

A Semidiscrete Model for Water and Solute Movement in Tile-Drained Soils

1. Governing Equations and Solution

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A finite element model has been developed to simulate solute transport in tile-drained soil-aquifer systems. Water flow in the unsaturated zone and to drains in the saturated zone was assumed to be at steady state. The model considers the transport of nonreactive solutes, as well as of reactive solutes whose behavior can be described by a distribution coefficient. The exact-in-time numerical solution yields explicit expressions for the concentration field at any future point in time without having to compute concentrations at intermediate times. The semidiscrete method involves the determination of an eigensystem of eigenvalues and eigenvectors of the coefficient matrix. The eigensystem may be complex (i.e., it may have imaginary components) due to asymmetry created by the convection term in the governing convection-dispersion equation. The proposed approach facilitates long-term predictions of concentrations in drainage effluents and of salt distributions in soil and groundwater. The accuracy of the model was verified by comparing model results with those based on an analytical solution for two-dimensional solute transport in groundwater.

INTRODUCTION

In arid areas, more irrigation water than is required for evapotranspiration must be added to the soil to avoid the accumulation of salts in the root zone. This excess irrigation water creates a downward flux of water and salts from the root zone to the underlying groundwater system, thus creating a potential for future groundwater salinization. A common method for avoiding groundwater salinization is to install a subsurface drainage system below the root zone to collect and remove drainage water and its dissolved constituents. The safe disposal of saline drainage water can pose serious environmental and economic challenges, as illustrated by as yet unresolved drainage water disposal problems in California, several parts of India, and many other arid and semiarid regions of the world [Suarez, 1989; Tanji, 1990; Boumans *et al.*, 1988]. Considering the potentially devastating consequences of the salinization of soil and water supplies in irrigated agriculture, the long-term effects of modern agricultural practices on groundwater quality must be evaluated. Predicting the long-term consequences of often short-term decisions regarding irrigation and drainage management in salt-affected areas is essential for the safe operation of irrigation projects and can best be achieved with the help of conceptually based simulation models.

A variety of numerical models involving finite difference or finite element techniques have been developed for simulating saturated-unsaturated water flow [Freeze, 1971; Todsen, 1973; Neuman, 1973; Tang and Skaggs, 1977; Skaggs, 1978] and solute transport [Duguid and Reeves, 1976; Pickens *et al.*, 1979; Freeze and Cherry, 1979; Yeh and Ward, 1981]. Of these the water flow models of Tang and Skaggs [1977] and Skaggs [1978] and the solute transport model of

Pickens *et al.* [1979] are directly applicable to subsurface drainage systems. Recently, Nour el-Din *et al.* [1987a, b] presented a comprehensive salinity management model for simulating salt accumulation and transport in irrigated croplands, including salt loadings of drainage effluents. While theoretically sound, the input data requirements appear prohibitive for application of the model on a routine basis. Also, simulations were made for time durations of the order of only one growing season.

Standard finite difference and finite element techniques transform the governing partial differential equations into a finite number of approximate algebraic equations. Discretization of the time and spatial derivatives leads to solution matrix equations which are solved sequentially for each time step to obtain the hydraulic head or concentration distributions at future times. Alternatively, it is also possible to use a semidiscrete approach which discretizes only the space domain but uses an exact-in-time analytical solution of the system of ordinary differential equations to advance in time. This alternative approach yields explicit expressions for the concentration or the hydraulic head at each nodal point as a function of time. The semidiscrete method requires less computer time and often yields smaller truncation errors for long-term predictions as compared to the standard numerical approach. The method entails first the calculation of an eigensystem (involving eigenvalues and eigenvectors) for the coefficient matrix resulting from the spatial discretization. Time integration subsequently leads to an exponential matrix equation. For solute transport, the eigensystem may be complex (i.e., it may have imaginary components) due to asymmetry created by the convection term in the governing solute transport equation.

Guymon [1970] applied the semidiscrete approach to the one-dimensional transport equation. By using a finite element method based on an equivalent variational approach and a special transformation, the matrix to be exponentiated was made symmetric, resulting in a real eigensystem. The approach was extended to the two-dimensional solute transport equation without mixed partial derivatives [Guymon *et al.*, 1970] and later also to a transport equation with mixed partial derivatives [Nalluswami *et al.*, 1972]. Kuiper [1973] and Sahuquillo [1983] successfully applied the semidiscrete technique to the solution of groundwater flow problems.

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head distributions $\phi_1(x, y)$ and $\phi_2(x, y)$ in the two horizontal layers composing the flow domain ABCDFA. Both analyses consider the flow of water in the arch-shaped saturated region above the drain axis to be vertically downward. The drain tube in each case was replaced by a strip sink of zero thickness and width a in the x direction. Solutions are directly applicable to the other half of the domain between the two drains because of symmetry.

The steady water table configuration, which is obtained from the computed $z(x)$ values at various points along the drain axis ($0 \leq x \leq S$), serves as a reference level for computing the volumetric water content at any point in the unsaturated zone by means of (1) and the adopted relationship for the soil water retention curve $\theta(h)$. From the hydraulic head distributions in the saturated zone the hydraulic gradients $\partial\phi/\partial x$ and $\partial\phi/\partial y$ for the homogeneous aquifer and the gradients $\partial\phi_1/\partial x$, $\partial\phi_1/\partial y$, $\partial\phi_2/\partial x$, and $\partial\phi_2/\partial y$ for the two-layered aquifer could be evaluated. The components q_x and q_y of the specific discharge q in the x and y directions, respectively, were subsequently computed for the region ($0 \leq x \leq S$, $0 \leq y \leq D$) with the help of Darcy's law [Kamra, 1989].

Final expressions for the height of the water table $z(x)$ above the drain axis and the components q_x and q_y of the specific discharge for the homogeneous and two-layered aquifers are given below.

Homogeneous aquifer.

$$z(x) = \frac{2RS}{K_s\pi(1 - R/K_s)} \left\{ \ln \left[\frac{\sin(\pi x/2S)}{\sin(\pi r/2S)} \right] + \sum_{m=1}^{\infty} \frac{1}{m} [\cos(m\pi r/S) - \cos(m\pi x/S)] \cdot [\coth(m\pi D/S) - 1] \right\} \quad (5)$$

$$q_x(x, y) = -2R \left\{ \frac{\sin(\pi x/S)/2}{\cosh(\pi y/S) - \cos(\pi x/S)} + \sum_{m=1}^{\infty} \frac{\cosh(m\pi y/S)}{\sinh(m\pi D/S)} e^{-m\pi D/S} \sin(m\pi x/S) \right\} \quad (6)$$

$$q_y(x, y) = -2R \left\{ \frac{[\sinh(\pi y/S) - \cosh(\pi y/S) + \cos(\pi x/S)]/2}{\cosh(\pi y/S) - \cos(\pi x/S)} - \sum_{m=1}^{\infty} \frac{\cos(m\pi x/S)}{\sinh(m\pi D/S)} e^{-m\pi D/S} \sinh(m\pi y/S) \right\} \quad (7)$$

where x and y are the horizontal and vertical coordinates (being positive toward the right and vertically downward, respectively), r is the radius of the drain, $2S$ is the drain spacing, K_s is the saturated hydraulic conductivity of the aquifer, R is the steady rainfall or recharge rate (equal to q in the unsaturated zone), and D is the depth of the impervious

layer below the drain axis. The origin of the coordinate system is at the center of the drain. For the strip sink (the tile drain), $q_x = 0$ and $q_y = RS/a$. In this study, a was taken equal to one fourth of the circumference of the tile and its envelope.

Layered aquifer. The geometry of the parallel tile drainage system in a layered aquifer is the same as for a homogeneous aquifer, except that the flow region now consists of two layers. The hydraulic conductivity of the upper layer is K_1 and that of the lower one is K_2 . Both layers are assumed to be homogeneous and isotropic. The upper layer extends to a distance A below the drain axis, and the lower one terminates at an impermeable layer located at a finite distance D below the drain axis (Figure 1). Results for the two-layered aquifer are

$$z(x) = \frac{2RS}{K_1\pi(1 - R/K_1)} \left\{ B_0 - \sum_{m=1}^{\infty} \frac{1}{m} \left[\cos(m\pi x/S) \coth(m\pi A/S) - B_m \frac{\cos(m\pi x/S)}{\sinh(m\pi A/S)} \right] \right\} \quad (8)$$

$$q_{x1}(x, y) = -2R \sum_{m=1}^{\infty} \left[\frac{\sin(m\pi x/S)}{\sinh(m\pi A/S)} \cdot \{ \cosh[m\pi(A - y)/S] - mB_m \cosh(m\pi y/S) \} \right] \quad (9)$$

$$q_{y1}(x, y) = -2R \sum_{m=1}^{\infty} \left[\frac{\cos(m\pi x/S)}{\sinh(m\pi A/S)} \cdot \{ \sinh[m\pi(A - y)/S] + mB_m \sinh(m\pi y/S) \} \right] \quad (10)$$

$$q_{x2}(x, y) = -2R \cdot \sum_{m=1}^{\infty} \left\{ mC_m \sin(m\pi x/S) \frac{\cosh[m\pi(D - y)/S]}{\cosh[m\pi(D - A)/S]} \right\} \quad (11)$$

$$q_{y2}(x, y) = -2R \cdot \sum_{m=1}^{\infty} \left\{ mC_m \cos(m\pi x/S) \frac{\sinh[m\pi(D - y)/S]}{\cosh[m\pi(D - A)/S]} \right\} \quad (12)$$

where

$$B_0 = \ln \left[\frac{1}{2 \sin(\pi r/2S)} \right] + \sum_{m=1}^{\infty} \left\{ \frac{1}{m} \cos(m\pi r/S) [\coth(m\pi A/S) - 1] - B_m \frac{\cos[(m\pi r)/S]}{\sinh[(m\pi A)/S]} \right\} \quad (13)$$

$$B_m = \left[m \sinh (m\pi A/S) \left\{ \frac{K_1}{K_2} \coth [m\pi(D-A)/S] + \coth (m\pi A/S) \right\} \right]^{-1} \quad (14)$$

$$C_0 = (K_2/K_1)B_0 \quad (15)$$

$$C_m = \left[m \sinh (m\pi A/S) \left\{ \frac{K_1}{K_2} + \tanh [m\pi(D-A)/S] \cdot \coth (m\pi A/S) \right\} \right]^{-1} \quad (16)$$

and where the subscripts 1 and 2 correspond to the upper and lower layers, respectively.

SOLUTE TRANSPORT IN A TILE-DRAINED SOIL-AQUIFER SYSTEM

Consider the governing equation for two-dimensional solute transport in unsaturated-saturated porous media during steady state water flow [Kamra, 1989]:

$$\begin{aligned} \theta R_f \frac{\partial c}{\partial t} = & \frac{\partial}{\partial x} \left(\theta D_{xx} \frac{\partial c}{\partial x} + \theta D_{xy} \frac{\partial c}{\partial y} \right) \\ & + \frac{\partial}{\partial y} \left(\theta D_{yx} \frac{\partial c}{\partial x} + \theta D_{yy} \frac{\partial c}{\partial y} \right) \\ & - \frac{\partial(q_x c)}{\partial x} - \frac{\partial(q_y c)}{\partial y} + \Phi(x, y, t) \end{aligned} \quad (17)$$

in which c is the dissolved solute concentration (ML^{-3}), R_f is the retardation factor, θ is the volumetric water content (equal to the porosity in the saturated zone) (L^3L^{-3}); D_{xx} , D_{xy} , D_{yx} , and D_{yy} are the components of the dispersion coefficient tensor (L^2T^{-1}), q_x and q_y are the Darcian specific discharge components (LT^{-1}), and $\Phi(x, y, t)$ is a source or sink term, being positive for sources and negative for sinks ($ML^{-3}T^{-1}$). The retardation factor R_f in (17) accounts for linear equilibrium interactions between the solute and the porous medium and is given by $R_f = 1 + \rho K_d/\theta$ where ρ is the bulk density of the medium (ML^{-3}) and K_d a solute distribution coefficient (L^3M^{-1}).

The dispersion coefficients for a two-dimensional isotropic porous medium were given by Scheidegger [1961] as

$$D_{xx} = D_L(q_x^2/q^2) + D_T(q_y^2/q^2) \quad (18)$$

$$D_{yy} = D_T(q_x^2/q^2) + D_L(q_y^2/q^2) \quad (19)$$

$$D_{xy} = D_{yx} = (D_L - D_T)(q_x q_y / q^2) \quad (20)$$

in which

$$D_L = \alpha_L q / \theta \quad (21)$$

$$D_T = \alpha_T q / \theta \quad (22)$$

where α_L and α_T are the longitudinal and transverse dispersivities (L), respectively.

Let L denote the operator on c such that (17) becomes

$$L(c) + \Phi(x, y, t) = 0 \quad (23)$$

The finite element method assumes that the concentration distribution $c(x, y, t)$ can be approximated by a trial solution of the form

$$\hat{c}(x, y, t) = \sum_{i=1}^{NN} C_i(t) N_i(x, y) \quad (24)$$

in which $C_i(t)$ is a finite set of unknown time-dependent coefficients representing concentrations at the nodes in the solution domain, $N_i(x, y)$ are the interpolation (or basis) functions, and NN is the total number of nodal points in the flow domain. Substituting (24) in (23) results in a residual equal to $L(\hat{c}) + \Phi(x, y, t)$. The Galerkin finite element method requires this residual to be orthogonal to each of the basis functions, that is,

$$\langle [L(\hat{c}) + \Phi(x, y, t)], N_i(x, y) \rangle = 0 \quad (25)$$

$$i = 1, 2, \dots, NN$$

Integrals in (25) are evaluated using Green's theorem (see Pinder and Gray [1977] or Kamra [1989] for details). The procedure results in a matrix differential equation of the following form:

$$[AM]\{dC/dt\} = [DM]\{C\} + \{F\} \quad (26)$$

where $[AM]$ is a $NN \times NN$ symmetric coefficient matrix, $[DM]$ is an $NN \times NN$ nonsymmetric matrix involving the convection and dispersion parameters, $\{F\}$ is a $NN \times 1$ force vector representing the contributions from solute sources, sinks, and boundary conditions imposed on the transport equation, and $\{C\}$ is a $NN \times 1$ vector of nodal concentrations. Typical elements of these matrices are given by

$$AM_{ij} = \sum_{e=1}^{NE} \langle N_i, \theta R_f N_j \rangle \quad (27)$$

$$\begin{aligned} DM_{ij} = & \sum_{e=1}^{NE} \left[\left\langle \frac{\partial N_i}{\partial x}, \left(-\theta D_{xx} \frac{\partial N_j}{\partial x} - \theta D_{xy} \frac{\partial N_j}{\partial y} + q_x N_j \right) \right\rangle \right. \\ & \left. + \left\langle \frac{\partial N_i}{\partial y}, \left(-\theta D_{yx} \frac{\partial N_j}{\partial x} - \theta D_{yy} \frac{\partial N_j}{\partial y} + q_y N_j \right) \right\rangle \right] \end{aligned} \quad (28)$$

$$F_i = F_{si} - F_{wi} \quad (29)$$

where

$$\begin{aligned} F_{si} = & \sum_{e=1}^{NB} \int_{B_e} \left[\left(\theta D_{xx} \frac{\partial c}{\partial x} + \theta D_{xy} \frac{\partial c}{\partial y} - q_x c \right) n_x \right. \\ & \left. + \left(\theta D_{yx} \frac{\partial c}{\partial x} + \theta D_{yy} \frac{\partial c}{\partial y} - q_y c \right) n_y \right] N_i dB \end{aligned} \quad (30)$$

$$F_{wi} = \sum_{e=1}^{NE} \langle \Phi(x, y, t), N_i(x, y) \rangle \quad (31)$$

The line integral in (30) accounts for the different boundary conditions. In the above equations, NE is the total number of elements in the flow domain, NB is the number of elements located on flow boundary B , B_e represents the sides of elements located on a boundary, and n_x and n_y are the directional cosines of the outward normal with respect to the x and y coordinate axes, respectively. Equation (31) represents salt removal by a well or other drainage facility installed in the interior of the flow domain (in our study, $F_{wi} = 0$ for all i). Finally, notice that the time variable t has been left continuous in (26), thus resulting in a space-discretized system of ordinary differential equations.

Initial and Boundary Conditions

Initial condition. The measured solute concentration distribution C^0 in the flow domain just before the start of the simulation is taken as the initial condition:

$$c(x, y, 0) = C^0(x, y) \quad t = 0 \quad (32)$$

Cauchy boundary conditions. Cauchy boundary conditions are used to implement solute inflow boundary fluxes. In our study the land surface represented by the segment GO (Figure 1) acts as a Cauchy boundary during the infiltration phase. If C_e is the concentration of the incoming fluid, and if a boundary side of length l connecting the k th and $(k + 1)$ th nodes is subjected to an inflow boundary flux with horizontal and vertical components $(n_x q_x C_e)$ and $(n_y q_y C_e)$, respectively, the line integral F_i in (29) yields [Desai, 1979; Kamra, 1989]

$$F_k = F_{k+1} = \frac{1}{2} (q_x n_x + q_y n_y) C_e \quad (33)$$

Neumann boundary conditions. Neumann boundaries are those along which the normal gradient of the concentration is prescribed. Neumann boundary conditions are imposed on flow-through boundaries with outflow from the region, and on impervious boundaries. The latter case leads to a zero value for the line integral in (30). In this study, sides BA (the bottom layer; see Figure 1), OA (the plane of symmetry), and BC and DG (streamlines) behave as impervious boundaries and the corresponding entries in F_i become zero. The tile surface CD and the land surface GO during evaporation are outflow boundaries. For these boundaries the normal gradient of the concentration becomes zero, and the line integral in (30) reduces to

$$-\sum_{e=1}^{NBO} \int_{B_e} (q_x n_x + q_y n_y) N_i N_j C_j dB = [G]\{C\} \quad (34)$$

where $[G]$ is a $NN \times NN$ matrix to be added to coefficient matrix $[DM]$ in (26), and NBO is the number of boundary elements along the outflow boundaries. The corresponding entries of F_i in (29) are again zero.

Dirichlet boundary conditions. Dirichlet boundary nodes are those for which the concentration is prescribed. An identity equation is generated for each node involved and (29) does not need to be evaluated. Detailed descriptions on how to implement this type of boundary condition can be found elsewhere [e.g., Yeh and Ward, 1981]. No Dirichlet boundaries were present for the flow domain of the tile-drained soil-aquifer system shown in Figure 1. However,

Dirichlet boundary conditions were implemented in an example problem to compare model results with those obtained with an analytical solution for two-dimensional solute transport in groundwater.

SOLUTION OF THE VECTOR-MATRIX DIFFERENTIAL EQUATION

For time-variant (transient) boundary conditions the solution of the inhomogeneous vector-matrix differential equation (26) is given by Bellman [1970] as

$$\{C\} = e^{[H]t} \{C^0\} + \int_0^t e^{[H](t-s)} [AM]^{-1} \{F(s)\} ds \quad (35)$$

where $[H]$ is a $NN \times NN$ matrix equal to $[AM]^{-1}[DM]$. The coefficient matrix $[DM]$ is asymmetric and contains the effects of dispersion, convective transport, and outflow through the boundaries, whereas $\{C^0\}$ represents the nodal values of initial concentration. The term $e^{[H]t}$ is referred to as the matrix exponential and is a matrix of the same dimensions as $[H]$. The eigenvalue-eigenvector method of Euler is generally used to compute the matrix exponential. In order to compute the matrix exponential, let us first consider the homogeneous vector-matrix differential equation

$$\{dC/dt\} = [H]\{C\} \quad (36)$$

All eigenvalues τ_k and associated linearly independent eigenvectors $\{Z^k\}$ of the matrix $[H]$ must be first computed. Because of its asymmetry, the matrix $[H]$ has real as well as complex eigenvalues. Let τ_k and $\{Z^k\}$ be the N real eigenvalues and associated linearly independent eigenvectors of the matrix. Then the product

$$\{C_i(t)\} = \{Z^k\} e^{(\tau_k t)} \quad i = 1, 2, \dots, N \quad (37)$$

represents N linearly independent real vector solutions of the homogeneous differential equation (36).

Let $\tau_j = a_j + ib_j$ be a complex eigenvalue of $[H]$ with eigenvector $\{Z^j\} = \{Z^{1j}\} + i\{Z^{2j}\}$. The complex solution corresponding to this complex eigensystem gives rise to the following two linearly independent real solutions, $\{C_{1j}(t)\}$ and $\{C_{2j}(t)\}$, of (36) [Braun, 1978]:

$$\{C_{1j}(t)\} = \{\cos b_j t \{Z^{1j}\} - \sin b_j t \{Z^{2j}\}\} e^{(a_j t)} \quad (38)$$

$$\{C_{2j}(t)\} = \{\sin b_j t \{Z^{1j}\} + \cos b_j t \{Z^{2j}\}\} e^{(a_j t)} \quad (39)$$

The same real solutions are also obtained from the corresponding complex conjugate eigensystem. This results in NN linearly independent real solutions of (36). Using the EISPACK computer package [Smith et al., 1976], the real and imaginary parts of all eigenvalues of the real general matrix $[H]$ may be evaluated and the output of eigenvectors stored in the matrix $[Z]$. If the i th eigenvalue τ_i is real, the i th column of matrix $[Z]$ contains its eigenvector $\{Z^i\}$. If the j th eigenvalue τ_j is complex with positive imaginary part, the j th and $(j + 1)$ th columns of $[Z]$ contain, respectively, the real and imaginary parts of the associated eigenvector $\{Z^j\}$.

Let $[C(t)]$ be a square matrix whose columns are linearly independent solutions $\{C_1(t)\}$, $\{C_2(t)\}$, $\dots$, $\{C_{NN}(t)\}$ of (36). Such a matrix is called the fundamental matrix solution [Braun, 1978]. The product of any fundamental matrix

solution of (36) with its inverse at $t = 0$ yields the matrix exponential $e^{[H]t}$. Hence

$$e^{[H]t} = [C(t)][C(0)]^{-1} \quad (40)$$

Substituting $t = 0$ in (37), (38) and (39) gives

$$[C(0)] = [Z] \quad (41)$$

If the i th and j th eigenvalues are real and complex, respectively, then the structure of $[Z]$ and (37)–(39) enable one to write the fundamental matrix $[C(t)]$ as the product of $[Z]$ and a tridiagonal matrix solution $[QD]$. The elements of $[QD]$ are given by

$$QD_{ii} = e^{\tau_i t}$$

$$QD_{jj} = QD_{j+1,j+1} = e^{a_j t} \cos b_j t \quad (42)$$

$$QD_{j,j+1} = e^{a_j t} \sin b_j t$$

$$QD_{j+1,j} = -e^{a_j t} \sin b_j t$$

$$QD_{ij} = 0 \quad \text{all other } i, j$$

In these equations, i can assume any integer value from 1 to NN and j from 1 to $(NN - 1)$. Thus $[QD]$ is of size $(NN \times NN)$. In view of the preceding discussion and (40) and (41), one finds

$$e^{[H]t} = [Z][QD][Z]^{-1} \quad (43)$$

Finally, the general solution (35) of the inhomogeneous matrix-vector equation (26) for time-invariant boundary conditions becomes

$$\{C\} = e^{[H]t} \{ \{C^0\} + [DM]^{-1}\{F\} - \{[DM]^{-1}\{F\} \} \} \quad (44)$$

The matrix exponential evaluated from (43) at any t is a square matrix with real numbers. Its substitution in (44) results in a column vector which represents the solute concentration at all finite element nodes.

COMPARISON OF NUMERICAL AND ANALYTICAL SOLUTIONS

In this section we give examples comparing the accuracy of the numerical solution with results based on analytical solutions derived by *Bruch and Street* [1967] and *Cleary and Ungs* [1978] for solute transport in a two-dimensional system. The saturated flow domain consists of a rectangular 240×60 m homogeneous isotropic medium with unidirectional steady flow along the x axis. The initially solute-free medium is subjected at time $t = 0$ to a strip type Dirichlet boundary condition (of concentration $C_e = 1000$ mg/L) along the inflow boundary ($x = 0, 0 \leq y \leq 15$ m). The mathematical problem was formulated by *Bruch and Street* [1967] as follows:

$$\frac{\partial c}{\partial t} = D_{xx} \frac{\partial^2 c}{\partial x^2} + D_{yy} \frac{\partial^2 c}{\partial y^2} - v \frac{\partial c}{\partial x} \quad (45a)$$

$$0 \leq y \leq 60; x > 0; t > 0$$

$$\begin{aligned} c(0, y, t) &= 1000 & 0 \leq y \leq 15 \\ c(0, y, t) &= 0 & 15 < y \leq 60 \end{aligned} \quad (45b)$$

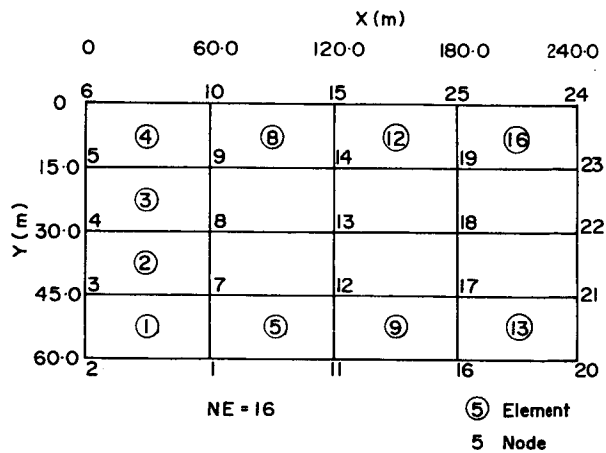


Fig. 2. Finite element discretization of the flow domain into 16 elements for comparison with an analytical solution.

$$\frac{\partial c}{\partial y}(x, 0, t) = 0 \quad t > 0 \quad (45c)$$

$$\frac{\partial c}{\partial y}(x, 60, t) = 0 \quad t > 0 \quad (45d)$$

$$|C(\infty, y, t)| \quad \text{is bounded} \quad (45e)$$

$$c(x, y, 0) = 0 \quad x > 0; 0 \leq y < 60 \quad (45f)$$

where $v = q_x/\theta$.

The flow region was divided into 16, 32, and 64 rectangular elements. The finite element discretization of the flow domain into 16 elements is shown in Figure 2. For $NE = 32$ and 64, the grid system was doubled and quadrupled, respectively. Numerical solutions using linear basis functions were obtained for 0.25, 0.5, 1.0, 2.0, 3.0, and 4.0 years with assumed constant values of the dispersion coefficients D_{xx} and D_{yy} and the seepage velocity v . We point out that the numerical solution is bounded by the rectangular region shown in Figure 2, whereas the analytical solution holds for a semiinfinite system subject to boundary condition (45e) which requires that the solution remain finite as $x \rightarrow \infty$. The numerical solution for this example was obtained by invoking a first-type (Dirichlet) boundary condition of zero concentration along the outflow boundary at $x = 240$ m.

The L_2 norm was taken as a measure of the error between the analytical and numerical solutions. The L_2 norm of a function $f(x, y)$ is defined as [Prenter, 1975]

$$\|f\|_2 = \frac{1}{[(Y_2 - Y_1)(X_2 - X_1)]^{1/2}} \cdot \left\{ \int_{X_1}^{X_2} \int_{Y_1}^{Y_2} [f(x, y)]^2 dy dx \right\}^{1/2} \quad (46)$$

where for our example $f(x, y)$ represents the difference in concentration computed with the analytical and numerical solutions, and where X_1, X_2 and Y_1, Y_2 are the limits of the flow domain in the x and y directions, respectively. Equation (46) was numerically integrated by using Simpson's quadrature formula [Demidovich and Maron, 1976], which is appli-

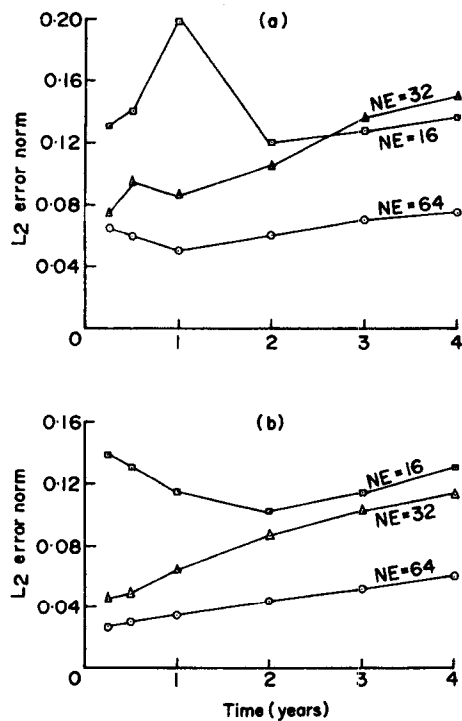


Fig. 3. Error in the numerical solution for different finite element discretizations assuming (a) $D_{xx} = 0.5 \text{ m}^2/\text{d}$ and (b) $D_{xx} = 2.0 \text{ m}^2/\text{d}$ ($D_{yy} = 0.1 D_{xx}$ and $v = 0.1 \text{ m/d}$).

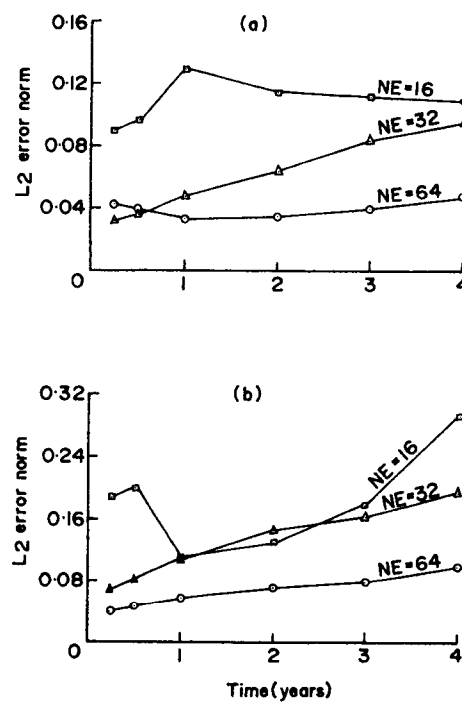


Fig. 4. Error in the numerical solution for different finite element discretizations assuming (a) $v = 0.05 \text{ m/d}$ and (b) $v = 0.2 \text{ m/d}$ ($D_{xx} = 1 \text{ m}^2/\text{d}$, $D_{yy} = 0.1 \text{ m}^2/\text{d}$).

cable to equispaced nodes in the x and y directions of the solution domain.

The L_2 error norm as a function of time for the three finite element discretizations ($NE = 16, 32$, and 64) is plotted in Figures 3 and 4 for several combinations of D_{xx} , D_{yy} , and v . The results show that as the number of elements in the domain increases, the difference between analytical and numerical results decreases. Some oscillations are apparent for the coarser grid ($NE = 16$) at relatively early times. All discretizations show an increase in the error when time progresses. This is a consequence of the fact that the numerical and analytical solutions implement different exist boundary conditions. For large times the finite domain ($0 \leq x < 240 \text{ m}$) can no longer accurately approximate the semi-infinite domain ($0 \leq x \leq \infty$).

An important feature evident from Figures 3 and 4 is the relative significance of the longitudinal dispersion coefficient D_{xx} and the seepage velocity v in the numerical simulation. The numerical error apparently decreases with increasing value of D_{xx} and decreasing v . Sensitivity analyses of various model parameters (Figure 5) using the finer finite element mesh ($NE = 64$) also showed that the error in the numerical solution is relatively more sensitive to variations in the seepage velocity than to variations in the longitudinal and transverse dispersion coefficients. This sensitivity is attributed to the fact that when linear basis functions are used in the finite element approximation, the velocity field is constant inside each element but discontinuous across the boundary from one element to another. Discontinuities in the velocity field often create problems for an accurate representation of the convection term in the solute transport equation.

Finally, Figure 6 compares numerically calculated solu-

tions with results based on an analytical solution derived by Cleary and Ungs [1978] and discussed further by Javandel *et al.* [1984]. The solution applies to the same problem as above (equations (45a)–(45f)), except that the lateral dimension y is allowed to go to infinity, that is, boundary conditions (45c and 45d) are replaced by the condition $\partial c(x, \pm\infty, t)/\partial y = 0$. The numerical solution was obtained for an x - y flow domain of size $360 \times 220 \text{ m}$ assuming a Dirichlet boundary condition of unit concentration over the strip $\{x = 0, |y| < 50 \text{ m}\}$.

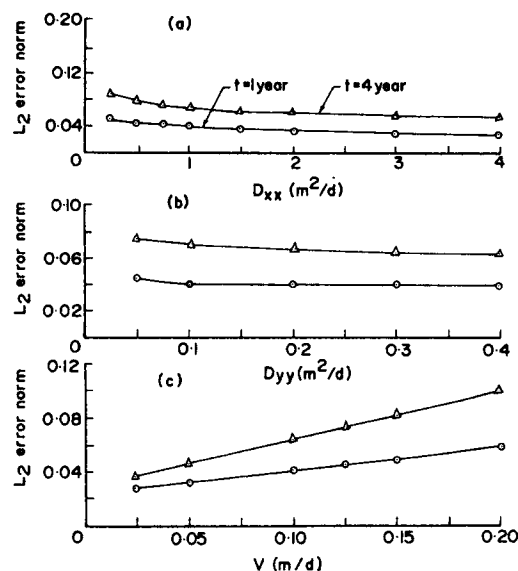


Fig. 5. Error in the numerical solution ($NE = 64$) as affected by (a) D_{xx} ($D_{yy} = 0.1 D_{xx}$, $v = 0.1 \text{ m/d}$), (b) D_{yy} ($D_{xx} = 1 \text{ m}^2/\text{d}$, $v = 0.1 \text{ m/d}$), and (c) v ($D_{xx} = 1 \text{ m}^2/\text{d}$, $D_{yy} = 0.1 \text{ m}^2/\text{d}$).

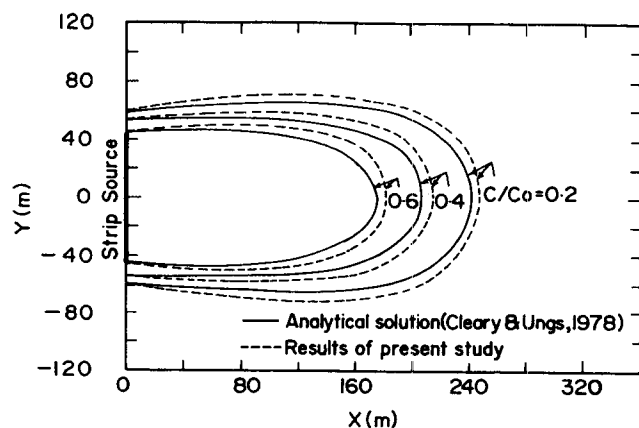


Fig. 6. Comparison of numerical results with the analytical solution of Cleary and Ungs [1978] assuming $v = 0.5$ m/d, $D_{xx} = 5.0$ m²/d, $D_{yy} = 0.5$ m²/d, and $t = 365$ days.

Figure 6 shows relative concentrations (C/C_0) after $t = 365$ days, assuming $v = 0.5$ m/d, $D_{xx} = 5.0$ m²/d, $D_{yy} = 0.5$ m²/d, and $R_f = 1$, and using a discretization ($NE = 64$) which is similar to that shown in Figure 2, except for the slightly larger flow domain. The numerical and analytical solutions results show close agreement, especially in view of the relatively coarse finite element grid system used for the numerical calculations.

SUMMARY AND CONCLUSIONS

A semidiscrete model for solute transport in a tile drained soil-aquifer system has been developed. Water flow in the unsaturated and saturated domains of the flow system was assumed to be at steady state. The water flow velocity field in the unsaturated zone was assumed to be vertically downward and in magnitude equal to the net steady downward flux of water. Water content distributions in the unsaturated domain were obtained by numerically integrating Darcy's law and incorporating appropriate models for the unsaturated hydraulic functions. The components of the Darcian flux in the saturated domain were computed using analyses by Kirkham [1958] and Toksöz and Kirkham [1971] for water flow to drains in homogeneous and two-layered aquifers, respectively. The semi-discrete solution of the transport equation requires only a discretization of the spatial derivatives (in this study using linear finite elements), whereas exact-in-time solutions for the concentration field at any future time were obtained without having to march through the intermediate time intervals. The proposed model compared favorably with results based on analytical solutions for two-dimensional solute transport in groundwater. A preliminary analysis of various model parameters showed that the error in the numerical solution was relatively sensitive to seepage velocity but fairly insensitive to variations in the longitudinal and transverse dispersion coefficients.

Results of a field validation experiment of the composite unsaturated-saturated solute transport model for tile-drained soils are presented in part 2 [Kamra et al., this issue] of this study.

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