A quasi three-dimensional approach for simulating water flow and solute transport in the vadose zone and phreatic aquifer

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Movement of solutes through the vadose zone and groundwater is of increasing concern because of environmental problems. Many theoretical models describing flow, solute transport and physico-chemical processes in soil, have been developed in recent years. Fully 3-D saturated-unsaturated flow and transport models (e.g., Panday *et al.*, 1993) give the full simulation extent of the problem. However, they require considerable computation time and thus their use for management problems is usually restricted. To circumvent these difficulties, the dimension of the equations is reduced to quasi three-dimensional case. Quasi three-dimensional models of flow for heterogeneous multiaquifer systems were developed by Bredehoeft and Pinder (1970), Herrera and Yates (1977), Neuman *et al.* (1982), etc. Pikul *et al.* (1974) coupled the one-dimensional Richards equation in vertical direction for the unsaturated zone with the one-dimensional Boussinesq equation in the horizontal direction for the phreatic aquifer. In order to link the rate of drainage out of the saturated zone to the change of height of the water table, Pikul *et al.* (1974) had to introduce the concept of the dynamic storage coefficient. As was noted by Vachaud and Vauclin (1975), such an approach is physically incorrect, and the use of a linked system of equations resting on the concept of storage coefficient may not yield simplification. Another recent development is given by Kool *et al.* (1994) which is a three-dimensional composite approach for subsurface flow and transport. However, this model considers steady state flow conditions and ignores the saturation variation in the vadose zone and in the capillary fringe above the phreatic surface.

In this paper we present a quasi three-dimensional model of flow based on coupling of the one-dimensional Richards equation in the unsaturated zone and the plane two-dimensional flow equation in the saturated zone. This is similar to the model developed by Pikul *et al.* (1974), but does not require the introduction of the storage coefficient. A three-dimensional transport equation is used to simulate the movement of solutes.

Governing equations

The motion of water in the unsaturated-saturated zone of soil can be described by the 3-D Richards equations. Let us introduce the following simplified assumptions to reduce the problem to a quasi 3-D case: 1) The flow in the unsaturated zone is in the vertical direction only; 2) Water is practically incompressible and soil matrix is rigid; 3) The Dupuit assumption of the essentially horizontal flow is valid in the saturated zone.

The equation that describes the phreatic surface reads

$$h(x,y,t) - z = 0 \tag{1}$$

where h is the elevation of the phreatic surface, x and y are the planar coordinates, z is the vertical coordinate (positive upward), and t is time.
In the unsaturated zone the model is presented by series of vertical 1-D Richards equations evaluated at points throughout the areal plane, i.e.

$$c\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial \psi}{\partial z} + K_{zz}\right) \tag{2}$$

where c is the water capacity, ψ is the matric pressure head, and K_{zz} is the vertical component of **K**, the hydraulic conductivity tensor.

The 2-D averaged flow equation for the saturated zone can be obtained by integrating the 3-D flow equation over the vertical direction (Bear and Verruijt, 1987)

$$\int_{\eta(x,y)}^{h(x,y,t)} (\nabla \cdot \mathbf{q} + I)dz = 0 \tag{3}$$

where η is the elevation of the bottom of the aquifer, $\mathbf{q}$ is the water flux vector, and I is an internal sink-source term. By employing Leibnitz rule we write (3) in the form

$$\nabla' \cdot (h-\eta)\tilde{\mathbf{q}}' + \mathbf{q}|_h \cdot \nabla(z-h) - \mathbf{q}|_\eta \cdot \nabla(z-\eta) + \tilde{I} = 0 \tag{4}$$

where

$$\tilde{\mathbf{q}}' = \frac{1}{h-\eta}\int_\eta^h \mathbf{q}'dz \quad \text{and} \quad \tilde{I} = \int_\eta^h I dz$$

in which $(\ )'$ denotes a property defined only in the xy-plane. The $\mathbf{q}|_h$ and $\mathbf{q}|_\eta$ denote the water flux vectors at the phreatic surface and at the aquifer bottom, respectively. The first term in (4) can be presented as (Bear and Verruijt, 1987)

$$\nabla' \cdot (h-\eta)\tilde{\mathbf{q}}' = -\nabla' \cdot \left[\mathbf{K}'(h-\eta)\nabla' h\right] \tag{5.1}$$

Taking into account that the normal fluxes at both sides of the phreatic surface (1) are equal, we write

$$-K_{zz}\left(\frac{\partial \psi}{\partial z} + 1\right)\Bigg|_{z=h^+} = \mathbf{q}|_{h^-} \cdot \nabla(z-h) \tag{5.2}$$

The last term in (4) we present in the form

$$\tilde{I} = -\sum_l P_w(x_l, y_l, t)\delta(x - x_l, y - y_l) \tag{5.3}$$

where P_w is the rate of the flux source located at a point (x_l, y_l) and δ is the Dirac delta function. The water flux at the bottom of the aquifer, $\mathbf{q}|_\eta$, can be either prescribed, or calculated using known head values at the top of the underlying confined aquifer (Bear and Verruijt, 1987). In view of (5), we rewrite (4) in the form

$$-K_{zz}\left(\frac{\partial \psi}{\partial z} + 1\right)\Bigg|_{z=h} = \nabla' \cdot \left[\mathbf{K}'(h-\eta)\nabla' h\right] + \mathbf{q}|_\eta \cdot \nabla(z-\eta) + \sum_l P_w(x_l, y_l, t)\delta(x - x_l, y - y_l) \tag{6}$$

The main difference of (6) from the Boussinesq equation for a leaky-phreatic aquifer, is that it does not contain a term with specific yield and a source term for natural replenishment. However it explicitly models a vertical flux at the phreatic surface. We note, that (6) refers to a nonsteady state, since ψ, the matric pressure head, is a function of time. The position of the moving phreatic surface is found by

$$\psi(x,y,z,t)\big|_{z=h}=0 \tag{7}$$

As a result, we decompose the 3-D flow problem to a 1-D vertical direction presented by (2) for the unsaturated zone, and to 2-D horizontal plane for the saturated zone presented by (6).

The transport of contaminant species is described by the advection-dispersion equation

$$\frac{\partial(\theta C_i)}{\partial t}+\rho_s(1-n)\frac{\partial F_i}{\partial t}=\nabla\cdot(\mathbf{D}_i\theta\nabla C_i-\mathbf{q}C_i)-\sum_m \mu_{im}+ \\ \sum_l\left[\tilde{C}_{wi}H(P_w)-C_iH(-P_w)\right]P_w(x_l,y_l,t)\delta(x-x_l,y-y_l,z-z_l) \tag{8}$$

where C_i and F_i are the concentration of the ith component in the liquid and on the adsorbed phases, respectively, ρ_s is the solid phase density, n is soil porosity, θ is the soil water content, $\mathbf{D}_i$ is the apparent dispersion tensor, μ_{im} is the sink-source term associated with the mth transformation reaction, e.g. decay, mineralization, immobilization etc., $\tilde{C}_{wi}$ is the concentration of the ith component in the injected water, and H is the Heaviside step function.

Numerical algorithm

To solve (2) and (6) to (8), we had implemented a finite differences grid in a three-dimensional space. We solved (2) along the vertical coordinate z at every J nodal point situated at (x_j, y_j) on the horizontal plane. Equation (6) is considered as the lower boundary condition for (2). The RHS of (6) is approximated by finite differences on a horizontal part of the 3-D grid.

The algorithm for solving (2) and (6) to (8) is described as follows:
1) Use the prescribed distribution of capillary pressure head $\psi(z_i,t^k)$ at the previous time level t^k and at each node J situated at (x_j, y_j) to find the height Z_J at which $\psi(Z_J,t^k)=0$. Knowing this height, constitutes the phreatic surface h_J at every node J (i.e., $h_J(x_j,y_j,t^k)=Z_J$).
2) Calculate the RHS of (6) using h_J. This will constitute the flux at the phreatic surface, which is the lower boundary for the solution of (2). This boundary condition can also be projected from the phreatic surface to the bottom of the aquifer, since the vertical component of Darcy's velocity is constant in the saturated zone when considering the 1-D Richards equation.
3) Given also the boundary condition at the soil surface, solve for $\psi(z_i,t^{k+1})$ using (2).
4) Evaluate the vertical component of Darcy's velocity in the unsaturated zone, and the vertical and horizontal components of the Darcy's velocity in the saturated zone, at the t^{k+1} time level.
5) Solve the three-dimensional transport problem (3), at the t^{k+1} time level.
Since (2) and (6) are nonlinear, an iterative procedure is required.

The vertical component of the water flux in the saturated zone can be approximately found by integrating the equation of continuity from the bottom to the top of the aquifer (Polubarinova-Kochina, 1977; Strak, 1984), i.e.,

$$q_z=\int(\nabla'\cdot\mathbf{q}'+I)dz+A \tag{9}$$

where A is a constant which can be found using the value of the water flux at the bottom of the aquifer.

To introduce the soil water retention curve and the unsaturated hydraulic conductivity we refer to the van Genuchten's relations (van Genuchten, 1980), namely

$$S_e = \left[1 + (-\alpha\psi)^{n_V}\right]^m \quad (9)$$

$$K = K_s S_e^{0.5}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \quad (10)$$

where $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$, θ_r is irreducible water content, θ_s is the water content at saturation, K_s is the saturated hydraulic conductivity of the soil, α and n_V are model parameters, and m=1-1/ n_V.

Examples

To test the ability of the model to simulate flow and transport in the unsaturated zone and in the phreatic aquifer, we compared the model's quasi 2-D predictions with those obtained by a fully 2-D unsaturated-saturated flow and transport equations which were simulated by the SUTRA (Voss, 1984) and 2DSOIL (Pachepsky et. al., 1993) numerical codes. Note, that the flow in the unsaturated zone is vertical only, while in the saturated zone it is essentially horizontal. Therefore, we consider, for the quasi 2-D case, these two direction as the principal axes of the dispersion (i.e., D_{xz}=D_{zx}=0). This allows us to use the Operator Splitting Methods to solve a 2-D transport equation (Samarsky, 1977). The two remaining components are given by (Bear and Verruijt, 1987)

$$D_{xx} = D_m\tau_c + \left(\alpha_T V_z^2 + \alpha_L V_x^2\right)/V \text{ and } D_{zz} = D_m\tau_c + \left(\alpha_L V_z^2 + \alpha_T V_x^2\right)/V \quad (11)$$

where D_m is molecular diffusion coefficient, τ_c is tortuosity factor, α_L and α_T are the longitudinal and the transverse dispersivities of soil, respectively, V_x,, V_z and $V\left(=\sqrt{V_x^2 + V_y^2}\right)$ are the horizontal and vertical components of the average water velocity vector and its module, respectively.

In all examples, we considered a homogeneous isotropic porous media and the transport of a single solute without any chemical reaction.

1. <u>Spread of the groundwater 'stripe'</u>

The groundwater level at the initial time is given as a step function

$$h(x,t_0) = h_0 \quad \text{if } |x| \geq R \text{, and } h(x,t_0) = h_0 + \Delta h \text{ if } |x| < R \quad (12)$$

where h_0 and the step $\Delta h \times R$ are prescribed. The analytical solution of the linearized 1-D Boussinesq equation for this case, has the form (Polubarinova- Kochina, 1977) of

$$h(x,t) = h_0 + \frac{\Delta h}{2}\left(\operatorname{erf}\frac{R-x}{2\sqrt{at}} + \operatorname{erf}\frac{R+x}{2\sqrt{at}}\right) \quad (13)$$

where $a = K_s/\left(S_y\tilde{h}\right)$, S_y is the specific yield and $\tilde{h}$ is the average groundwater level.

We carried out simulations for the silt loam GE 3 soil (van Genuchten, 1980) for which θ_s=0.369, θ_r=0.131, K_s=0.0496 m/day, α=0.423 m^{-1} and n_V=2.06. The longitudinal and transversal dispersivities were α_L=1.0 m and α_T=0.1 m, respectively. The simulated domain was presented by a rectangle of height 4 m (from bottom of the aquifer to the soil surface) and 40 m length. The assigned initial conditions were h_0= 2.0 m, $\Delta h = 0.5$ m, and R=5.0 m. We note the symmetry of (13) at x=0, hence, accordingly the $\partial h/\partial x = 0$ condition was assigned. No flow condition was also specified at z=0 and z=4 m. At x=40 m we prescribed a constant head h=2 m. The initial solute concentration was set to be C_0=1 for $0 \le x \le R$ and $h_0 \le z \le h_0 + \Delta h$, and C_0=0 elsewhere. A finite differences grid of 17×17 nodes was used to solve the quasi 2-D (QUASI2D) problem. An equivalent finite elements grid was implemented for simulation with SUTRA and 2DSOIL. The time step increased by a factor of 1.1 starting from 10^{-6} day. The simulated groundwater level, on the basis of (2) and (6), was between the analytical solution of the linearized Boussinesq equation and the numerical solution of the 2-D Richards equation, however, closer to the latter one (Fig. 1a). The simulated distribution of the water content in the unsaturated zone was consistent with the one obtained on the basis of the 2-D Richards equation. The concentration obtained by the quasi 2-D approach and the fully 2-D flow and transport, were also in good agreement (Fig. 1b).

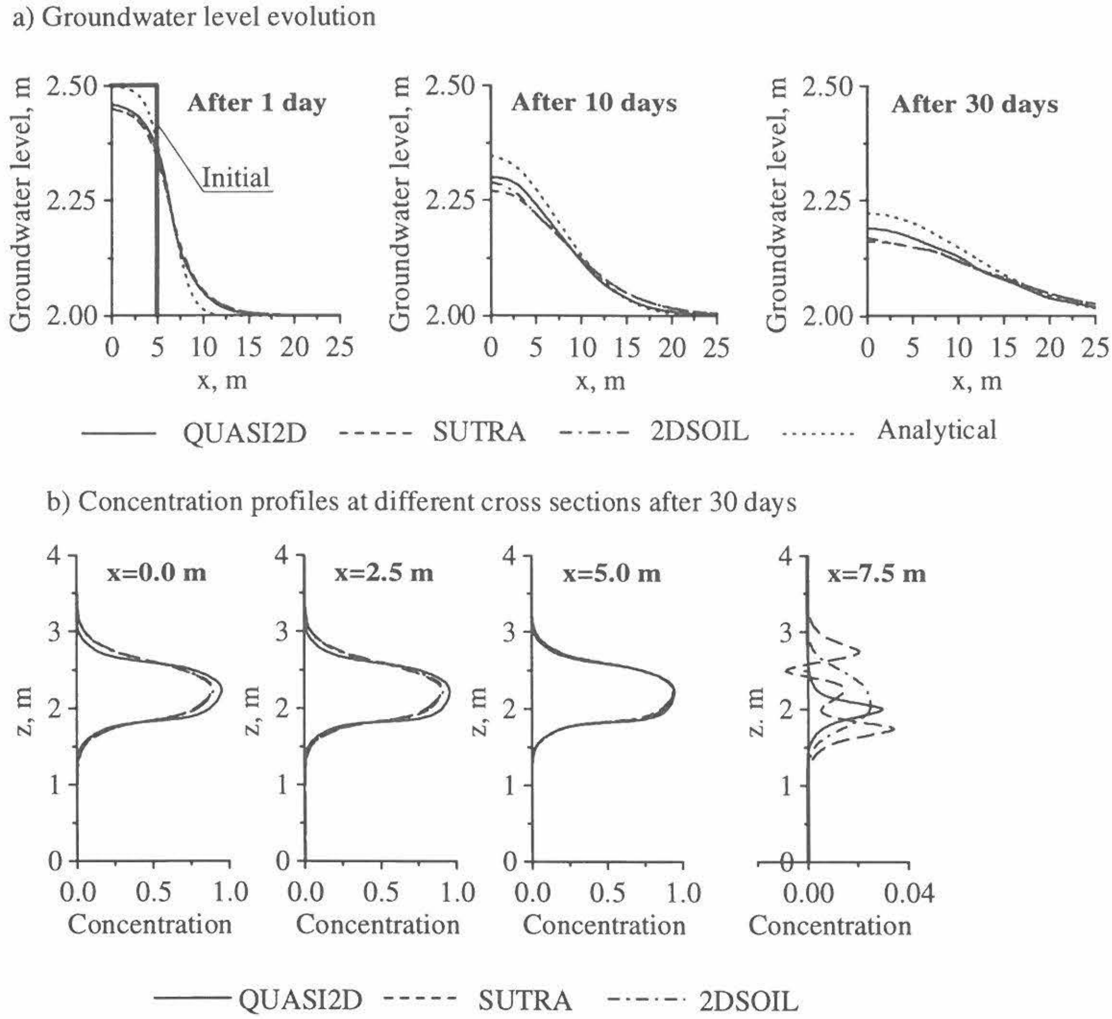

Figure 1. Groundwater level (a) and concentration profiles (b) for the problem of the 'stripe' spread.

The computation time for the period of 30 days using a Pentium/120 PC, was **12**, **60**, and **600** sec for the QUASI2D, 2DSOIL and SUTRA, respectively.

2. *Infiltration from the soil surface*

A problem of time dependent water infiltration and solute transport through the soil surface was considered. The simulations were carried out for the Guelph loam soil (van Genuchten, 1980) for which θ_s=0.520, θ_r=0.218, K_s=0.316 m/day, α=1.15 m^{-1}, n_V=2.03. The longitudinal and transversal dispersivities were α_L=5.0 m and α_T=1.0 m, respectively. The simulated domain was presented by a rectangle of height 10 m (from bottom of the aquifer to the soil surface) and 300 m length. Initial groundwater level was h_0= 4 m. Initial solute concentration was equal to zero. The flux boundary condition was assigned at the soil surface for the segment $110<x<170$ m. During the first 3 years, the intensity of the flux was 2 mm/day with a concentration of the solute in water equal to 1; during the next 3 years, these were 0.2 mm/day and 0, respectively; and during the last 4 years, no flow condition was implemented. The boundary conditions h=4.0 m for flow and $\partial C/\partial x = 0$ for transport, were assigned at x=0 m. The remaining part of the boundary was subject to no flow boundary condition. A finite differences grid of 16 × 18 nodes was used to solve the quasi 2-D problem. An equivalent finite elements grid was implemented for simulation with SUTRA and 2DSOIL. The time step increased by a factor of 1.5 starting from 10^{-6} day. The maximum value of the time step was 10 days. The simulated groundwater level, on the basis of (2) and (6), was closer to the one obtained by the 2DSOIL code (Fig. 2). The simulated distribution of water content in the unsaturated zone was consistent with the one obtained on the basis of the 2-D Richards equation. The contours of concentration, obtained by the quasi 2-D approach and the fully 2-D flow and transport, were also very similar (Fig. 3).

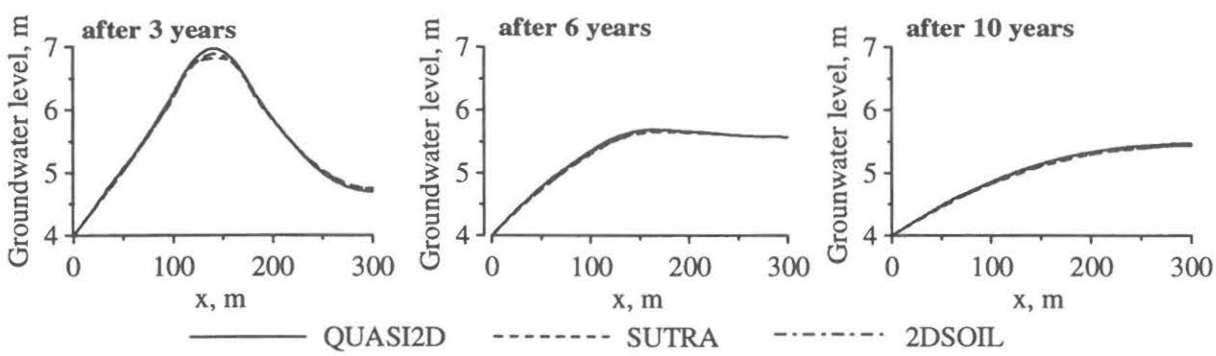

Figure 2. Groundwater level during infiltration from the soil surface.

The computation time for the total period of 10 years using a Pentium/120 PC, was **29**, **155**, and **871** sec for the QUASI2D, 2DSOIL and SUTRA, respectively.

Conclusion

The simulations for the quasi 2-D case proved to be computationally very effective for the modeling of flow and transport in the unsaturated soil and phreatic aquifer. It can, therefore, be speculated that it will even be more effective in compare to fully unsaturated-saturated flow and transport models, when considering the 3-D case. Limitations of the developed approach are that they assume a 1-D flow in the vadose zone and refers to small slopes of the phreatic surface. However, this model can be used for reliable solution of field scale flow and transport problems.

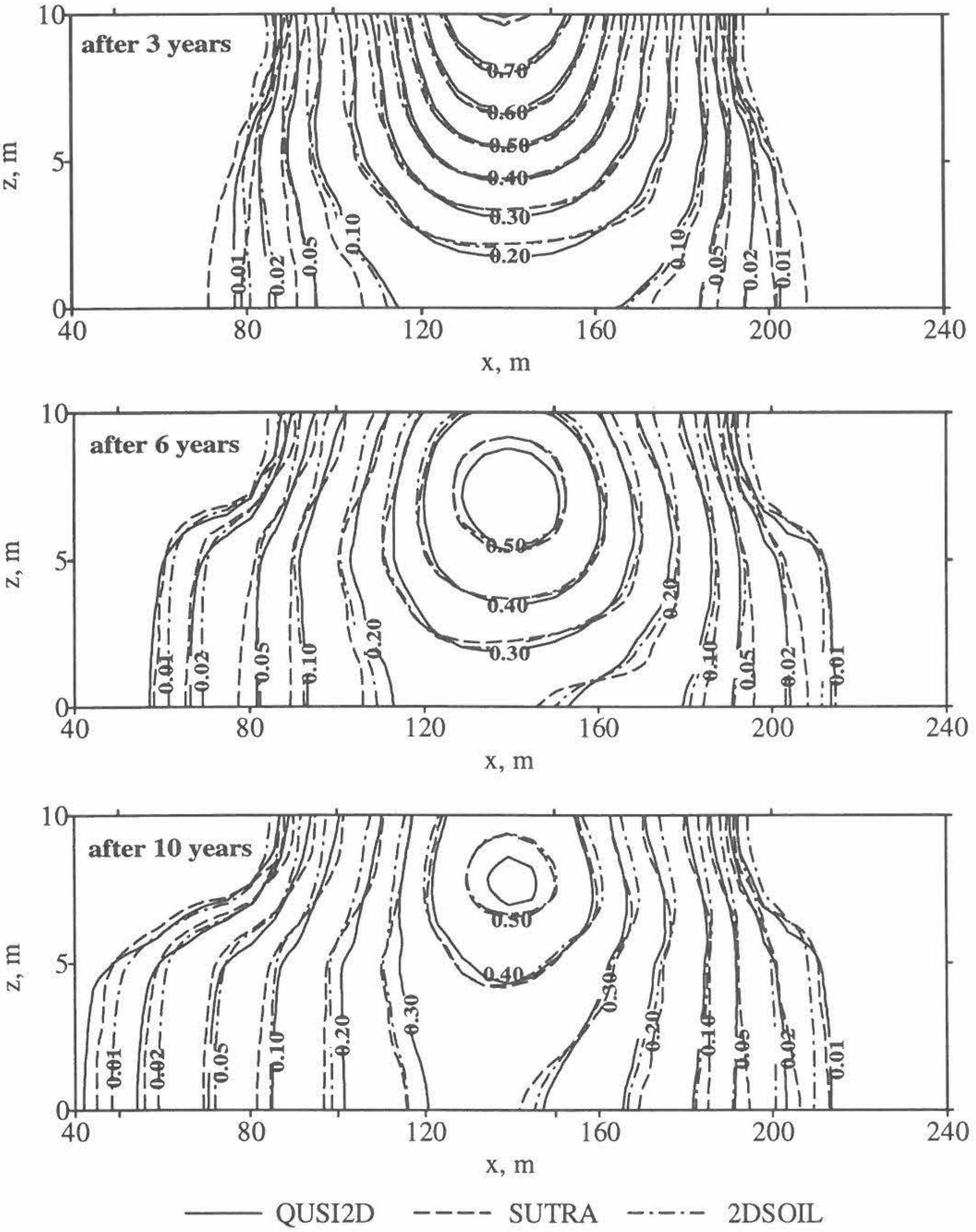

Figure 3. Contours of the solute concentration during infiltration from the soil surface.

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