One-dimensional Transient Water and Solute Transport In Soils

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Abstract: Water flow and solute transport processes in the vadose zone have become a focus of research, particularly in terms of water quality management, agricultural management and also the prevention of pollution of groundwater. This paper considers both the vertical and horizontal movement of water in soil, as described by Richard's equation. The transport equation is used to describe the movement of a solute by water through different soils. Numerical solutions are obtained for both the water content and also the concentration of the solute, using the Method of Lines technique. Special forms of the soil hydraulic diffusion and chemical diffusion functions are used to provide a closed form analytic solution for the solute profile in a horizontal flow situation. This analytic solution is used to verify the numerical method and estimate the accuracy of the numerical code. Numerical simulations are also carried out for the vertical flow case for more realistic forms of the soil hydraulic functions. The vertical infiltration of the water and solute profiles are obtained for two different soils subject to Dirichlet and Neumann conditions at the upper surface. The results show the propagation of the soil water front followed by a more diffuse solute profile into the soils. The method is readily applicable to the study of salt movement in clays and sandy soils.

Keywords: numerics, solute, transport, soils, transient flow

1. INTRODUCTION

A knowledge and understanding of water flow and solute transport processes in the vadose zone is becoming increasingly important especially in terms of water quality management, the management of saline soils, and the mitigation of groundwater pollution. The presence of different phases (air, water, salt, pollutant and the soil matrix) result in many different physical and chemical processes taking place. These processes are often complex and require simplifying assumptions to provide achievable and verifiable simulations in terms of water and solute solution profiles in the soil. To date, only a few analytical solutions have been found to describe water and solute transport in the vadose zone. There is the exact solution of Smiles et al [1978] developed for horizontal absorption in very fine textured soils where solute transport by molecular diffusion dominates that due to mechanical dispersion. There are also the approximate analytical solutions which include the dependence of flow velocity in the dispersion coefficient have been given by Smiles et al. [1981] and Bond [1986]. All these have been shown to give very good agreement with experimental data across a range of conditions.

This paper offers both a numerical model and an analytical solution to horizontal one-dimensional coupled transient water and solute transport in the vadose zone. The analytical solution for both the water and the solute profiles uses specific forms for the water diffusivity and solute dispersion functions. Numerical results are then obtained by the Method of Lines, and are compared to the analytical solution to validate the model. Finally, using more realistic soil hydraulic functions, some solutions are presented for the 1D vertical flow configuration.

2. GOVERNING PARTIAL DIFFERENTIAL EQUATIONS

The combination of water flow and solute transport processes are governed by a system of two coupled partial differential equations (PDEs). Under conditions of isothermal and incompressible flow, the movement of water is governed by

Richard's equation. When written in terms of the volumetric water content θ, it takes the form [Bear, 1979]

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left(D\frac{\partial\theta}{\partial z}\right)-\frac{\partial K}{\partial z}, \qquad (1)$$

where $D = D(\theta)$, is the hydraulic diffusivity $[L^2T^{-1}]$, $K = K(\theta)$, is the hydraulic conductivity $[LT^{-1}]$, z is a vertical space coordinate [L], and t is time [T]. Note that $D = K/C$, where $C = C(h) = d\theta/dh$.

The convection-dispersion equation in an incompressible homogeneous porous medium in the absence of sink terms, is given by Bear [1979]

$$\frac{\partial c}{\partial t}=\frac{1}{\theta}\left(\frac{\partial}{\partial z}\left(D_S\theta\frac{\partial c}{\partial z}\right)-q\frac{\partial c}{\partial z}\right), \qquad (2)$$

where c is the solute concentration $[ML^{-3}]$, q is the Darcy flux $[LT^{-1}] = -D\partial\theta/\partial z + K$ and D_S is the coefficient of dispersion $[L^2T^{-1}]$. Note that $q = V\theta$, where V is the velocity of flow in the z direction, and the D_S is given by

$$D_S = D_m + \alpha|V| = D_m + \alpha\frac{|q|}{\theta}, \qquad (3)$$

with α (L) being the longitudinal dispersivity and D_m is the molecular diffusivity of the solute.

3. NUMERICAL METHOD OF LINES

The NUMOL (Numerical Method of Lines) consists of a finite difference discretisation on the spatial derivatives of an evolution equation [PDE] on a discrete set of nodes while the time derivative is left in a continuous form [Schiesser, 1991]. This transformation of the PDE leads to a coupled system of ordinary differential equations (ODE). An ODE integrator is then used to integrate the system to obtain the solution at each nodal point of the domain. Lee et al. [1998] have shown that a template leading to a differentiation matrix can be used to automate the NUMOL. It has also been shown that this flexible template can be applied successfully to sets of partial equations in one, two or more spatial dimensions. The vector capabilities of MATLAB [2000], can be used to automate the template and the NUMOL.

Equations (1) and (2) were discretised using the template approach of Lee et. al. [1998], and a 4^{th} order finite difference scheme to represent the space derivatives. The MATLAB suite of ODE solvers, particularly ODE45 with relative and absolute error tolerances of order 10^{-10}, were used to integrate the resultant sets of ODEs.

4. MODEL VERIFICATION

When they are available, analytical solutions offer a means of validating a numerical code and numerical solution. Lee et al. [1998] used the analytical solution from Sander et. al. [1988] to validate the use of NUMOL in solving soil water problems. Excellent accuracy was obtained using the 4^{th} order finite difference representations of the spatial derivatives.

4.1 Analytical Solution Based on Brutsaert's Profile

An exact solution to the horizontal transient flow of water and solute can be derived using assumptions about flow conditions and the shape of the profiles of both the water content and solute concentration. This is based on the approach of a Brutsaert profile [Brutsaert, 1976] for describing both the water and solute profiles.

Consider the reduced variables defined by:

$$\bar{\theta}=\frac{\theta-\theta_i}{\theta_s-\theta_i}, \qquad (4a)$$

$$\bar{c}=\frac{c-c_i}{c_s-c_i}, \qquad (4b)$$

where θ_i and θ_s are the initial and saturated volumetric water contents, and c_i and c_s ($c_s > c_i$) are the initial and surface solute concentrations respectively. With x as the horizontal space coordinate, (2) can be written in terms of the reduced variable $\bar{\theta}$ in the form

$$\frac{\partial\bar{\theta}}{\partial t}=\frac{\partial}{\partial x}\left(D(\bar{\theta})\frac{\partial\bar{\theta}}{\partial x}\right). \qquad (5)$$

In the same way, the solute transport equation may be written as

$$\left(\bar{\theta}+\frac{\theta_i}{\theta_s-\theta_i}\right)\frac{\partial\bar{c}}{\partial t}= \left[\frac{\partial}{\partial x}\left(D_s^*(\bar{\theta})\frac{\partial\bar{c}}{\partial x}\right)+D(\bar{\theta})\frac{\partial\bar{\theta}}{\partial x}\frac{\partial\bar{c}}{\partial x}\right], \qquad (6)$$

where $D_s^* = \theta D_s$. By introducing the Bolztman variable $\eta=\frac{x}{\sqrt{t}}$ [Smiles et al., 1978] (5) and (6) become respectively;

$$\frac{d}{d\eta}\left(D\frac{d\bar{\theta}}{d\eta}\right)+\frac{\eta}{2}\frac{d\bar{\theta}}{d\eta}=0, \qquad (7)$$

and

$$\frac{d}{d\eta}\left(D_s^*(\bar{\theta})\frac{d\bar{c}}{d\eta}\right)+\frac{G}{2}\frac{d\bar{c}}{d\eta}=0, \qquad (8)$$

with

$$G=\left(\bar{\theta}+\frac{\theta_i}{\theta_s-\theta_i}\right)\eta+2D\frac{d\bar{\theta}}{d\eta}= \left(\bar{\theta}+\frac{\theta_i}{\theta_s-\theta_i}\right)\eta-\int_0^{\bar{\theta}}\eta du, \qquad (9)$$

Here, a solution to (7) and (8) is sought subject to the boundary conditions of $\bar{\theta}=\bar{c}=1$ at $\eta=0$ and $\bar{\theta}=\bar{c}=0$ as $\eta\to\infty$ (Table 1). Thus, after integrating (7) and (8), the water diffusivity and chemical dispersion coefficient may also be obtained in the form

$$D(\bar{\theta})=-\frac{1}{2}\frac{d\eta}{d\bar{\theta}}\int_0^{\bar{\theta}}\eta du, \qquad (10)$$

and

$$D_s^*(\bar{\theta})=-\frac{1}{2}\frac{d\eta}{d\bar{c}}\int_0^{\bar{c}}G du, \qquad (11)$$

if both $\bar{\theta}(\eta)$ and $\bar{c}(\eta)$ are known. For a constant D_s*, Smiles et al [1978] provide a simple exact solution to (8), using the boundary conditions from Table 1, for any $\eta(\bar{\theta})$ satisfying (7). However, in the case of a non constant D_s*, there does not appear to be any solution to (8) in the literature. In this section we provide such a solution to (8) by following the technique of Brutsaert [1976]. For sharp moving water and solute fronts we take the profiles [Brutsaert, 1976]

$$\bar{\theta}(x,t)=\bar{\theta}(\eta)=\left(1-\eta/\eta_{wf}\right)^{1/N_w}, \qquad (12a)$$

$$\bar{c}(x,t)=\bar{c}(\eta)=\left(1-\eta/\eta_{sf}\right)^{1/N_s}, \qquad (12b)$$

where η_i is the position for the water front (i = wf) and solute front (i = sf) and N_i is a curve fitting parameter for the water profile (i = w) and solute profile (i = s). While (12a) has been successfully used to match water data [Brutsaert, 1976], (12b) has not been used on solute data. Since (12b) cannot model a tail in the solute profile it is only suitable for modeling flows where very abrupt solute fronts occur. However, the aim here is only to have a simple solution which captures the general physical features of an advancing solute profile that is easy to use for checking the efficiency and accuracy of a numerical solution. Other functional forms for $\bar{c}(\eta)$ could also be used if required, to more accurately match experimental data. Physically, the only restrictions on N_i and η_i in (12) are that, N_i is greater than one and $\eta_{sf}\le\eta_{wf}$. For algebraic simplicity only, we take $N_w = N_s$ and $\eta_{sf}=\eta_{wf}=1$ in (12). Using (12) and integrating (10) and (11) gives the following functional forms for D and D_S*

$$D(\bar{\theta})=\frac{N}{2}\bar{\theta}^N\left(1-\frac{\bar{\theta}^N}{N+1}\right), \qquad (13)$$

and

$$D_s^*(\bar{\theta})=\frac{\theta_i}{\theta_s-\theta_i}D(\bar{\theta})-\frac{N^2}{2(N+1)(N+2)}\bar{\theta}^{2N+1} \qquad (14)$$

and, since $D_s^*(\bar{\theta})\ge 0$, then $\theta_i>\frac{\theta_s}{N+3}$. In summary then, for D and D_s* as given by (13) and (14), the solution of (7) and (8) or (5) and (6) is given by (12).

Table 1. Initial and boundary conditions.

	Variables		Reduced variables	
$t=0$	$\theta=\theta_i$	$c=c_i$	$\bar{\theta}=0$	$\bar{c}=0$
$x\to\infty$	$\theta=\theta_i$	$c=c_i$	$\bar{\theta}=0$	$\bar{c}=0$
$x=0$	$\theta=\theta_s$	$c=c_s$	$\bar{\theta}=1$	$\bar{c}=1$

The parameter N plays a major role in the accuracy of the numerical code. Indeed, the higher the value of N, the steeper the profile for both the water content and solute concentration profiles which led to increased difficulties in obtaining accurate numerical solutions.

4.2 Accuracy of the Numerical Code

The numerical results obtained, using the NUMOL, were compared with the analytic solution, in terms of water content, concentration and mass conservation by integrating $\bar{\theta}$ and $\bar{\theta}\bar{c}$ over the full domain L. For N=2, 3, 4 and 5, good agreement is found between both the numerical and analytical solutions for the water and solute profiles. For a step size of 0.025 over a domain of length L = 5, the errors in the results at different x coordinates are low (3 to 4 significant figures for N = 2) since neither the wetting or solute front is too sharp. Indeed, the accuracy remains acceptable at 3 significant figures for the much steeper fronts occurring in both profiles for N =5. The relative errors in term of water and solute mass balances are negligible (order of 10^{-4}). Obviously smaller step sizes improved these results.

5. VERTICAL FLOW AND SOLUTE TRANSPORT

5.1 Conditions of Simulation

Numerical solutions are now presented for the vertical flow problem defined by (1) and (2), using NUMOL. We consider two soils, a coarse textured soil as used by Inoue et al (2000) (INU) and Yolo light clay (YLC) as given by Fuentes et al. [1992].

The Van Genuchten equation [Van Genuchten, 1980]

$$\frac{\theta-\theta_r}{\theta_s-\theta_r}=\left(1+\left(\frac{h}{h_g}\right)^n\right)^{-m} \quad , \qquad (15)$$

was used for the water retention curve for both soils. The Brooks and Corey function

$$\frac{K}{K_s}=\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{\beta} \quad , \qquad (16)$$

was used for the YLC hydraulic conductivity with

$$\beta=\frac{2}{mn}+2+p \quad , \qquad (17)$$

whereas the Mualem [1976] model

$$K(h)=K_s\overline{\theta}^{\ell}[1-(1-\overline{\theta}^{1/m})^m]^2 \quad , \qquad (18)$$

is used for the INU soil.

In (15) to (18), K_s represents the saturated hydraulic conductivity, and h_g, β, ℓ m, n and p are shape and scale parameters depending upon the nature of the soil. The values used for these parameters are given in Table 2, with ℓ = -1.16 for INU and p = 1.907 for YLC..

Three different numerical simulations were conducted, each with a free drainage condition at the bottom boundary for water and a zero concentration gradient for the solute. The water boundary condition at the upper surface was taken as either a Dirichlet condition with the soil moisture at the surface held constant, or as a Neumann condition with the. water flux prescribed. The surface solute boundary condition was either a fixed concentration or a flux condition (see Table 3). Constant initial conditions were taken for both the water content (or pressure) and solute concentration.

5.2 Results

Figures 1a to 1f show the profiles of water and solute concentration calculated at various times for the different soils and boundary conditions listed in Table 3. For all cases a value of D_m = 1.9x10^{-9} m^{2}s^{-1} was used while the dispersivity values were α = 0.221 cm for INU and α = 0.02cm for YLC. In Inoue et al (2000) neither the water or solute profiles were given, but instead the breakthrough curves for h, θ and c at z = 23cm were provided in their fig. 6. As a further check on the numerical solution we compared the breakthrough curves obtained at z = 23cm from figs 1a and b with Inoue et al (2000) and found excellent agreement.

For the INU soil, transport by mechanical dispersion completely dominates that due to molecular diffusion. This is shown by the ratio $\alpha V/D_m$ being of the order of 100. This is not surprising where you have a coarse textured soil with a high conductivity and flow velocity V. By comparison in the clay soil, YLC, molecular diffusion is essentially always the dominant transport process. Following calculations in Smiles et al. [1978], D_s may be taken independent of flow velocity for the YLC for infiltration times greater than 4 seconds. The other feature apparent in fig 1, that is also well known in the literature, is the lagging of the solute front behind the water front due to the piston like displacement of the initial water in the soil by the infiltrating water [Smiles et al, 1978].

6. CONCLUSION

The development of an analytical solution for a one dimensional horizontal transient flow and transport problem has provided a way to check the efficiency, accuracy, and the robustness of numerical models of coupled water and solute transport. The NUMOL technique is shown to be an effective tool for modeling coupled water flow and solute transport in one dimension. The method has also been applied successfully to coupled water and solute movement in the vertical direction. The results replicate experimental observations reported in the literature.

Table 2. Values of hydraulic parameters for YLC and INU soils

	θ_s	θ_r	$-h_g$ cm	m	n	K_s cm h^{-1}
YLC	0.495	0	19.31	0.0995	2.22	0.0443
INU	0.31	0.027	7.25	0.502	2.01	162

Figures 1a, b, c and d. Water and solute profiles reached at different infiltration times for INU (1a,b) and YLC (1c,d,e,f) soils as defined in Table 3 for a step size of 0.3cm

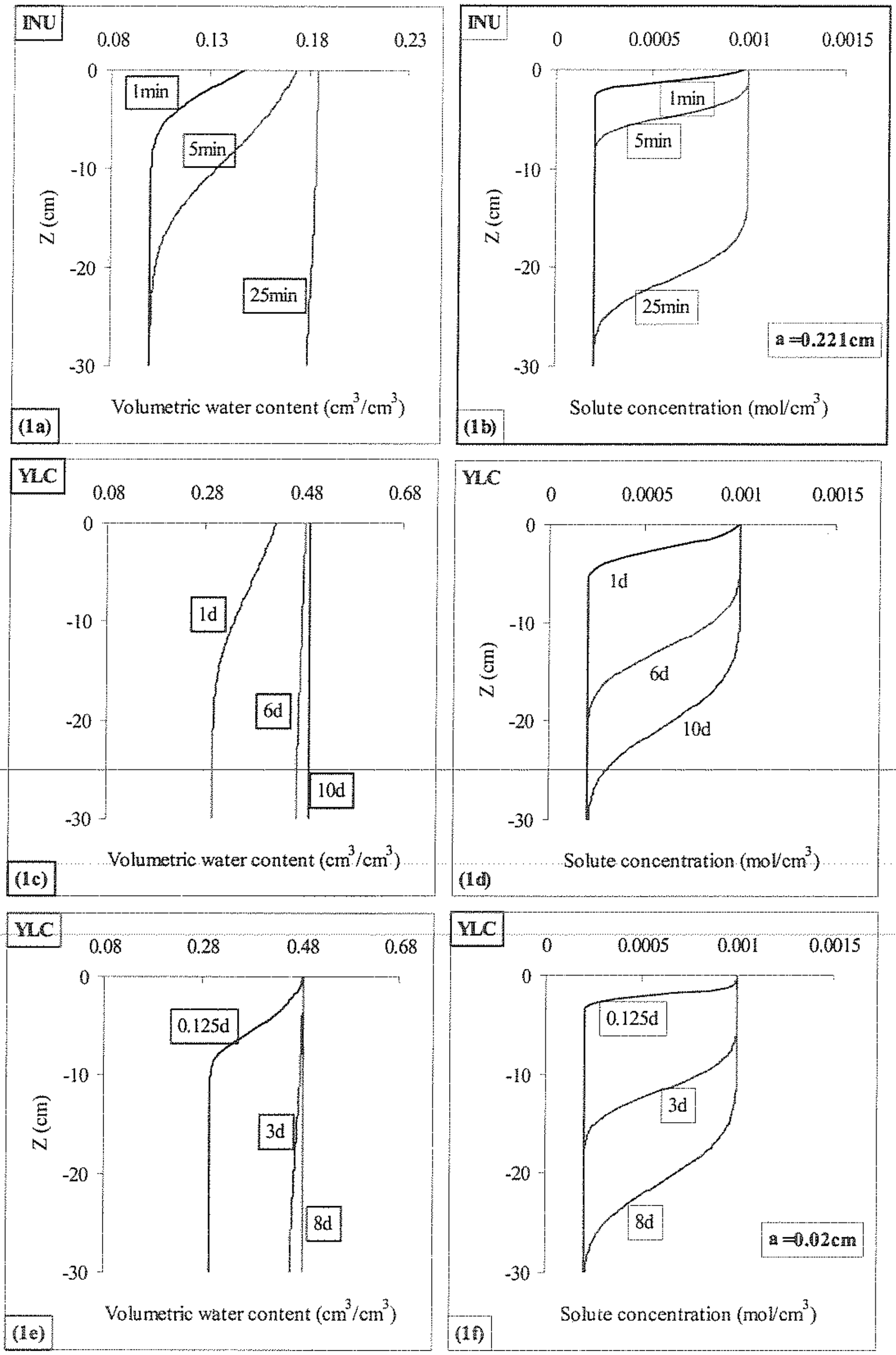

Table 3. Initial and boundary conditions tested for a domain of length L = 30cm; Units are h [cm] ; q_o [cm/min] and c [mole/l]

Test	Soil	Initial conditions	Boundary conditions	
		$0 \le z \le L$	$z = 0$	$z = L$
1 (fig.1a,b)	INU	h = -26.8 c = 0.02	$q_o = 0.155$ $c_o = 0.1$ $-\theta D_s \frac{\partial c}{\partial z} + qc = q_o c_o$	$\frac{\partial h}{\partial z} = 0 \quad \frac{\partial c}{\partial z} = 0$
2 (fig.1c,d)	YLC	h = -200 c = 0.0002	h = -10 c = 0.001	$\frac{\partial h}{\partial z} = 0 \quad \frac{\partial c}{\partial z} = 0$
3 (fig.1e,f)	YLC	h = -200 c= 0.0002	$q = 7x10^{-4}$ c =0.001	$\frac{\partial h}{\partial z} = 0 \quad \frac{\partial c}{\partial z} = 0$

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