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WATER AND CHLORIDE TRANSPORT IN A FINE-TEXTURED SOIL: FIELD EXPERIMENTS AND MODELING

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Numerical models are being used increasingly to simulate water and solute movement in the subsurface for a variety of applications in research and soil/water management. Although a large number of models of varying degrees of complexity have been developed over the years, relatively few have been tested under field conditions. We tested the performance of the HYDRUS-1D computer model to simulate variably saturated water flow and chloride transport in a fine-textured Italian soil subject to a fluctuating saline groundwater table. The model was also used for estimating solute transport parameters using an inverse optimization scheme. Our results indicate that including the effects of immobile water produced better predictions of chloride transport compared with the traditional convection-dispersion transport approach. Including anion exclusion as well did not improve the model predictions appreciably. Occasional deviations between model prediction and field observation were attributed to unrepresented lateral groundwater flow processes and to preferential flow through macropores or other structural voids. The HYDRUS-1D model was found to be very useful for analyzing the relatively complex flow and solute transport processes at our field site and for estimating model parameters using inverse procedures. (Soil Science 2000;165:624–631)

Key words: Water flow, chloride transport, numerical modeling, shallow groundwater table.

MOST coastal zones of Italy are subject to relatively high phreatic groundwater tables, often occurring within 2 m of the soil surface. Such shallow water tables can have considerable impact on both the growth of agricultural crops, and the preservation of soil and groundwater environmental resources. Consequently, optimal agronomic techniques (irrigation, fertilization, and tillage) must be based on a precise understanding of the water and salt balances in the vadose zone and shallow groundwater.

The ability to predict water flow and solute transport into and through the vadose zone accurately is essential for effective management of soil and groundwater. A large number of analytical models, and especially numerical models, have been developed during the past several decades for predicting water flow in the vadose zone at the field scale (e.g., Belmans et al., 1983; Hopmans, 1988; Hopmans and Stricker, 1989; de Jong and Kabat, 1990; Johnsen et al., 1995; Ould Mohamed et al., 1997). By comparison, relatively few field-scale model application studies have been carried out to date by soil scientists and hydrologists. Mohanty et al. (1997 and 1998) recently used a two-dimensional numerical model with bimodal hydraulic functions to predict field-scale preferential flow and nitrate transport in a structured agricultural soil in New Mexico. Although they were reasonably successful in simulating flow and transport at their experimental field site, based on several site-specific findings, they recommended further testing of the model under different hydrologic, soil, and climatic conditions.

In this paper we evaluate the utility of a numerical model, HYDRUS-1D (Šimůnek et al., 1998), for simulating long-term (3 year) water flow and chloride transport in an Italian soil sub-

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ject to a shallow, saline groundwater table. As a secondary objective we analyzed a limited data set from the field to obtain solute transport parameters in the governing convection-dispersion solute transport equation (CDE) with and without accounting for the presence of immobile liquid zones and anion exclusion.

FIELD SITE AND HYDROLOGIC MONITORING

The experimental field (15 m × 15 m) is located at the experimental farm of the Istituto Sperimentale Agronomico, situated in the coastal area of the Basilicata region in Southern Italy (Metaponto: lat. 40° 24′ N and long. 16° 48′ E). The climate of this region is classified as "accentuated thermomediterranean" (according to the UNESCO-FAO classification), with mean monthly temperatures of 5 °C in the winter and 26 °C in the summer. The mean annual precipitation (1981–1998) at the experimental farm is 476 mm, with more than 77% of the rainfall occurring during the winter months (September through March). Typically, a substantial proportion of the annual rain comes in a few days, thereby creating a rapid rise in the groundwater table during the winter period (Fig. 1). Another feature of the climate at our field site is the high annual potential evaporation rate, with a mean annual pan evaporation rate of 1535 mm. Evaporation rates are maximum during the months of June, July, and August, with mean daily rates of 7.4, 8.4, and 7.3 mm, respectively. The soil is classified as a Typic Epiaquerts, similar to those formed on the silty-clay and clay lagoon sediments of the Oleocene that are present over large portions of the alluvial basin between the Basento and Bradano rivers. The original sediment affected its evolution and current functional characteristics strongly since it consists mostly of swelling clays. The soil, poorly drained with strong medium angular blocky structure, is relatively low in nitrogen and organic matter and is classified as alkaline (pH = 8.4). The clay and silt contents, as well as the electrical conductivity, increase with depth, whereas the organic matter content and the bulk density decrease with depth (Table 1).

In November 1993, five sets of nested

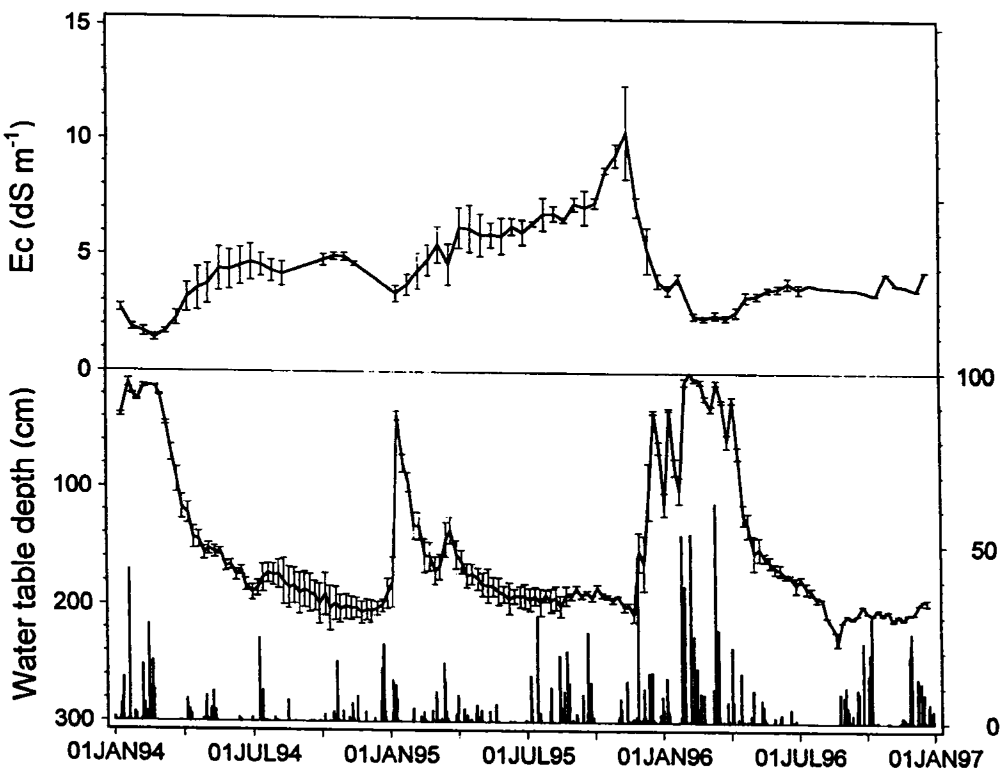

Fig. 1. Water table depth, daily rainfall (needle), and groundwater salinity at 3 m during the entire period of study. The bars indicate ± standard error of the field means.

TABLE 1
Selected soil properties at the experimental site

Layer cm	Horizon	Particle size distribution			Dry bulk density g cm^{-3}	Electrical conductivity (1:2) dS m^{-1}	Cation exchange capacity $cmol_c kg^{-1}$	Organic matter %
		Clay (%)	Silt (%)	Sand (%)				
0–50	Ap	58.8	35.8	5.50	1.38	0.53	13.37	1.48
50–70	Abss	60.0	35.8	4.23	1.21	0.77	11.47	0.83
70–100	Abssk	60.2	36.4	3.51	1.19	1.41	9.68	0.61
100–170	Bw	67.7	30.8	1.53	1.15	3.51	10.28	0.72
170–210	Btg	77.2	22.0	0.84	1.10	2.38	16.31	0.57

piezometers were installed, each set consisting of five piezometers (120-mm i.d.) located at depths of 0.5, 1, 1.5, 2, and 3 m. The piezometers were used for measuring hydrostatic pressure heads and collecting water samples for chemical analysis. To prevent clogging, the lower parts of the piezometers were lined with glass wool and enveloped by a layer of sand and siliceous fine gravel. Before installation of the piezometers, a pit was excavated to a depth of 3 m in order to determine variations in the unsaturated soil hydraulic property versus depth. Three replicates of 5-cm-diameter and 5-cm-long undisturbed soil cores were taken from each layer. Soil water retention data were obtained by using a sand and kaolin box apparatus (from saturation to −300 cm of water) and pressure plates (between −300 cm and −15000 cm).

Between January 1994 and December 1996, soil water pressure heads were measured on a weekly basis. Ground water samples were taken every 2 weeks to determine the bulk electrical conductivity and concentrations of chlorides, sulphates, carbonates, bicarbonates, sodium, magnesium, and calcium ions. Figure 1 shows the trend of the measured water table depth and the electrical conductivity at 3-m depth. During the summer months the water table remained nearly constant at a depth of 1.8 to 2 m, whereas during the winter months the water table rose to a depth of 0.2 to 0.4 m below the soil surface as a result of heavy rains. An increase in the evaporative demand of the atmosphere following the summer of 1995 caused the groundwater table to go down and its salinity to increase up to 10 dS m^{-1}. The electrical conductivity during the previous winter months, when the water table was shallow, ranged between 1 and 4 dS m^{-1}. Between January 1994 and October 1995, a slowly increasing trend in salinity was observed until a large amount of rainfall in 1996 decreased the electrical conductivity to its background value (3 dS m^{-1}). In this study we consider only the chloride concentration, which was found to be strongly correlated ($r = 0.95$) with the electrical conductivity (Losavio et al., 1997).

The experimental field was kept weed free and no crop was grown.

NUMERICAL MODELING

The HYDRUS-1D computer model (Šimůnek et al., 1998) was used to simulate one-dimensional vertical isothermal variably-saturated flow at the experimental site. Simulations were performed for the period from January 11, 1994, to December 31, 1996. The one-dimensional flow domain extended to a depth of 3 m and was divided into five separate soil layers, as shown in Table 1, comprising a total of 100 finite elements. A finer discretization was used near the soil surface to accommodate relatively steep gradients in the pressure head.

On the basis of available profile information and hydraulic property data, the five soil layers were characterized in terms of their field-averaged hydraulic functions. For each layer, we optimized the hydraulic parameters in the retention equation of van Genuchten (1980) using the RETC nonlinear optimization code (van Genuchten et al., 1991). As the soil surface boundary condition (x=L), we used a system-dependent atmospheric condition in accordance with the approach of Feddes et al. (1974) and Šimůnek et al. (1998). Class A pan evaporation rates, recorded by an automated data-logger located at the experimental farm, were used to calculate potential evaporation rates on a daily basis. These data, combined with daily precipitation data from the same weather station, were used to define the transient top boundary condition. The bottom boundary condition (x=0) consisted of daily prescribed values of the pressure head [$h_i(t)$] obtained by linear interpolation from weekly measured data. The water table elevation measured on January 11, 1994, was used to define the initial condition [$h_0(x)$] for our simulations. Thus, the boundary and initial conditions for our calculations are

$$\left|-K\frac{\partial h}{\partial x}-K\right| \leq E \qquad \text{at } x = L \qquad (1)$$

$$h_A \leq h \leq h_S \qquad \text{at } x = L \qquad (2)$$

$$h(x,t) = h_i\,(t) \qquad \text{at } x = 0 \qquad (3)$$

$$h(x,t) = h_0\,(x) \qquad \text{at } t = 0 \qquad (4)$$

where t is the time (T), x is distance (positive upward) (L), E is the maximum potential rate of infiltration and evaporation under the prevailing atmospheric conditions (LT^{-1}), and h_A and h_S are, respectively, the minimum and maximum pressure heads allowed at the soil surface (L). The value of h_S was set to 0, whereas h_A was calculated using relationships given by Feddes et al. (1974).

HYDRUS-1D solves numerically the Richards equation (Richards, 1931) for variably saturated water flow and the convection-dispersion transport equation (CDE) of a single ion. The latter equation is given by:

$$\frac{\partial(\theta c)}{\partial t}=\frac{\partial}{\partial x}\left(\theta D^{w}\frac{\partial c}{\partial x}\right)-\frac{\partial qc}{\partial x} \qquad (5)$$

in which

$$\theta D^{w} = \lambda\,|q| + \theta D_w\,\tau_w \qquad (6)$$

where c is the solute concentration (ML^{-3}), θ is the water content (L^3L^{-3}), D^w is the effective dispersion coefficient (L^2T^{-1}), q is the Darcian fluid flux density (LT^{-1}), λ is the longitudinal dispersivity (L), D_W is the molecular diffusion coefficient (L^2T^{-1}) and τ_w is the tortuosity factor.

An option in HYDRUS-1D allows users to implement the concept of two-region or mobile-immobile solute transport (MIM: van Genuchten and Wierenga, 1976). The code for this purpose partitions the liquid phase into distinct mobile, θ_m (L^3L^{-3}), and immobile, θ_{im} (L^3L^{-3}), regions, with solute exchange between the two liquid regions modeled as an apparent first-order exchange process, i.e.,

$$\begin{aligned}&\frac{\partial\theta_m c_m}{\partial t}+\frac{\partial\theta_{im} c_{im}}{\partial t}=\frac{\partial}{\partial x}\left(\theta_m D^{w}\frac{\partial c_m}{\partial x}\right)-\frac{\partial qc_m}{\partial x}\\&\frac{\partial\theta_{im} c_{im}}{\partial t}=\alpha(c_m-c_{im})\end{aligned} \qquad (7)$$

where α is a mass transfer coefficient (T^{-1}).

We also incorporated anion exclusion (AE) concepts into the MIM approach. For this purpose we used the following transport equations (van Genuchten and Wierenga, 1976; van Genuchten, 1981)

$$\begin{aligned}&\frac{\partial(\theta_m+f\rho k)c_m}{\theta t}+\frac{\partial[\theta_{im}+(1-f)\rho k]c_{im}}{\partial t}=\\&\frac{\partial}{\partial x}\left(\theta_m D^{w}\frac{\partial c_m}{\partial x}\right)-\frac{\partial qc_m}{\partial x}\\&\frac{\partial[\theta_{im}+(1-f)\rho k]c_{im}}{\partial t}=\alpha(c_m-c_{im})\end{aligned} \qquad (8)$$

in which f is the fraction of the solid phase that equilibrates instantaneously with mobile fluid, ($1-f$) is the fraction that equilibrates with immobile liquid, ρ is the soil bulk density, and k is an empirical distribution coefficient ($L^3\,M^{-1}$). The value of k determines if chemical sorption ($k>0$) or anion exclusion ($k<0$) takes place. As shown by van Genuchten (1981), the above model resembles closely the anion exclusion model of Krupp et al. (1972), where anion exclusion is assumed to be restricted only to the immobile phase.

For chloride transport we implemented a no-flux boundary condition at the soil surface (which, in case of rainfall, assumes that the rain water is free of solute), whereas observed daily concentrations [$c_i(t)$] were used to define a time-variant bottom boundary condition (obtained by linear interpolation from biweekly measured data). Measured chloride concentrations [$c_0(x)$] from the piezometers on January 11, 1994, were used to define the initial concentration in the transport domain. The boundary and initial conditions of chloride transport can thus be written as:

$$-\theta D\frac{\partial c}{\partial x}+qc = 0 \qquad \text{at } x = L \qquad (9)$$

$$c(x,t) = c_i(t) \qquad \text{at } x = 0 \qquad (10)$$

$$c(x,t) = c_0(x) \qquad \text{at } t = 0 \qquad (11)$$

MODEL PARAMETER ESTIMATION

HYDRUS-1D includes a Marquardt-Levenberg parameter optimization algorithm for inverse estimation of transport parameters, based on minimization of an objective function that express the discrepancy between observed and predicted values. We used this procedure to estimate field-scale chloride transport parameters for the CDE, MIM, and MIM+AE modeling approaches. For our case the objective function, Φ, was taken as

$$\Phi(\mathbf{b},\mathbf{p}) = \sum_{i=1}^{n} w_i\left[c_i^*\,(x,t_i) - c_i\,(x,t_i,\mathbf{b})\right] \qquad (12)$$

where n is the number of measurements, c_i^* are the measured concentrations at time t_i and depth x, $c(x, t_i, \mathbf{b})$ are the corresponding model predic-

TABLE 2

Fitted van Genuchten retention parameters and regression coefficients for different soil horizons at the field site

Layer cm	θ_r cm^3 cm^{-3}	θ_s cm^3 cm^{-3}	α cm^{-1}	n	R^2
0–50	0	0.4791 (0.0054)§	0.0077 (0.0025)	1.1135 (0.0094)	0.986
50–70	0	0.5461 (0.0087)	0.0145 (0.0033)	1.1504 (0.0074)	0.996
70–100	0	0.5501 (0.0101)	0.0130 (0.0034)	1.1531 (0.0088)	0.996
100–170	0	0.5593 (0.0109)	0.0084 (0.0023)	1.1559 (0.0101)	0.993
170–210	0	0.5600 (0.0107)	0.0034 (0.0014)	1.4100 (0.0910)	0.900

§Values in parentheses are Standard Errors associated with the parameter.

tions for the optimized parameter vector **b**, and w_i is the weights associated with a particular measurement point, i. We assumed that all w_i's were equal to 1, indicating that the error variances for all measured concentrations remained the same. In this study, the vector of optimized parameters included λ for the CDE approach and θ_{im} and α for the MIM and MIM+AE approaches, in which we assumed that λ was known with sufficient accuracy from the CDE approach. Independent sensitivity analysis showed that λ had relatively little impact on the results. We utilized measured chloride data during the initial 100 days of the experiment for our inverse modeling. The parameter(s) estimated using this procedure were used later in the forward problem for simulating the entire 3-year period.

RESULTS AND DISCUSSION

Table 2 shows the field-average values of the different soil hydraulic parameters by soil horizons optimized with RETC from water retention measurements using soil cores. Since no measurements were made of the saturated hydraulic conductivity (K_s), we initially calibrated our simulation results to a reference K_s of 5 cm day^{-1}.

Table 3 shows average daily water fluxes across the top (evaporation and infiltration) and bottom (inflow to and outflow from the domain) boundaries calculated with HYDRUS-1D from December 10, 1994, to March 16, 1996. This simulation period was divided into five intervals characterized by different water table conditions. During the winter months of both years (December 10, 1994 to January 13, 1995 and November 26, 1995 to February 5, 1996), fluxes were directed predominantly into the flow domain because of infiltration through the surface and inflow through the bottom associated with a rising groundwater table. The drop in the groundwater table between January 14, 1995, and May 10, 1995, was caused primarily by outflow from the flow domain, but soil evaporation was also germane. During the summer months (May 11, 1995 to November 25, 1995), when the groundwater table was deep and relatively stable (about 200 cm from the soil surface), soil evaporation dominated all other fluxes. Finally, during the period between February 6, 1996, and March 16, 1996, net infiltration (infiltration-evaporation) across the top boundary equaled the outflow across the bottom boundary, thus defining an approximately stationary shallow groundwater table. Flux data such as those shown in Table 3 should be helpful for quantifying the impact of different agricultural management practices on the leaching of solutes to groundwater.

Table 4 shows the results of the parameter optimization utilizing measured chloride concentrations during the initial 100 days. For D_w we used a literature value of 1.7 cm^2 day^{-1} (van Rees et al., 1991). It is evident that the inclusion of the mobile-immobile water concept improves the correspondence between measured and simulated chloride concentrations at different depths (Fig. 2), as indicated by higher regression coefficient (R^2) and

TABLE 3

Average daily water fluxes across the top and bottom flow boundaries during part of simulation (Dec. 10, 1994 - Mar. 16, 1996) as calculated with HYDRUS-1D

Duration	Observed water table condition	Average daily fluxes (cm day^{-1})			
		Top boundary		Bottom boundary	
		Evaporation	Infiltration	Inflow to domain	Outflow from domain
Dec. 10, 94–Jan. 13, 1995	Rising	0.09	0.26	0.16	0.01
Jan. 14, 95–May 10, 1995	Falling	0.17	0.05	0.04	0.40
May 11, 95–Nov. 25, 1995	Deep	0.16	0.07	0.09	0
Nov. 26, 95–Feb. 5, 1996	Rising	0.08	0.28	0.12	0.15
Feb. 6, 96–Mar. 16, 1996	Shallow	0.01	0.32	0	0.31

TABLE 4

Results of transport parameter estimation from experimental concentration data

Approach	Constant parameters§	Estimated parameters§				R^2
			Initial Estimate	Final Estimates	Standard Error	
CDE	$D_w = 1.7, \theta_{im} = 0, \alpha = 0$	λ	10	0.78	0.001	0.41
MIM	$D_w = 1.7, \lambda = 10$	θ_{im}	0.1	0.209	0.012	0.91
		α	0.008	0.016	0.005	
MIM	$D_w = 1.7, \lambda = 20$	θ_{im}	0.1	0.210	0.012	0.91
		α	0.008	0.016	0.005	
MIM	$D_w = 1.7, \lambda = 30$	θ_{im}	0.1	0.210	0.012	0.91
		α	0.008	0.016	0.005	
MIM+AE	$D_w = 1.7, \lambda = 10, k = -0.01$	θ_{im}	0.1	0.203	0.012	0.91
		α	0.008	0.015	0.005	

§D_w ($cm^2 day^{-1}$), λ (cm), θ_{im} ($cm^3\ cm^{-3}$), α (day^{-1}), k ($cm^3\ g^{-1}$).

lower standard error compared with the CDE. The CDE actually posed convergence problems. With the MIM approach, θ_{im} and α were estimated to be 0.21 and 0.016 day^{-1}, respectively, independent of the value of λ. In addition, incorporating anion exclusion in the MIM concept resulted in a slight decrease in θ_{im} with no improvement in R^2 or the standard error. This result suggests that anion exclusion is not as important a factor under transient field conditions as it is under the steady-state flow condition for which the concept was originally developed. Furthermore, our findings reconfirm the importance of the mobile-immobile water concept, which is used widely to characterize preferential transport in field soils. In addition by using different initial conditions, we were able to identify the (unique) transport parameters of the MIM approach.

Adopting the MIM approach (λ = 30 cm, θ_{im} = 0.211, and α = 0.016 day^{-1}), we carried out another independent simulation from January 10, 1995, to December 31, 1996, in order to test the performance of the model by comparing simulated and measured chloride concentrations at 50, 100, 150, and 200 cm depths. Results in Fig. 3 show that the model predictions agree reasonably well with the available data at different depths. The model underestimated and somewhat delayed the arrival of the chloride peak in October 1995 at the 200 cm depth. A similar trend was noticed for the other depths (results not shown). This finding suggests that several field-scale processes were not correctly represented in the HYDRUS-1D model.

The processes that were most likely not modeled correctly are (i) lateral groundwater flow,

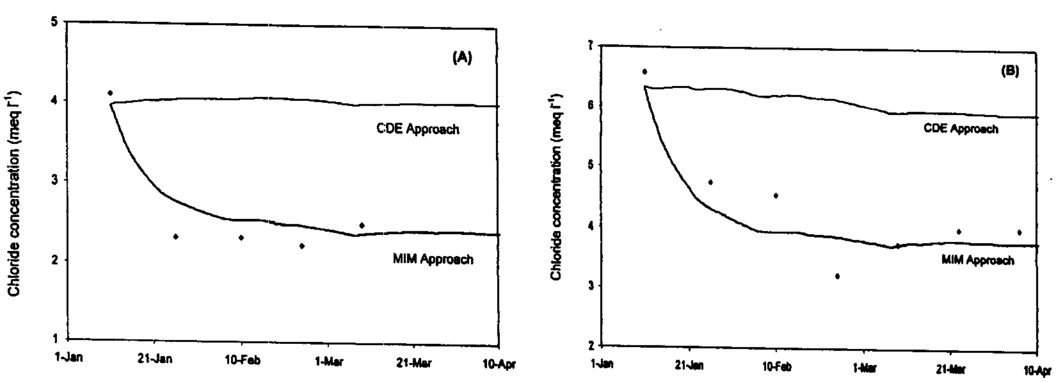

Fig. 2. Comparison of inverse analysis results of CDE (λ=0.78 cm) and MIM (λ=30 cm, θ_{im}=0.21 $cm^3\ cm^{-3}$, α=0.016 day^{-1}) approaches (solid lines) with measured (symbols) soil chloride concentrations at depths of 50 cm (A) and 200 cm (B).

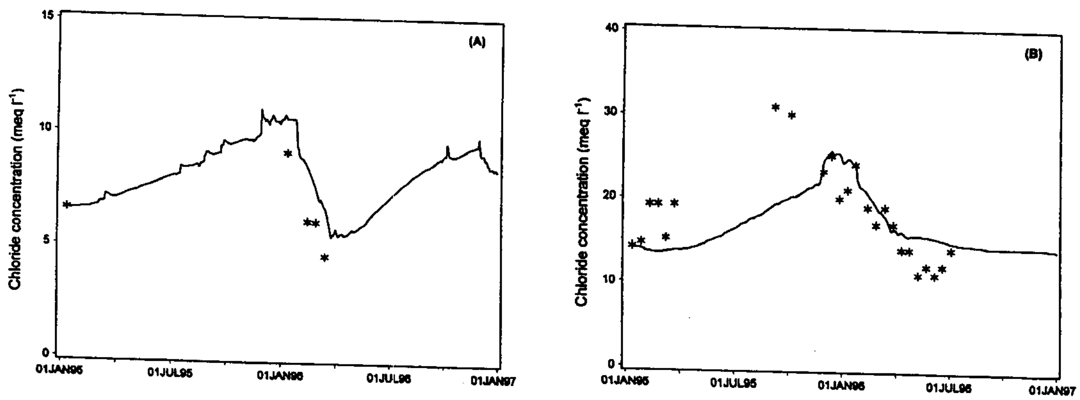

Fig. 3. Comparison of the simulated (solid line) and measured (symbols) soil chloride concentration at depths of 50 cm (A) and 200 cm (B).

and (ii) preferential flow through larger pores and structural cracks in the vadose zone. Our results agree with Zurmühl and Durner (1996) who showed that the MIM approach was not very effective in describing preferential transport under natural field conditions, unless bimodal functions of the hydraulic properties were considered in attempts to account for flow through the structured (macroporous) parts of the soils. The importance of using bimodal functions was confirmed by Mohanty et al. (1998), who simulated the preferential transport of nitrate in a field soil. Zurmühl and Durner (1996) also demonstrated that a better description of preferential transport in structured soils can be achieved when θ_{im} is defined as a transient variable that varies in time, depending on the slope of the unsaturated hydraulic conductivity curve. The current version of HYDRUS-1D assumes that immobile water content is constant. A follow-up paper will address some of these issues.

CONCLUSION

The performance and utility of the HYDRUS-1D model was assessed by simulating water flow and solute transport in a bare, fine-textured soil in Italy subject to transient water-table boundary conditions. The model, with estimated MIM transport parameters obtained from inverse modeling (based in part of available data), reproduced the general trends of measured chloride concentration at the field site fairly well, except for some underestimation and a delayed arrival of the concentration peaks. Possible reasons for this behavior could be unrepresented lateral groundwater flow and preferential flow through macropores and other structural voids. Considering the complexity of our field conditions, the HYDRUS-1D model was found to be a useful tool for analyzing solute transport data and estimating transport parameters.

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