ as

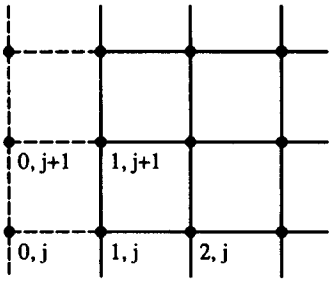


Fig. 3. Treatment of the Neumann boundary condition.

$$\left[\frac{\partial C}{\partial n}\right]_{1,j} = \left[\frac{\partial C}{\partial x}\right]_{1,j} = \frac{C_{2,j} - C_{0,j}}{2a}. \tag{26}$$

Therefore,

$$C_{0,j} = C_{2,j} - 2a\left[\frac{\partial C}{\partial x}\right]_{1,j}, \tag{27}$$

which is used to calculate the value of $\partial^2 C/\partial x^2$ at the boundary nodes. Unlike the forward difference scheme which results in the explicit finite difference formulation, the central and backward difference schemes lead to an implicit finite difference formulation. The advantage of an implicit formulation is that the time step may be chosen much larger than for the explicit one. The disadvantages are due to a greater complexity, and that the Gauss–Seidel iteration must be applied at each time step. The explicit formulation is particularly attractive for three-dimensional problems. The formulation may be adapted to three-dimensional mass transport problems in porous media simply by generating a three-dimensional mesh and changing the related expressions in eqn (24).

4. FINITE ELEMENT METHODS FOR MASS TRANSPORT PROBLEMS

The finite element method mainly differs from the finite difference method in the following two aspects: (1) the problem domain is discretized into a mesh of finite elements of any shape; (2) the governing differential equation of the problem is not solved directly but replaced by an approximate formulation. Although there exist various approximate procedures [27], the Galerkin weighted residual method may be the best one for dealing with mass transport problems in porous media.

As demonstrated in Sec. 2, the governing equation of mass transport in a two-dimensional porous media can be written as

$$D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} - \bar{v}_x\frac{\partial C}{\partial x} - \bar{v}_y\frac{\partial C}{\partial y} = \frac{\partial C}{\partial t}. \tag{28}$$

Using the Galerkin weighted residual method, eqn (28) can be rewritten for an element as

$$\iint_A [N]^{\mathrm{T}}\left[D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} - \bar{v}_x\frac{\partial C}{\partial x} - \bar{v}_y\frac{\partial C}{\partial y}\right]\mathrm{d}A - \iint_A [N]^{\mathrm{T}}\left\{\frac{\partial C}{\partial t}\right\}\mathrm{d}A = 0, \tag{29}$$

where $[N]$ is the weighting function matrix of the element, C is the trial function of the element and A is the area of the element:

$$C = [N]\{C\}^e, \tag{30}$$

where $\{C\}^e$ is the nodal concentration vector of the element at a given time.

Substituting eqn (30) into eqn (29), the following equation yields:

$$\left[\iint_A [N]^T\left(D_x\frac{\partial^2[N]}{\partial x^2}+D_y\frac{\partial^2[N]}{\partial y^2}-\bar{v}_x\frac{\partial[N]}{\partial x}-\bar{v}_y\frac{\partial[N]}{\partial y}\right)dA\right]\{C\}^e - \iint_A [N]^T[N]\left\{\frac{\partial C}{\partial t}\right\}^e A = 0. \tag{31}$$

Integrating by parts and applying Green's theorem to the second-order derivative, eqn (31) can be written as

$$[G_e]\{C\}^e + [H_e]\{C\}^e + [R_e]\left\{\frac{\partial C}{\partial t}\right\}^e = \{f\}^e, \tag{32}$$

where $[G_e]$, $[H_e]$ and $[R_e]$ are property matrices of the element and $\{f\}^e$ is a 'load' vector of the element. They can be expressed as

$$[G_e] = \iint_A \left(D_x\frac{\partial[N]^T}{\partial x}\frac{\partial[N]}{\partial x}+D_y\frac{\partial[N]^T}{\partial y}\frac{\partial[N]}{\partial y}\right)dA$$

$$[H_e] = \iint_A \left(\bar{v}_x[N]^T\frac{\partial[N]}{\partial x}+\bar{v}_y[N]^T\frac{\partial[N]}{\partial y}\right)dA$$

$$[R_e] = \iint_A [N]^T[N]\,dA$$

$$\{f\}^e = \int_S [N]^T\left(D_x\frac{\partial C}{\partial x}n_x + D_y\frac{\partial C}{\partial y}n_y\right)dS, \tag{33}$$

where S is the boundary of the element, n_x and n_y are the direction cosines of the outward unit normal vector on the boundary.

For the four-node two-dimensional isoparametric fiinte element shown in Fig. 4, the coordinate transform relationship between the global coordinate system xoy and the local coordinate system $\xi o\eta$ can be defined as

$$x = \sum_{i=1}^{4} N_i x_i$$

$$y = \sum_{i=1}^{4} N_i y_i, \tag{34}$$

where

$$N_1 = \tfrac{1}{4}(1+\xi)(1+\eta)$$

$$N_2 = \tfrac{1}{4}(1-\xi)(1+\eta)$$

$$N_3 = \tfrac{1}{4}(1-\xi)(1-\eta)$$

$$N_4 = \tfrac{1}{4}(1+\xi)(1-\eta). \tag{35}$$

The contaminant concentration field within the element can be defined as

$$C = \sum_{i=1}^{4} N_i C_i. \tag{36}$$

Comparing eqn (36) with eqn (30), the shape function matrix of the element can be written as

$$[N] = [N_1 \quad N_2 \quad N_3 \quad N_4]. \tag{37}$$

Following the differentiation rule in mathematics, the following relationships exist.

$$\frac{\partial[N]}{\partial\xi} = \frac{\partial[N]}{\partial x}\frac{\partial x}{\partial\xi}+\frac{\partial[N]}{\partial y}\frac{\partial y}{\partial\xi}$$

$$\frac{\partial[N]}{\partial\eta} = \frac{\partial[N]}{\partial x}\frac{\partial x}{\partial\eta}+\frac{\partial[N]}{\partial y}\frac{\partial y}{\partial\eta}. \tag{38}$$

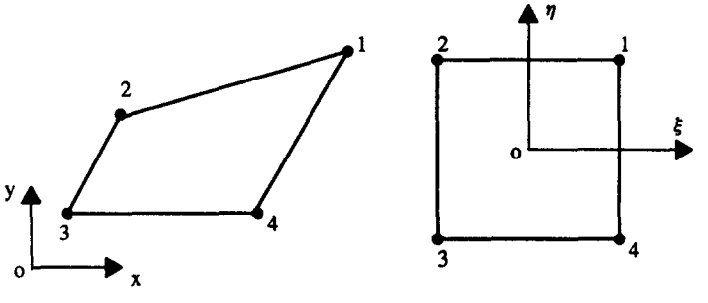


Fig. 4. Four-node two-dimensional isoparametric finite element.

Equation (38) can be written in a matrix form as

$$\begin{Bmatrix} \frac{\partial [N]}{\partial \xi} \\ \frac{\partial [N]}{\partial \eta} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} \begin{Bmatrix} \frac{\partial [N]}{\partial x} \\ \frac{\partial [N]}{\partial y} \end{Bmatrix}. \quad (39)$$

Therefore,

$$\begin{Bmatrix} \frac{\partial [N]}{\partial x} \\ \frac{\partial [N]}{\partial y} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix}^{-1} \begin{Bmatrix} \frac{\partial [N]}{\partial \xi} \\ \frac{\partial [N]}{\partial \eta} \end{Bmatrix}. \quad (40)$$

Finally, the property matrices of the element for mass transport in porous media can be expressed using the local coordinate as

$$[G_e] = \int_{-1}^{1}\int_{-1}^{1} \left(D_x \frac{\partial [N]^T}{\partial x}\frac{\partial [N]}{\partial x} + D_y \frac{\partial [N]^T}{\partial y}\frac{\partial [N]}{\partial y} \right) |J| \, d\xi \, d\eta$$

$$[H_e] = \int_{-1}^{1}\int_{-1}^{1} \left(\bar{v}_x [N]^T \frac{\partial [N]}{\partial x} + \bar{v}_y [N]^T \frac{\partial [N]}{\partial y} \right) |J| \, d\xi \, d\eta$$

$$[R_e] = \int_{-1}^{1}\int_{-1}^{1} [N]^T [N] |J| \, d\xi \, d\eta, \quad (41)$$

where $|J|$ is the Jacobian determinant of the element.

It is noted that eqn (41) can be easily evaluated using numerical integration techniques. As a result, the global matrices of the system can be assembled using the standard technique in the finite element method. Thus, the global matrix equation for the mass transport in porous media can be expressed as

$$[A]\{C\} + [R]\left\{\frac{\partial C}{\partial t}\right\} = \{f\}, \quad (42)$$

where

$$[A] = [G] + [H]. \quad (43)$$

The solution of eqn (42) in the time domain can be carried out by the finite difference approach for $\{\partial C/\partial t\}$.

$$\left\{\frac{\partial C}{\partial t}\right\} = \frac{1}{\Delta t}(\{C\}^{t+\Delta t} - \{C\}^t), \quad (44)$$

where the superscript represents the time level and Δt is the time step.

Having used the finite difference approach for the first derivative of C with respect to t, it is necessary to specify the time level in the time interval between t and $t + \Delta t$ at which another term $\{C\}$ is evaluated. In general, the nodal contaminant concentration vector, $\{C\}$, can be approximate anywhere between t and $t + \Delta t$.

$$\{C\} = (1-\alpha)\{C\}^t + \alpha\{C\}^{t+\Delta t}, \quad (45)$$

where $0 \leqslant \alpha \leqslant 1$. If $\alpha = 1$, the solution is fully implicit. If $\alpha = 0$, the solution is fully explicit. In the case of $\alpha = 0$, eqn (44) is called a forward difference approximation relative to time t. In the case of $\alpha = 1$, eqn (44) is called a backward difference approximation relative to time $t + \Delta t$. However, if $\alpha = 0.5$, eqn (44) is called a central difference approximation relative to time.

The formula for the forward difference scheme can be derived by letting $\alpha = 0$ in eqn (45) and substituting eqns (44) and (45) into eqn (42).

$$[A]\{C\}^t + [R]\frac{1}{\Delta t}(\{C\}^{t+\Delta t} - \{C\}^t) = \{f\}^t. \quad (46)$$

Therefore,

$$[R]\{C\}^{t+\Delta t} = [R]\{C\}^t - \Delta t[A]\{C\}^t + \Delta t\{f\}^t. \quad (47)$$

Letting $\alpha = 1$ in eqn (45) and substituting eqns (44) and (45) into eqn (42), the formula for the backward difference scheme can be expressed as

$$[A]\{C\}^{t+\Delta t} + [R]\frac{1}{\Delta t}(\{C\}^{t+\Delta t} - \{C\}) = \{f\}^{t+\Delta t}. \quad (48)$$

Thus

$$\left([A] + \frac{1}{\Delta t}[R]\right)\{C\}^{t+\Delta t} = \frac{1}{\Delta t}[R]\{C\}^t + \{f\}^{t+\Delta t}. \quad (49)$$

Similarly, letting $\alpha = 0.5$ in eqn (45) and substituting eqns (44) and (45) into eqn (42), the formula for the central difference scheme can be written as

$$[A](\tfrac{1}{2}\{C\}^t + \tfrac{1}{2}\{C\}^{t+\Delta t}) + [R] \times \frac{1}{\Delta t}(\{C\}^{t+\Delta t} - \{C\}^t) = \{f\}^{t+0.5\Delta t}. \quad (50)$$

Equation (50) can be further written as

$$\left(\tfrac{1}{2}[A] + \frac{1}{\Delta t}[R]\right)\{C\}^{t+\Delta t} = \left(\frac{1}{\Delta t}[R] - \tfrac{1}{2}[A]\right)\{C\}^t + \{f\}^{t+0.5\Delta t}. \quad (51)$$

Apparently, if the contaminant concentration distribution of a system is known for a time instant t, the contaminant concentration distribution of the system for another time instant $t + \Delta t$ can be found using eqn (47), eqn (49) or eqn (51), depending on whichever difference scheme is chosen.

If the advection terms in eqn (28) play a predominant role in the mass transport process, the Galerkin finite element approach as mentioned above fails to solve the problem because its solution exhibits pronounced oscillatory behaviour and excessive numerical dispersion. These oscillations and numerical dispersion can only be avoided by using a drastic refinement of the finite element mesh, which makes the conventional Galerkin finite element approach inefficient in calculation. In order to overcome this problem, Huyakorn [28], Huyakorn and Nilkuhua [29] presented an upwind finite element scheme. This scheme differs from the conventional Galerkin scheme in the following two aspects: (1) spatial discretization is performed through a general weighted residual technique which employs asymmetric weighting functions and yields an upwind weighting effect for the advection term in the mass transport equation; (2) the time derivative term of the equation is weighted using the standard trial functions which are symmetric functions.

Using the upwind finite element scheme, eqn (28) can be written for an element as

$$\iint_A [W]^{\mathrm{T}}\left[D_x\frac{\partial^2 C}{\partial x^2}+D_y\frac{\partial^2 C}{\partial y^2}-\bar{v}_x\frac{\partial C}{\partial x}-\bar{v}_y\frac{\partial C}{\partial y}\right]\mathrm{d}A - \iint_A [N]^{\mathrm{T}}\left\{\frac{\partial C}{\partial t}\right\}\mathrm{d}A = 0, \quad (52)$$

where $[W]$ is the upwind weighting function matrix of the element, while $[N]$ is the conventional weighting function matrix as shown in eqn (29).

Using the same procedure as in the conventional Galerkin finite element approach, the property matrices of the upwind finite element can be derived as

$$[G_e] = \iint_A \left(D_x\frac{\partial [W]^{\mathrm{T}}}{\partial x}\frac{\partial [N]}{\partial x}+D_y\frac{\partial [W]^{\mathrm{T}}}{\partial y}\frac{\partial [N]}{\partial y}\right)\mathrm{d}A$$

$$[H_e] = \iint_A \left(\bar{v}_x[W]^{\mathrm{T}}\frac{\partial [N]}{\partial x}+\bar{v}_y[W]^{\mathrm{T}}\frac{\partial [N]}{\partial y}\right)\mathrm{d}A$$

$$[R_e] = \iint_A [N]^{\mathrm{T}}[N]\,\mathrm{d}A$$

$$\{f\}^e = \int_S [W]^{\mathrm{T}}\left(D_x\frac{\partial C}{\partial x}n_x+D_y\frac{\partial C}{\partial y}n_y\right)\mathrm{d}S. \quad (53)$$

It is noted that from the computational point of view, all procedures employed in the Galerkin finite element approach can be directly used in the upwind finite element scheme so long as the weighting function matrix $[N]$ is replaced by the upwind weighting function matrix $[W]$ in the appropriate positions. Therefore, the following discussion is focused on the construction of the upwind weighting functions of the element.

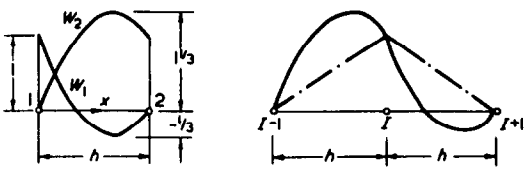


Fig. 5. One-dimensional upwind finite element.

For a one-dimensional transport problem, a linear element is shown in Fig. 5. It is assumed that the flow velocity is in the positive direction from node 1 to node 2. Let the upwind weighting functions for nodes 1 and 2 be expressed in the form:

$$W_1(x) = N_1(x) - F(x)$$

$$W_2(x) = N_2(x) + F(x), \quad (54)$$

where

$$F(x) = a\frac{x^2}{h^2}+b\frac{x}{h}+c \quad (0 \leqslant x \leqslant h), \quad (55)$$

and x is a coordinate and $F(x)$ is a piecewise quadratic function with a, b and c as undetermined coefficients; h is the length of the element. The function $F(x)$ must be chosen to satisfy the following requirements:

$$F(0) = F(h) = 0. \quad (56)$$

Substituting eqn (56) into eqn (55) yields

$$F(x) = b\left(-\frac{x^2}{h^2}+\frac{x}{h}\right), \quad (57)$$

where b is the remaining undetermined coefficient. For convenience in performing subsequent mathematical analysis, the following parameter is introduced:

$$\alpha = \frac{b}{3}. \quad (58)$$

Substituting eqns (57) and (58) into eqn (54) yields

$$W_1(x) = N_1(x) + 3\alpha\frac{x^2}{h^2} - 3\alpha\frac{x}{h}$$

$$W_2(x) = N_2(x) - 3\alpha\frac{x^2}{h^2} + 3\alpha\frac{x}{h}, \quad (59)$$

where $N_1(x)$ and $N_2(x)$ are the conventional shape functions and given by

$$N_1(x) = 1 - \frac{x}{h}$$

$$N_2(x) = \frac{x}{h}. \quad (60)$$

For a value of $\alpha = 1$, the corresponding upwind weighting functions are shown in Fig. 5. It is evident that when α is non-zero, the upwind weighting function for any node I in the mesh is asymmetric with respect to the node. More weighting is given to the upstream portion of the line segment consisting of nodes $I-1$, I and $I+1$ when α is positive. For $\alpha = 1$, it can be proven that

$$\int_{x_{I-1}}^{x_I} W_I(x)\,dx = \int_0^h W_2(x)\,dx = h$$

$$\int_{x_I}^{x_{I+1}} W_I(x)\,dx = \int_0^h W_1(x)\,dx = 0. \qquad (61)$$

The numerical experience indicated that to dampen the numerical oscillation, the sigh of α must be chosen in accordance with the sense of the direction of the flow velocity, i.e., $\alpha > 0$ when $\bar{v}_x > 0$ and vice versa. Thus, for any node I in the mesh, greater weighting must always be given to the upstream element which contributes to that node, if the oscillation is to be dampened. In view of this, the weighting functions so determined are termed upwind weighting functions. Besides, it has been demonstrated from a steady-state one-dimensional mass transport problem that the numerical solution is free of oscillation if $\alpha \geqslant 1$ or $(1-\alpha)(\bar{v}_x h/D_x) < 2$ when $\alpha < 1$. Since α directly controls oscillation, it may be termed a damping factor.

To establish numerical stability with minimum loss of accuracy, the value of α must be carefully chosen. The expression for optimum α was obtained theoretically from a steady-state one-dimensional mass transport problem by Christie *et al.* [30]. It can be written in the following form:

$$\alpha_{\text{opt}} = \coth\left(\frac{\bar{v}_x h}{2D_x}\right) - \frac{2D_x}{\bar{v}_x h}, \qquad (62)$$

where coth stands for hyperbolic cotangent.

For the quadrilateral element shown in Fig. 6, let $\xi o \eta$ represent a local isoparametric coordinate system. Since the element belongs to the Lagrangian family, its upwind weighting functions can be obtained by taking appropriate products of functions in each coordinate. In the process of forming such products, the fact that the damping factor α can vary from one element side to another should be taken into account. Thus, four different damping factors, namely $\bar{\alpha}_1$, $\bar{\beta}_1$, $\bar{\alpha}_2$ and $\bar{\beta}_2$, are assigned to sides 3–4, 4–1, 2–1 and 3–2 of the element in Fig. 6, respectively. The sense of direction of the flow velocity which corresponds to the positive values of the damping factors needs also to be considered for each side so that $\bar{\alpha}_i$ and $\bar{\beta}_i$ $(i = 1, 2)$ can be expressed as

$$\bar{\alpha}_i = \alpha_i^{\text{opt}} \operatorname{sign}(\bar{v})$$

$$\bar{\beta}_i = \beta_i^{\text{opt}} \operatorname{sign}(\bar{v}), \qquad (63)$$

where α_i^{opt} and β_i^{opt} $(i = 1, 2)$ are the optimal values of the upwind parameters for the related element sides; $\bar{v}$ is the corresponding average scalar velocity of the element side and can be determined using the following formula:

$$\bar{v} = \tfrac{1}{2}(\{v_i\} + \{v_j\}) \cdot \{l_{ij}\}, \qquad (64)$$

where i and j are the node numbers of the element side, $\{v_i\}$ and $\{v_j\}$ are the velocities of nodes i and j respectively, $\{l_{ij}\}$ is a direction vector of this particular side in the local coordinate system and its positive direction is coincident with that of the local coordinate system of the element.

Taking node 1 as an example, the upwind weighting function for this node can be expressed as

$$W_1(\xi, \eta) = F_1(\xi, \bar{\alpha}_2) F_2(\eta, \bar{\beta}_1), \qquad (65)$$

where the expressions for F_1 and F_2 can be derived directly from the one-dimensional upwind weighting function in eqn (59) in terms of ξ as follows:

$$F_1(\xi, \bar{\alpha}_2) = \frac{x}{h} - 3\bar{\alpha}_2 \frac{x^2}{h^2} + 3\bar{\alpha}_2 \frac{x}{h}, \qquad (66)$$

where

$$\frac{x}{h} = \frac{\xi + 1}{2}. \qquad (67)$$

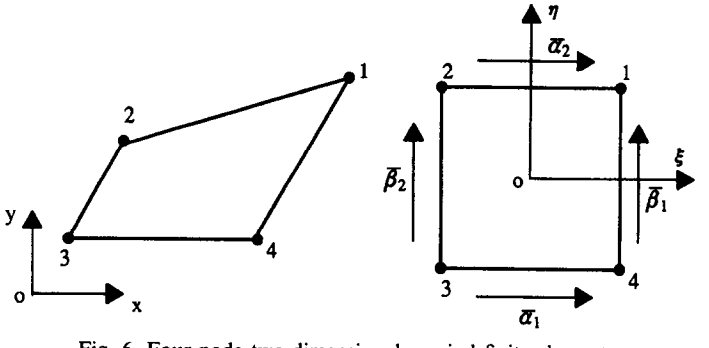


Fig. 6. Four-node two-dimensional upwind finite element.

Substituting eqn (67) into eqn (66) yields

$$F_1(\xi, \bar{\alpha}_2) = \tfrac{1}{4}[(1+\xi)(-3\bar{\alpha}_2\xi + 3\bar{\alpha}_2) + 2]. \quad (68)$$

Similarly, $F_2(\eta, \bar{\beta}_1)$ can be derived as

$$F_2(\eta, \bar{\beta}_1) = \tfrac{1}{4}[(1+\eta)(-3\bar{\beta}_1\eta + 3\bar{\beta}_1) + 2]. \quad (69)$$

Thus, eqn (65) can be further written as

$$W_1(\xi, \eta) = \tfrac{1}{16}[(1+\xi)(-3\bar{\alpha}_2\xi + 3\bar{\alpha}_2) + 2] \times [(1+\eta)(-3\bar{\beta}_1\eta + 3\bar{\beta}_1) + 2]. \quad (70)$$

In the same manner, $W_2(\xi, \eta)$, $W_3(\xi, \eta)$ and $W_4(\xi, \eta)$ can be derived as follows:

$$W_2(\xi, \eta) = \tfrac{1}{16}[(1+\xi)(3\bar{\alpha}_2\xi - 3\bar{\alpha}_2 - 2) + 4] \times [(1+\eta)(-3\bar{\beta}_2\eta + 3\bar{\beta}_2 + 2)]$$

$$W_3(\xi, \eta) = \tfrac{1}{16}[(1+\xi)(3\bar{\alpha}_1\xi - 3\bar{\alpha}_1 - 2) + 4] \times [(1+\eta)(3\bar{\beta}_2\eta - 3\bar{\beta}_2 - 2) + 4]$$

$$W_4(\xi, \eta) = \tfrac{1}{16}[(1+\xi)(-3\bar{\alpha}_1\xi + 3\bar{\alpha}_1 + 2)] \times [(1+\eta)(3\bar{\beta}_1\eta - 3\bar{\beta}_1 - 2) + 4]. \quad (71)$$

It should be noted that in order to obtain satisfactory solutions, the derivatives, $\partial W_i/\partial\xi$ and $\partial W_i/\partial\eta$ ($i = 1, 2, 3, 4$), of the element must be evaluated in such a way that when differentiation is taken with respect to one particular coordinate, the values of the upwind parameters along the remaining coordinate must be set to zero. Therefore, the derivatives of the upwind weighting functions of the element can be expressed as:

$$\frac{\partial W_1}{\partial\xi} = -\tfrac{1}{4}(1+\eta)(3\bar{\alpha}_2\xi - 1)$$

$$\frac{\partial W_2}{\partial\xi} = \tfrac{1}{4}(1+\eta)(3\bar{\alpha}_2\xi - 1)$$

$$\frac{\partial W_3}{\partial\xi} = \tfrac{1}{4}(1-\eta)(3\bar{\alpha}_1\xi - 1)$$

$$\frac{\partial W_4}{\partial\xi} = -\tfrac{1}{4}(1-\eta)(3\bar{\alpha}_1\xi - 1) \quad (72)$$

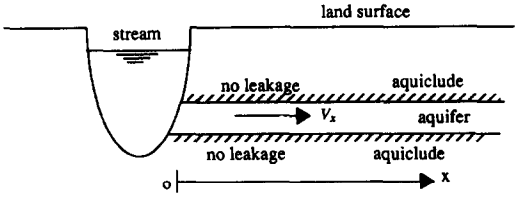


Fig. 7. Physical model of a solute transport problem.

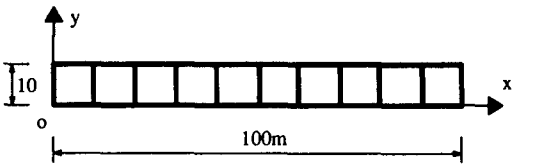


Fig. 8. Discretized model of a solute transport problem.

and

$$\frac{\partial W_1}{\partial\eta} = -\tfrac{1}{4}(1+\xi)(3\bar{\beta}_1\eta - 1)$$

$$\frac{\partial W_2}{\partial\eta} = -\tfrac{1}{4}(1-\xi)(3\bar{\beta}_2\eta - 1)$$

$$\frac{\partial W_3}{\partial\eta} = \tfrac{1}{4}(1-\xi)(3\bar{\beta}_2\eta - 1)$$

$$\frac{\partial W_4}{\partial\eta} = \tfrac{1}{4}(1+\xi)(3\bar{\beta}_1\eta - 1). \quad (73)$$

Having obtained the upwind weighting functions of the element and their derivatives, the property matrices of the upwind finite element can be straightforwardly evaluated using the same procedure as described in the conventional finite element method. Thus, the solution for the mass transport problems in a porous medium can be obtained.

5. NUMERICAL EXAMPLE AND DISCUSSION

In order to illustrate how the finite element method is applied to solve mass transport problems in porous media, a practical problem, which is sea water or contaminant water intrusion into an aquifer of fresh groundwater in a lowland area, is considered in this section.

Figure 7 shows the physical model for this illustrative example. This problem can be simplified as a one-dimensional solute transport problem. Supposing the solute is located on the surface at $x = 0$ and that the unidirectional flow is along the horizontal direction, the problem is discretized into finite elements as shown in Fig. 8, where the solute will propagate from its source ($x = 0$) to the boundary ($x = 100$ m) due to advection and dispersion. Since two-dimensional rectangular elements are used in the analysis, no-flow conditions along the two boundaries ($y = 0$ and $y = 10$ m) should be imposed for the calculation. To avoid the influence of the artificial boundary at $x = 100$ m on the numerical results, the time range of interest and the location of the artificial boundary should be chosen appropriately. The problem is discretized by 10 two-dimensional upwind finite elements and the related boundary conditions are

$$C(x, t) = C_0 = 10\ \text{mg/cm}^3 \quad \text{at } x = 0$$

$$C(x, t) = 0 \quad \text{at } x = 100\ \text{m}. \quad (74)$$

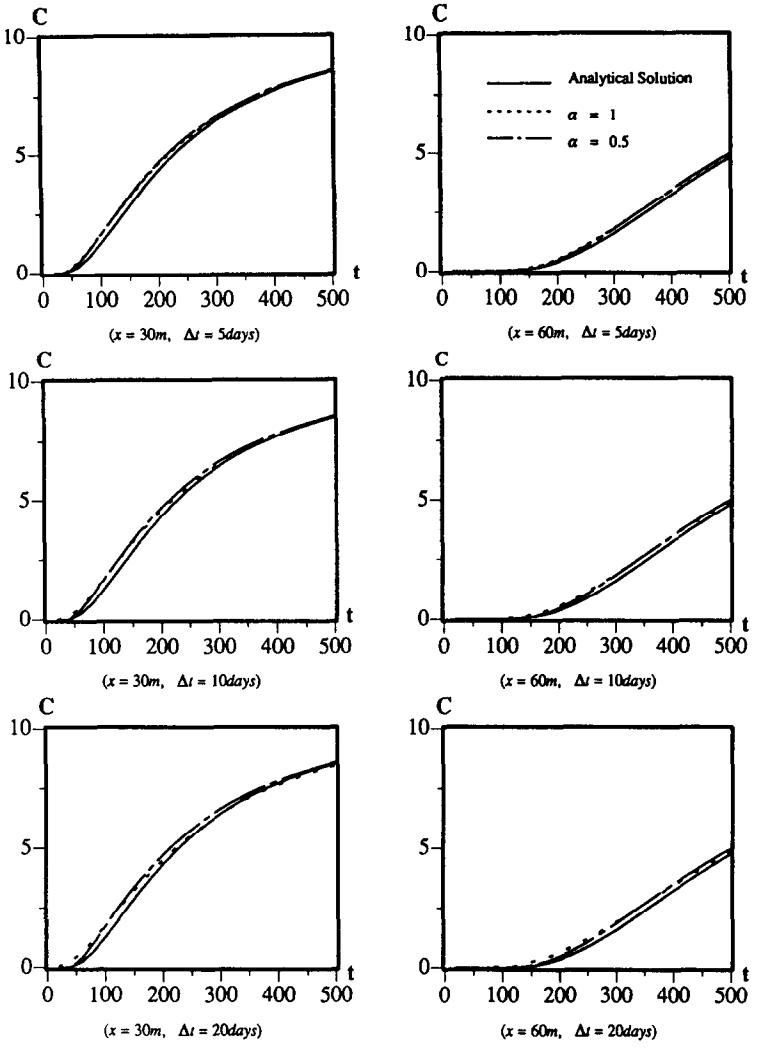


Fig. 9. Concentration versus time for the solute transport problem.

The analytical solution for this problem is available [31] and can be written as:

$$C(x,t)=\frac{C_0}{2}\left[\exp\left(\frac{\bar{v}_x x}{D_x}\right)\operatorname{erfc}\left(\frac{x+\bar{v}_x t}{2\sqrt{D_x t}}\right)+\operatorname{erfc}\left(\frac{x-\bar{v}_x t}{2\sqrt{D_x t}}\right)\right], \quad (75)$$

where erfc is the complementary error function and can be expressed as

$$\operatorname{erfc}(z)=\frac{2}{\sqrt{\pi}}\int_z^\infty \exp(-u^2)\,du. \quad (76)$$

For the purpose of numerical calculation, the following parameters are used in the analysis: the average velocity of flow in the x direction, $\bar{v}_x = 0.1$ m/day; the dispersion coefficient $D_x = 1$ m^2/day. Three different time intervals, namely $\Delta t = 5$ days, 10 days and 20 days, are considered to examine the effect of time intervals on the numerical results. For the discretization of time, the forward difference scheme ($\alpha = 0$), the central difference scheme ($\alpha = 0.5$) and the backward difference scheme ($\alpha = 1$) are used in the calculation. Figure 9 shows the concentration through time for the solute transport problem. The detailed discussions about the numerical results and analytical solutions for this problem were reported in a previous paper [14]. According to the related discussion, the following conclusions have been obtained: (1) the finite element method can provide valuable solutions for mass/contaminant transport problems in porous media; (2) either the central difference scheme or the backward difference scheme is suitable for the upwind finite element simulation of mass/contaminant transport problems since the CPU time can be reduced due to the use of a large time increment; (3) compared to the central difference scheme or the backward difference scheme, the forward difference scheme is not accurate enough for the upwind finite element analysis except when using smaller time intervals.

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