WATER RESOURCES RESEARCH, VOL. 27, NO. 9, PAGES 2439–2447, SEPTEMBER 1991

A Semidiscrete Model for Water and Solute Movement in Tile-Drained Soils
1. Governing Equations and Solution

S. K. Kamra,[1] Sita Ram Singh,[2,3] K. V. G. K. Rao,[1] and M. Th. van Genuchten[4]

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.* [1987*a*, *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.

[1]Central Soil Salinity Research Institute, Karnal, India.
[2]Department of Soil and Water Engineering, Punjab Agricultural University, Ludhiana, India.
[3]Now at Water Technology Centre for Eastern Region, Nayapalli, Bhubaneswar, India.
[4]U.S. Salinity Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Riverside, California.

Paper number 91WR01242.
0043-1397/91/91WR-01242$05.00

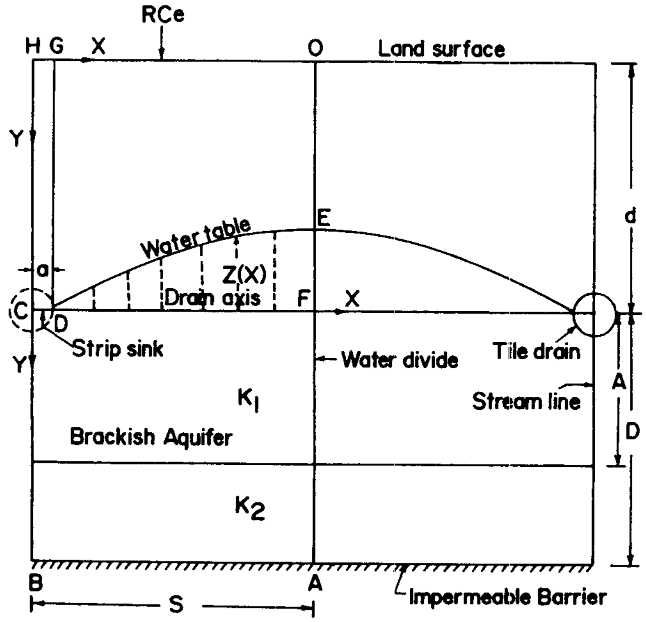

Fig. 1. Schematic of the flow domain for solute transport in a two-layered tile-drained soil-aquifer system. For a homogeneous aquifer, $K_1 = K_2$ or $A = D$.

Hwang et al. [1984] subsequently used the method for a two-dimensional solute transport problem with transient boundary conditions and variable source loads. They solved the eigensystem using complex arithmetic, which made it possible to decouple concentrations at different spatial grid nodes and to solve for these concentrations separately. More recently, *Umari and Gorelick* [1986] presented an algorithm that uses real arithmetic to convert a complex eigensystem into an equivalent real eigensystem.

To our knowledge, the semidiscrete method has not yet been applied to transport in the unsaturated zone. In this paper we will use the approach with real arithmetic to obtain an exact-in-time numerical solution of a two-dimensional finite element model for solute transport in a tile-drained soil-aquifer system. The model considers steady state water flow in the unsaturated and saturated zones and includes the effects of convective transport, dispersion, and linear equilibrium reactions between the solute and the porous medium (characterized by a distribution coefficient) on solute transport. This part 1 presents the development of the model, its numerical solution, and comparisons with a two-dimensional analytical solution for solute transport in a groundwater aquifer. Part 2 [*Kamra et al.*, this issue] presents a field validation of the composite unsaturated-saturated solute transport model for a tile-drained soil, as well as a detailed sensitivity analysis of several model parameters.

WATER FLOW IN A TILE-DRAINED SOIL-AQUIFER SYSTEM

Figure 1 schematically shows the movement of water and dissolved solutes to parallel drains in a tile-drained soil-aquifer system. The horizontal spatial coordinate x is taken to be positive toward the right, whereas y is positive downward. Infiltrating rain and irrigation water is assumed to flow vertically downward through the unsaturated soil profile before reaching the arch-shaped steady state groundwater table, DE. After reaching the water table, water and dissolved salts move two-dimensionally toward the parallel drains.

Wierenga [1977] and *Beese and Wierenga* [1980] have shown that relatively simple transport models based on steady state water flow can produce solute concentration distributions that are comparable to those obtained with transient water flow models, but with considerably less input data than the transient models. Steady state formulations can be particularly useful for making long-term predictions by ignoring the often highly dynamic but short-term oscillations in water content and solute concentration near the soil surface. Since the objective of this study was to make long-term predictions of salt transport in a tile-drained soil-aquifer system, and since the mathematical description of the problem could be simplified dramatically, we decided to implement steady state water flow models for both the unsaturated and saturated zones.

Unsaturated Zone

The steady state pressure head distribution during vertical water flow to or from a water table can be derived from Darcy's law as [e.g., *Raats and Gardner*, 1974]

$$z(h) = \int_0^h \frac{-1}{1 + q/K(h)} \, dh \tag{1}$$

where K is the unsaturated hydraulic conductivity (LT^{-1}) as a function of the pressure head $h(L)$, z is distance (L) above the water table (positive upward), and q is the fluid flux or specific discharge (LT^{-1}). If the water retention $\theta(h)$ and hydraulic conductivity $K(h)$ curves of the soil are available, (1) may be integrated numerically to determine the water content θ at any point z above the water table in a soil profile during steady upward ($+q$) or downward ($-q$) water flow. The functional forms of the unsaturated hydraulic properties used in this study were those of *van Genuchten* [1978]:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^m} \qquad (\theta_r \le \theta \le \theta_s) \tag{2}$$

$$K(\theta) = K_s \sqrt{S_e}[1 - (1 - S_e^{1/m})^m]^2 \tag{3}$$

$$S_e = (\theta - \theta_r)/(\theta_s - \theta_r) \tag{4}$$

where θ_r and θ_s are the residual and saturated water contents, respectively, α and n are empirical shape parameters to be estimated by fitting (2) to experimental retention data, $m = 1 - 1/n$, K_s is the saturated hydraulic conductivity, and S_e is effective fluid saturation ($0 \le S_e \le 1$).

Saturated Zone

The mathematical analyses of *Kirkham* [1958] and *Toksöz and Kirkham* [1971] were used to describe the steady two-dimensional flow of water to drains in homogeneous and two-layered aquifers, respectively. For homogeneous aquifers, approximate analytical solutions of the Laplace equation give the height z of the water table above the drain axis, as well as the hydraulic head ϕ distribution in the flow domain ABCDFA below the drain axis (Figure 1). Similarly, analytical solutions for the two-layered aquifer give the height of water table z above the drain axis and the hydraulic 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.

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

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

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

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

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

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

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

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

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

where

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

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

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

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

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]:

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

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,

$$\langle [L(\hat{c}) + \Phi(x, y, t)], N_i(x, y) \rangle = 0 \qquad i = 1, 2, \ldots, NN \quad (25)$$

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

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

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

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

where

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

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

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:

$$c(x, y, 0) = C^0(x, y) \qquad t = 0 \tag{32}$$

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 kth 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]

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

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

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

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

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

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

$$\{dC/dt\} = [H]\{C\} \tag{36}$$

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

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

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]:

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

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

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 ith eigenvalue τ_i is real, the ith column of matrix $[Z]$ contains its eigenvector $\{Z^i\}$. If the jth eigenvalue τ_j is complex with positive imaginary part, the jth 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 $\{C_1(t)\}, \{C_2(t)\}, \cdots, \{C_{NN}(t)\}$ 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

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

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

$$[C(0)] = [Z] \tag{41}$$

If the ith and jth 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

$$\begin{aligned} QD_{ii} &= e^{\tau_i t} \\ QD_{jj} &= QD_{j+1,j+1} = e^{a_j t} \cos b_j t \\ QD_{j,j+1} &= e^{a_j t} \sin b_j t \\ QD_{j+1,j} &= -e^{a_j t} \sin b_j t \\ QD_{ij} &= 0 \qquad \text{all other } i, j \end{aligned} \tag{42}$$

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

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

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

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

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 ($x = 0$, $0 \le y \le 15$ m). The mathematical problem was formulated by *Bruch and Street* [1967] as follows:

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

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

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

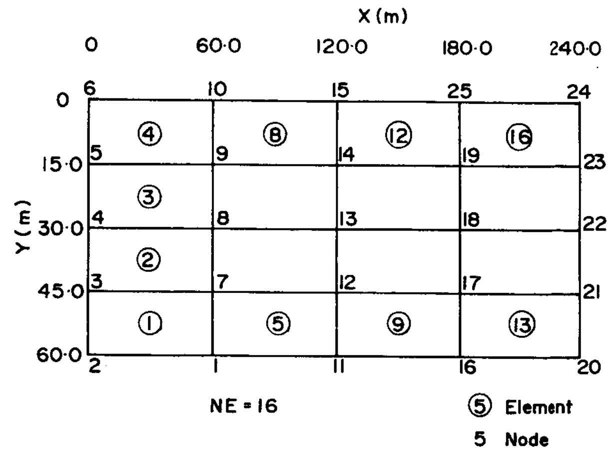

Fig. 2. Finite element discretization of the flow domain into 16 elements for comparison with an analytical solution.

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

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

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

$$c(x, y, 0) = 0 \qquad x > 0;\ 0 \le y < 60 \tag{45f}$$

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 $x \to \infty$. 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 $L2$ norm was taken as a measure of the error between the analytical and numerical solutions. The $L2$ norm of a function $f(x, y)$ is defined as [*Prenter*, 1975]

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

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-

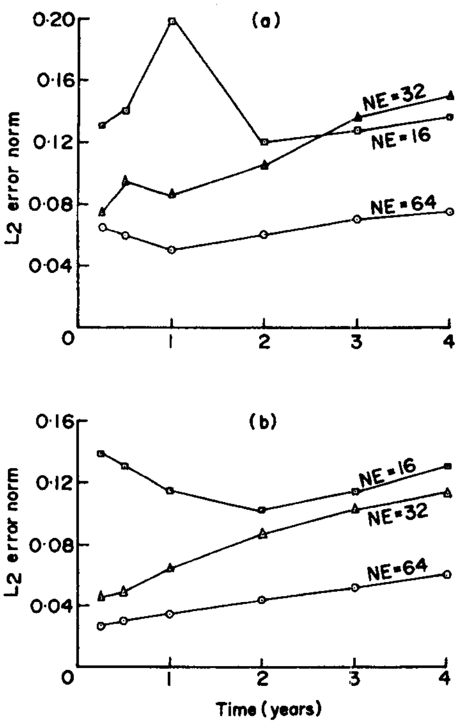

Fig. 3. Error in the numerical solution for different finite element discretizations assuming (*a*) $D_{xx} = 0.5$ m^2/d and (*b*) $D_{xx} = 2.0$ m^2/d ($D_{yy} = 0.1\ D_{xx}$ and $v = 0.1$ m/d).

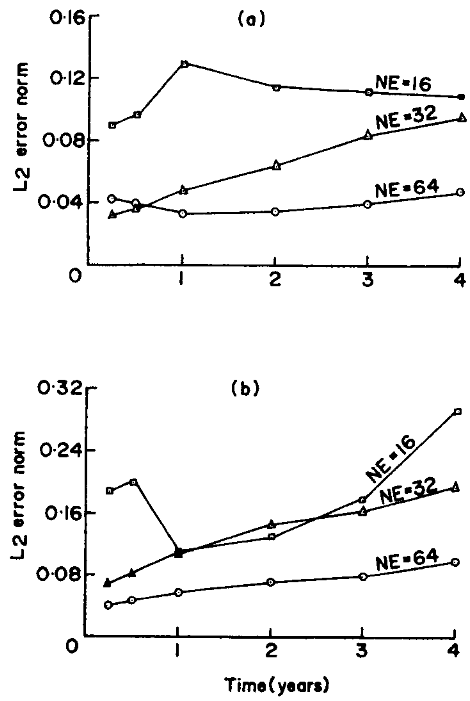

Fig. 4. Error in the numerical solution for different finite element discretizations assuming (*a*) $v = 0.05$ m/d and (*b*) $v = 0.2$ m/d ($D_{xx} = 1$ m^2/d, $D_{yy} = 0.1$ m^2/d).

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

The $L2$ 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 ($0 \leq x < 240$ 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 solutions 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 (45*a*)–(45*f*)), except that the lateral dimension y is allowed to go to infinity, that is, boundary conditions (45*c* and 45*d*) 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 × 220 m assuming a Dirichlet boundary condition of unit concentration over the strip $\{x = 0, |y| < 50 \text{ m}\}$.

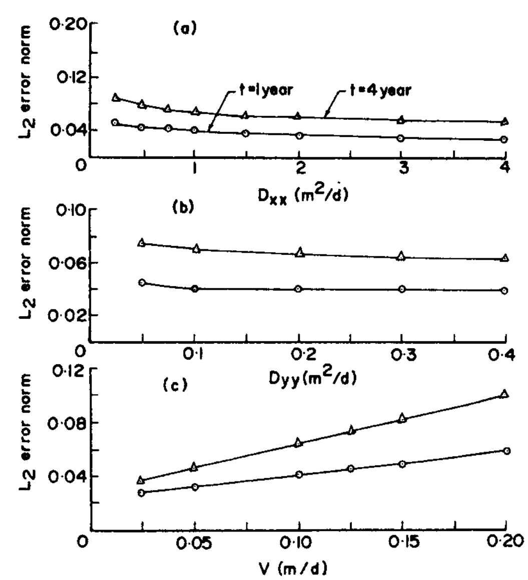

Fig. 5. Error in the numerical solution (NE = 64) as affected by (*a*) D_{xx} ($D_{yy} = 0.1\ D_{xx}$, $v = 0.1$ m/d), (*b*) D_{yy} ($D_{xx} = 1$ m^2/d, $v = 0.1$ m/d), and (*c*) v ($D_{xx} = 1$ m^2/d, $D_{yy} = 0.1$ m^2/d).

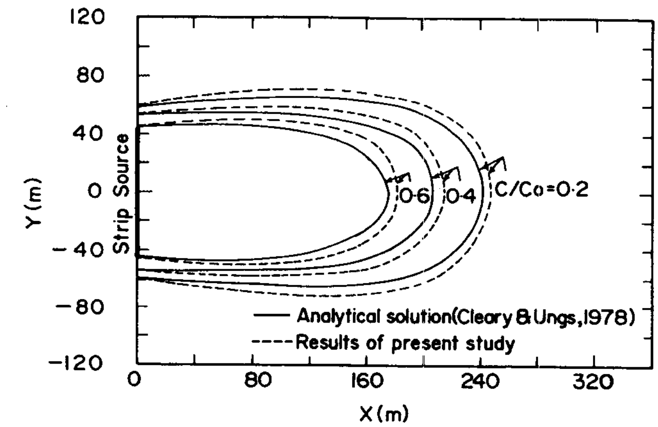

Fig. 6. Comparison of numerical results with the analytical solution of *Cleary and Ungs* [1978] assuming v = 0.5 m/d, D_{xx} = 5.0 m^2/d, D_{yy} = 0.5 m^2/d, and t = 365 days.

Figure 6 shows relative concentrations (C/C^0) after t = 365 days, assuming v = 0.5 m/d, D_{xx} = 5.0 m^2/d, D_{yy} = 0.5 m^2/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.

Acknowledgments. This research was conducted at the Department of Soil and Water Engineering, Punjab Agricultural University, Ludhiana, India, with financial support of PL 480 grant FG-IN-609, IN-ARS-200, through a collaborative project between the Indian Council of Agricultural Research and the United States Department of Agriculture. The authors are thankful for the assistance. The authors are also thankful to I. P. Abrol, Deputy Director General of the Indian Council of Agricultural Research, New Delhi, India, and N. T. Singh, Director of the Central Soil Salinity Research Institute, Karnal, India, for their constant encouragement and support of this study.

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S. K. Kamra and K. V. G. K. Rao, Central Soil Salinity Research Institute, Karnal 132001, India.

S. R. Singh, Water Technology Centre for Eastern Region, N-2/94, Nayapalli, Bhubaneswar, 751012, India.

M. Th. van Genuchten, U.S. Salinity Laboratory, Agricultural Research Service, U.S Department of Agriculture, 4500 Glenwood Drive, Riverside, CA 92501.

(Received January 5, 1990;
revised April 24, 1991;
accepted May 1, 1991.)