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A NUMERICAL MODEL FOR INCORPORATING VADOSE ZONE TRANSPORT INTO THE GLEAMS ROOT ZONE MODEL

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ABSTRACT

Formulation of a one-dimensional unsaturated advection-diffusion numerical model is presented. The model uses a linear finite element numerical solution to coupled moisture and solute transport. The model can be used with the GLEAMS root zone model to examine the complete transport process through an agricultural soil. Results of model verification and testing are presented. Testing indicates good agreement between model predictions and both analytical and observed data.

INTRODUCTION

Since its introduction in 1986, (Leonard et al., 1987), the GLEAMS model has been widely applied and tested for assessing the impact of management practices on pesticide movement in the root zone. Leonard et al. (1988) extended the model to include pesticide metabolite transport and demonstrated how the model can be used to predict secondary product transport as well as that of the parent compounds. Leonard and Knisel (1988a) demonstrated how the GLEAMS model can be used to estimate the groundwater loadings of herbicides, thereby classifying the chemicals into groups of potential hazard. The model has also been used to examine the effectiveness of controlled-release pesticides as a means to decrease agricultural chemical transport beyond the root zone (Leonard and Knisel, 1988b). Analysis has shown the model to be sensitive to physical processes occurring in the soil, and simulation results are within the variability of field data (Leonard et al., 1987).

Widespread acceptance of the GLEAMS root zone model has created a need for a tool which can extend the prediction capabilities through the vadose zone (referred to here as the area between the root zone and the water table). This new tool should be capable of using output of the GLEAMS model as input for the vadose zone model. GLEAMS uses a water budget approach to calculate percolation in and through the root zone. Because the area below the root zone is normally at low levels of saturation, and flow velocities in this area are small, the water budget approach would not apply as well to the vadose zone. In addition, other processes which occur in the biologically active root zone may not be applicable in the vadose zone. For these reasons, a new method must be developed to simulate transport of water and solutes through the vadose zone. This paper presents a numerical model which incorporates vadose zone transport into GLEAMS.

OBJECTIVES

The primary objective of this research is to develop a vadose zone transport model which can be linked to the GLEAMS root zone model to simulate the movement of agricultural chemicals from the soil surface to the water table. The model should be physically based, and as such should accurately represent the simulated system. The model should be computationally efficient, and data requirements should be kept to a minimum. The parameters required by the model should, if possible, be physically based and easily obtainable. In addition, because of the move toward personal-computer (PC) based models, the model should be developed for PC compatibility.

Output of the GLEAMS model places constraints on the vadose zone model. Specifically, the daily time step of GLEAMS must be incorporated into the vadose zone component, or a method must be developed to disaggregate the daily outputs of GLEAMS.

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MODEL FRAMEWORK

With these objectives in mind, a numerical model of solute transport in the vadose zone was developed. A linear finite element formulation was selected because of its proven accuracy (van Genuchten, 1978; Huyakorn and Pinder, 1983; de Marsily, 1986). The numerical model can also be used as a starting point for future simplifications. With the type of model chosen, the goal was to develop an efficient computational scheme.

Moisture Flow

The processes which occur in the unsaturated zone include infiltration and redistribution of water and transport of chemicals or solutes. Water flow is controlled by the total soil water potential in the soil and is governed by Richards equation. Written in one-dimensional (1-D) form, this equation can be expressed as:

$$C \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left[K \frac{\partial}{\partial z} (\psi - z) \right] \qquad (1)$$

where C is specific moisture capacity (1/L), Ψ is matric pressure (L), t is time (T), K is unsaturated hydraulic conductivity (L/T), and z is the vertical coordinate, positive downward (L). Specific moisture capacity is defined as:

$$C = \frac{d\theta}{d\psi} \qquad (2)$$

where θ is volumetric moisture content (L^3/L^3). Equation (1) was solved using a finite element solution with linear basis functions.

The unsaturated hydraulic conductivity was related to the matric potential using van Genuchten's (1980) relation:

$$K = K_s \frac{\{1 - (\alpha h)^{n-1} [1 + (\alpha h)^n]^{-m}\}^2}{[1 + (\alpha h)^n]^{m/2}} \qquad (3)$$

where K_s is saturated hydraulic conductivity (L/T), h is matric suction, the absolute value of the matric pressure (L), and α, m, and n are fitted coefficients. The coefficient m can be expressed in terms of n as m = 1-1/n.

The moisture content was related to the matric pressure through the relation (van Genuchten, 1980):

$$\theta = \theta_r + (\theta_s - \theta_r) [1 + (\alpha h)^n]^{-m} \qquad (4)$$

where θ_r is residual moisture content (L^3/L^3), and θ_s is saturated moisture content (L^3/L^3). The specific moisture capacity can be evaluated by differentiating equation (4) with respect to Ψ or h:

$$C = - \frac{d\theta}{dh} = (\theta_s - \theta_r) (mn\alpha) [1 + (\alpha h)^n]^{-(m+1)} (\alpha h)^{n-1} \qquad (5)$$

One must iterate to solve equation (1) since the hydraulic conductivity and the specific moisture capacity are both functions of the dependent variable, Ψ. The Newton-Raphson iteration technique (Huyakorn and Pinder, 1983) was chosen for better convergence of the solution. This iterative technique requires the derivatives of the hydraulic conductivity and specific moisture capacity for solution. These derivatives are presented below.

$$\frac{dK}{d\psi} = - K_s \left[\left(\{1 - [(\alpha h)^{n-1}] [1 + (\alpha h)^n]^{-m}\}^2 \right) \right.$$
$$\left\{ \frac{-mn\alpha}{2} [1 + (\alpha h)^n]^{-(m/2+1)} (\alpha h)^{n-1} \right\}$$
$$+ (2 \{1 - [(\alpha h)^{n-1}] [1 + (\alpha h)^n]^{-m} \}$$
$$\{(1 - n) \alpha (\alpha h)^{n-2} [1 + (\alpha h)^n]^{-m}$$
$$+ mn\alpha [(\alpha h)^{n-1}]^2 [1 + (\alpha h)^n]^{-(m+1)}\})$$
$$\left. \{ [1 + (\alpha h)^n]^{-m/2} \} \right] \qquad (6)$$

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$$\frac{dC}{d\psi} = -([mn\alpha \ (\theta_s - \theta_r)]$$

$$\{\alpha(n-1) \ [1+(\alpha h)^n \ ]^{-(m+1)} \ (\alpha h)^{n-2}$$
$$+ \ [-n\alpha(m+1)] \ [(\alpha h)^{n-1}]^2 \ [1+(\alpha h)^n \ ]^{-(m+2)}\})$$

$$(7)$$

A specified matric pressure must be used to calculate the coefficients expressed in equations (3), (5), (6), and (7). That is, a choice must be made to evaluate these coefficients using the matric pressure calculated at the previous time step, using an average of the matric pressure values obtained from the current and previous time levels, leads to less oscillations and generally a much faster convergence (van Genuchten, 1978). For this reason, this averaging technique was employed in the developed model.

Solute Transport

The advection-diffusion equation for soluble chemical transport in 1-D can be written as:

$$\frac{\partial C_T}{\partial t} = -\frac{\partial J_T}{\partial z} + S_s \qquad (8)$$

where C_T is total mass of chemical stored per total volume of soil (M/L^3 total volume), J_T is total solute flux ($M/L^2/T$), and S_s is a source (+) or sink (-) term (M/L^3 total volume/T).

Total chemical concentration in the soil is composed of liquid, solid, and vapor phases. The vapor phase component was assumed to be small in comparison to the liquid and solid phases and was disregarded in the calculations. The total concentration can then be calculated as:

$$C_T = \rho_b \ C_s + \theta \ C_1 \qquad (9)$$

where ρ_b is soil bulk density (M soil/L^3 total volume), C_s is mass of chemical adsorbed per mass of soil (M/M soil), and C_1 is mass of chemical per volume of soil solution (M/L^3 solution). A linear adsorption isotherm was assumed, relating the liquid and solid concentrations:

$$C_s = k_d \ C_1 \qquad (10)$$

where k_d is the adsorption coefficient (L^3 solution/M soil). The total concentration can then be expressed as:

$$C_T = C_1 \ \theta \ R \qquad (11)$$

where:

$$R = 1 + \frac{\rho_b \ k_d}{\theta} \qquad (12)$$

The solute flux is composed of a vapor, a dispersive, a diffusive, and a mass or advective flux. For this analysis, the vapor flux was assumed negligible. The total solute flux can then be written as:

$$J_T = C_1 \ q - D_e \ \theta \ \frac{\partial C_1}{\partial z} \qquad (13)$$

where q is volumetric moisture flux or Darcy flux (L^3 solution/L^2/T) and D_e is the effective diffusion/dispersion coefficient (L^2/T). D_e is calculated as:

$$D_e = D_o \tau + \lambda |q/\theta| \qquad (14)$$

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where D_o is the chemical ionic or molecular diffusion coefficient (L^2/T), τ is the soil tortuosity factor, and λ is soil dispersivity (L). $|\ |$ denotes the absolute value.

Combining these equations, the advection-diffusion equation is:

$$\frac{\partial\,(\,\theta\,R\,C_1\,)}{\partial\,t} = \frac{\partial}{\partial\,z}\,(\,D_e\,\theta\,\frac{\partial\,C_1}{\partial\,z} - C_1\,q\,) + S_s$$

$$(15)$$

Sources and sinks can be expressed in terms of zero- and first-order decay terms (van Genuchten, 1978): ·

$$S_s = (\,\nu\,\theta + \beta\,\rho_b\,k_d\,)\,C_1 + \gamma\,\theta \quad (16)$$

where ν is a first-order rate constant for liquid phase solute generation ($1/T$), β is a first-order rate constant for solid phase solute generation ($1/T$), and γ is a zero-order rate constant for liquid phase solute generation ($M/L^3/T$).

Equation (15) was solved using a finite element solution with linear basis functions. Data requirements for the solute transport component of the model include ρ_b, τ, λ, k_d, ν, β, and γ for each soil layer and D_o for the solute. The soil tortuosity factor, τ, is an empirical factor smaller than unity which expresses the ratio of the straight-line length of a soil sample to the average roundabout path length through the water-filled pores. The dispersivity, λ, normally must be estimated from field observations. Davidson et al. (1975) suggest a dispersivity value of 0.08 (cm). The adsorption coefficient can be estimated from the equation (Rao and Davidson, 1982):

$$k_d = k_{oc}\,\frac{OC}{\cdot 100} \quad (17)$$

where k_{oc} is organic carbon adsorption coefficient (L^3/M), and OC is percent organic carbon in the soil. Neglecting zero-order chemical production, the degradation terms can be combined such that:

$$S_s = -\,\mu_e\,\theta\,C_1 \quad (18)$$

where:

$$\mu_e = \nu + \frac{\beta\,\rho_b\,k_d}{\theta} \quad (19)$$

μ_e is the effective first-order decay coefficient, which can be estimated from the half-life of the chemical in question, $t_{1/2}$

$$\mu_e = \frac{0.693}{t_{1/2}} \quad (20)$$

A sensitivity analysis will be performed in the future to evaluate the importance of each of the coefficients in the model.

Linking to the GLEAMS Model

The finite element solute transport (FEST) model can be linked to the GLEAMS model by using output from the pesticide component of GLEAMS. This output includes daily percolate volumes and concentrations of the solutes being modeled. These data can be read into the FEST model as an upper boundary condition. For the moisture transport portion of the model, the daily percolate volume represents the flux into the soil for a 24-hour period. On any day without percolation, the flux is assumed to be zero. Since no direct linkage is made with the GLEAMS model, no upward flux into the root zone is allowed. With the flux into the soil known and the concentration of that flux also

known, the mass loading into the upper boundary of the vadose zone can be calculated. The bottom of the vadose zone is defined by the water table. At this point the matric pressure and the spatial derivative of the solute concentration are assumed to be zero.

The FEST model uses 24-hour time steps to agree with GLEAMS output. In certain cases, this large time step can lead to instability in the solution of the transport equation. The FEST model checks for instability by calculating the peclet number and courant number at each node for each time step. The peclet number is calculated as:

$$Pe = \frac{q \; \Delta z}{\theta \; D_e} \qquad (21)$$

where Δz is the spatial increment between nodes (L), and D_e is the effective diffusion/dispersion coefficient (equation (14)). The courant number is calculated as:

$$Cr = \frac{q \; \Delta t}{\theta \; \Delta z} \qquad (22)$$

where Δt is the time increment (T). Huyakorn and Pinder (1983) recommend that the peclet number not exceed 2 and that the courant number not exceed 1. When the model calculates numbers which exceed these limits, the user is notified. In these cases, it will be necessary to reduce the time step of the FEST model and break down the daily inputs of the GLEAMS model into smaller time intervals.

MODEL VERIFICATION

Two tests were performed to mathematically verify computations made by the FEST model. The first verification test compared FEST results to an analytical solution for transport in a homogeneous soil with steady moisture flow (van Genuchten, 1978). The second verification test

compared FEST results for a simulation of transient flow and transport to results from a similar numerical model developed by van Genuchten (1978). The main differences between the two numerical models are in the methods used to determine the specific moisture capacity, the iteration methods, and the type of basis functions used in the finite element formulation. For both of the verifications tests, the simulations were performed without the GLEAMS root zone model, with the FEST model simulating transport from the soil surface down. Neither of the tests examined the effects of uptake by plant roots.

For the first verification test, transport of a solute pulse through a homogeneous soil was simulated. Two simulations were performed, the first with decay and adsorption, the second with only adsorption. The input data sets for the first verification tests are presented in table 1. A pulse of solute was introduced into the profile at a constant rate over the period from 0 to 5 days. During this period a constant solute flux was assumed for the upper boundary condition. Following this period a solute flux of zero was used. The moisture flux in the profile was constant. The time step and the spatial increment used for the simulation were 0.25 days and 2 cm, respectively. Results of the two simulations were presented in figure 1. FEST results compared well with the analytical results.

The second verification test examined transient flow and transport in a non-homogeneous soil profile. In brief, the soil profile consisted of ten layers of different soil types. The top layer was a clay loam, which extended down to 25 cm. Under the clay loam was a sandy loam which changed gradually to a sand at 68 cm. There was a dense soil layer from 75 to 87 cm, underlain by a sand which extended to the bottom of the profile at 170 cm. Each of these layers were characterized by different hydraulic and transport characteristics. A pulse of solute at a concentration of 20 meq/l was introduced into the profile from time 0 to half a day, after which the solute concentration in the infiltrating water became zero. The infiltration rate during this period was 25 cm/day and continued for one day. Following the infiltration period, the soil experienced constant evaporation
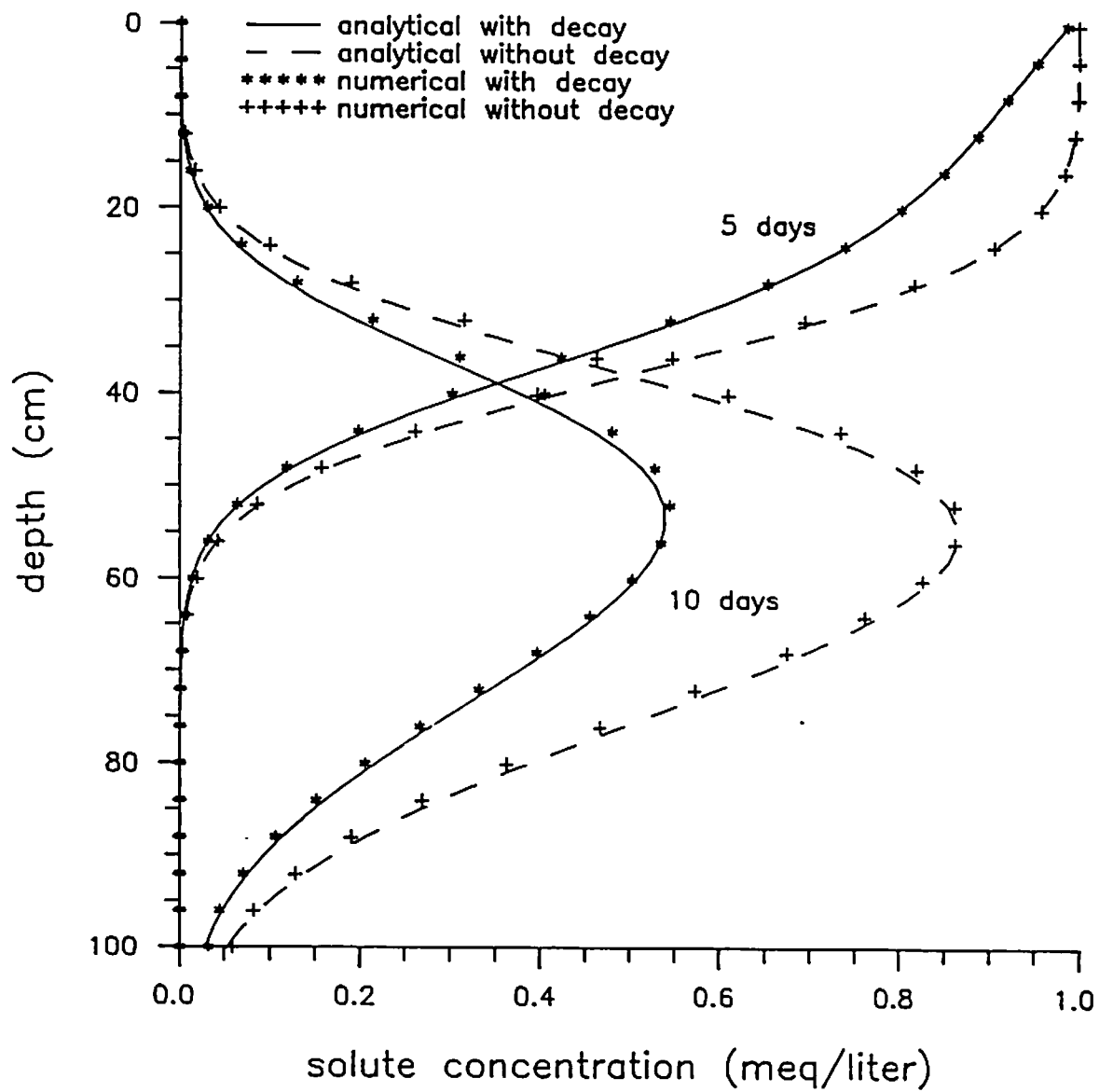
Figure 1. Calculated solute concentrations versus depth for a chemical undergoing linear adsorption and linear decay during constant velocity infiltration.

at a rate of 0.5 cm/day from the surface. A complete description of this example, as well as the input characteristics of each of the soil layers, is given in van Genuchten (1978).

For the FEST simulation, the upper boundary condition for the matric pressure solution was set by the infiltration rate. Free drainage was assumed at the bottom of the profile, that is $d\psi/dz = 0$ at $z = 170$ cm. The upper boundary condition for solution of the advection-diffusion equation was set by the known solute flux at that point. The concentration gradient, dC_i/dz, at the bottom of the profile was assumed to be zero. A

Table 1. Parameter set for the first verification tests.

Parameter	Value
Profile pore velocity	25.0 cm/day
Profile moisture content	0.30 cm³/cm³
Initial concentration in profile	0.0 meq/l
Inflow concentration	1.0 meq/l $\quad 0 < t \leq 5$ days 0.0 meq/l $\quad\quad t > 5$ days
Bulk density	1.40 gm/cm³
Absorption coefficient	0.50 gm/cm³
Solid phase first-order rate constant	-0.05 1/day with decay 0.00 1/day without decay
Effective diffusion coefficient	37.5 cm²/day
Liquid phase first-order rate constant	-0.10 1/day with decay 0.00 1/day without decay
Liquid phase zero-order rate constant	0.0 meq/l/day
Δt	0.25 day
Δz	2.00 cm

time step of 0.001 days and a spatial increment of 1 cm were used for this simulation.

Figures 2 and 3 present comparisons of the matric potentials calculated by the FEST model to those calculated by the van Genuchten (1978) model. As the figures show, the models predicted slightly different results for this complex soil profile. These differences should be expected because of the differences in the formulations of the two models. The magnitude of the differences decreased at the end of the 8-day simulation. Figures 4 and 5 present comparisons of the solute concentrations predicted by the two models. The rate of advance of the solute front predicted by the two models was approximately the same. The overall decay rate was also quite close.

The sharp breaks at 75 cm in the matric potential and the solute concentration curves coincide with the dense soil layer in the profile. In the case of the matric potential curve, the break occurs within the soil layer and is caused by differences in the moisture characteristics of this layer. For the concentration profile, the break occurs directly above the soil layer. The break in the concentration profile appears to be caused by a change in the hydraulic gradient within the dense soil layer. This changes the direction of the flow in this area and alters the advective flux.

MODEL TESTING

A data set published by Warrick et al. (1971) was used to conduct a preliminary test of the model accuracy. The data is from a field study in which the concentration of chloride was measured during infiltration into a 125 cm deep homogeneous Panoche clay loam. The initial and boundary conditions were estimated from information in the publication. The initial matric pressure at the soil surface was -270 cm, decreased linearly down to -159 cm at 60 cm below the surface, and remained constant from 60 cm down. The initial concentration in the soil was 0 meq/l. The soil surface was ponded with water with a chloride concentration of 209 meq/l for 2.8 hours after which time pure water was applied. Constant matric pressures of 0 cm and -159 cm were assumed at the upper and lower
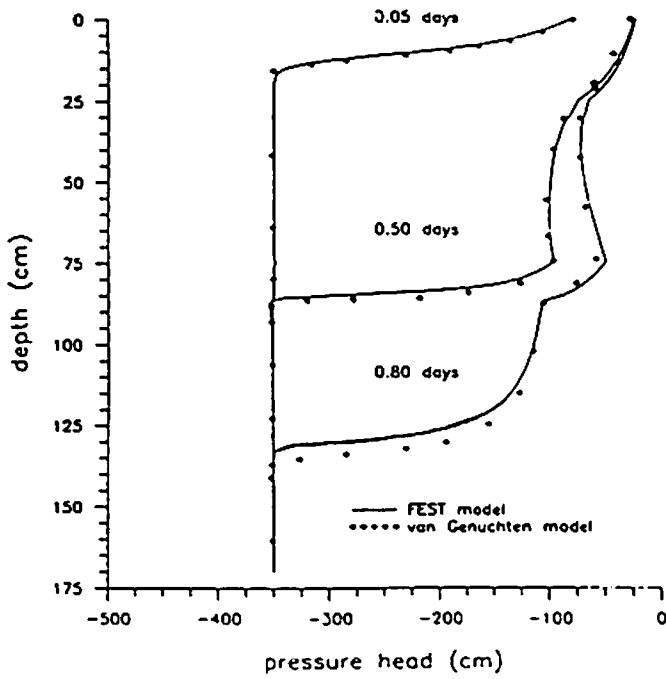
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Figure 2. Calculated pressure distributions during infiltration for the 10-layer verification test profile.
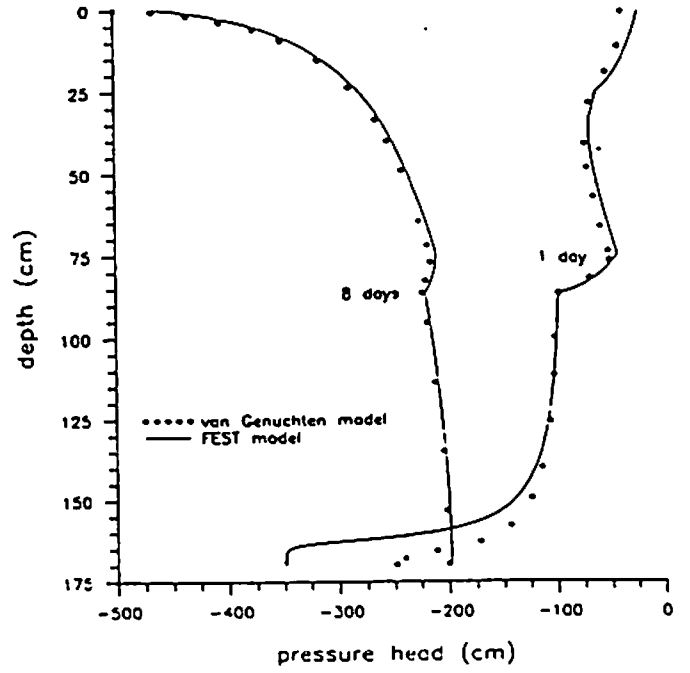

Figure 3. Calculated pressure distributions during evaporation for the 10-layer verification test profile.
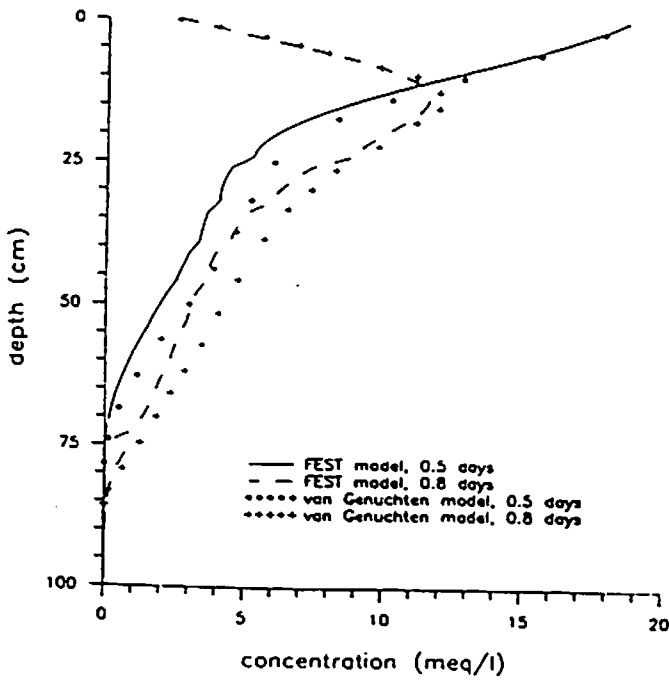

Figure 4. Calculated concentration distribution during infiltration for the 10-layer verification test profile.
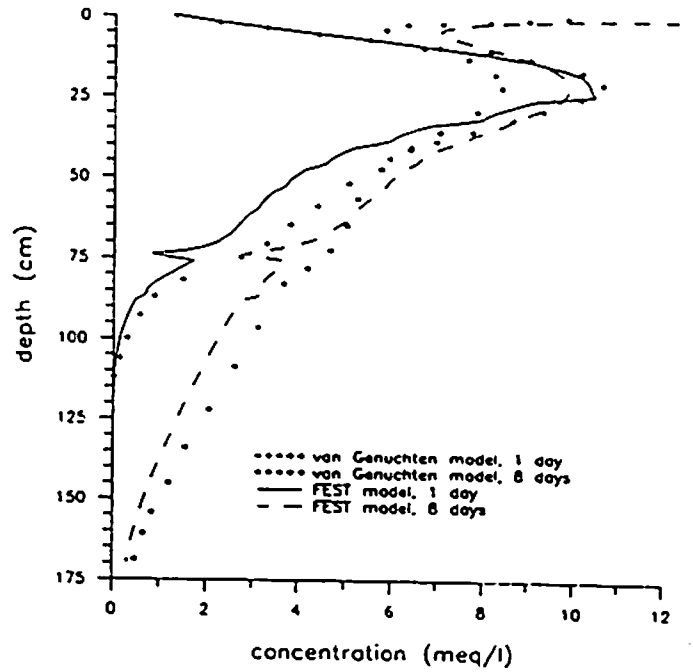

Figure 5. Calculated concentration distributions during evaporation for the 10-layer verification test profile.

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boundaries, respectively. A solute flux boundary condition was assumed at the upper boundary and the spatial derivative of the concentration gradient at the bottom of the profile was assumed to be zero. The adsorption coefficient and the decay rate were set at Hx zero since the solute (chloride) is conservative. The other input parameters for this simulation are listed in table 2. This simulation was also performed without the GLEAMS linkage since there were no plants on the field site.

Results of the matric potential simulation for the Panoche soil are shown in figure 6. The figure presents a comparison of observed data to predictions made by the model at 2, 9, and 17 hours. The model tended to underpredict the rate of advance of the moisture front. This could be attributed to inaccuracy of the fit of the van Genuchten K-ψ relation, equation (3), for this

Table 2. Parameter set for the Panoche clay loam simulation

Parameter	Value
Saturated moisture content	0.38 cm^3/cm^3
Residual moisture content	0.15 cm^3/cm^3
Saturated hydraulic conductivity	0.026 cm/min
n, soil moisture parameter	1.4
α, soil moisture parameter	0.064
Bulk density	1.22 gm/cm^3
Adsorption coefficient	0.00 gm/cm^3
Effective decay coefficient	0.00 1/min
Effective diffusion coefficient	0.07 cm^2/min
Δt	0.50 min
Δz	1.00 cm

particular soil. It appears that the equation underpredicted the hydraulic conductivity in the soil as it was wetting, thus reducing the rate at which the moisture front advanced. Better results have been obtained by using the K-ψ relation for this soil developed by Warrick et al. (1971) (Bosch, 1988). However, this would not be testing the complete model as it was intended to be used.

Results of the transport simulation for the Panoche soil are shown in figure 7. The model underpredicted the rate of advance of the solute plume as well as the magnitude of the plume, e.g. see 17 hour data. This can be related back to the underprediction of the rate of advance of the moisture front. Since the rate of advance of the moisture front was underpredicted, the total flux into the soil was also underpredicted. This decreased the mass of chemical brought into the soil during the period from 0 to 0.5 hours. The total mass of chloride in the soil was thus underpredicted. Without adsorption, the rate of advance of the solute plume is directly related to the rate of advance of the moisture front. In addition, some inaccuracies may have occurred because the transport conditions in this experiment may not have followed classical advection-diffusion theory.

SUMMARY

A finite element model for predicting transport of solutes through the vadose zone has been presented. The model was developed to be linked to the GLEAMS root zone model, and can use GLEAMS output in the pesticide pass file as input. The model can be set to work on a daily time step to be compatible with the time steps used in the GLEAMS model. The model was verified using an analytical solution for transport of solutes in the unsaturated zone and through comparison with a similar numerical model.

Testing of the model has indicated some areas which require additional analysis. Testing indicated that obtaining a good characterization of the hydraulic characteristics of the soil is critical. Since the hydraulics drive the transport process, any inaccuracies in the moisture flow
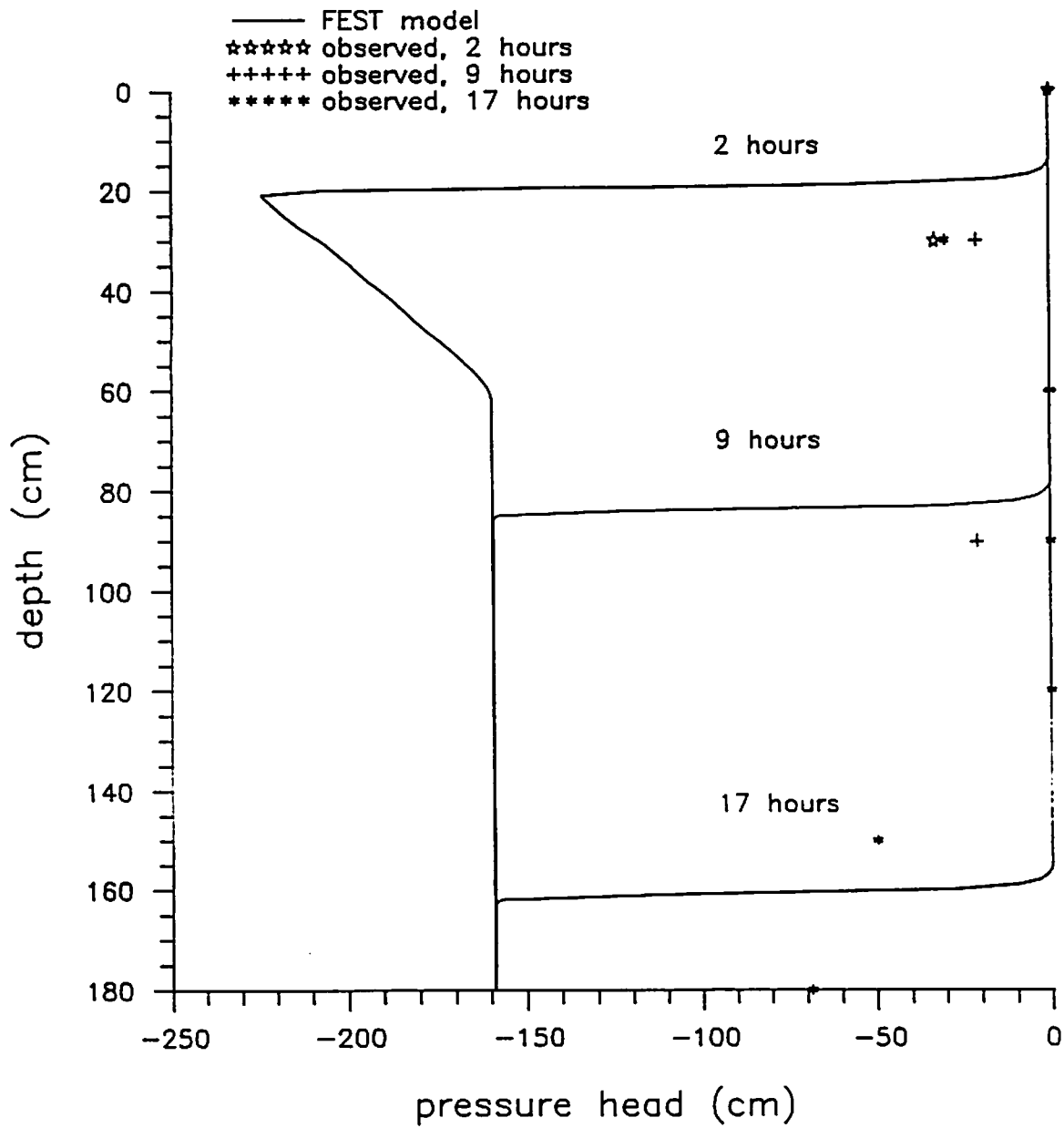
Figure 6. Calculated and observed pressure distributions for the Panoche silt loam soil.
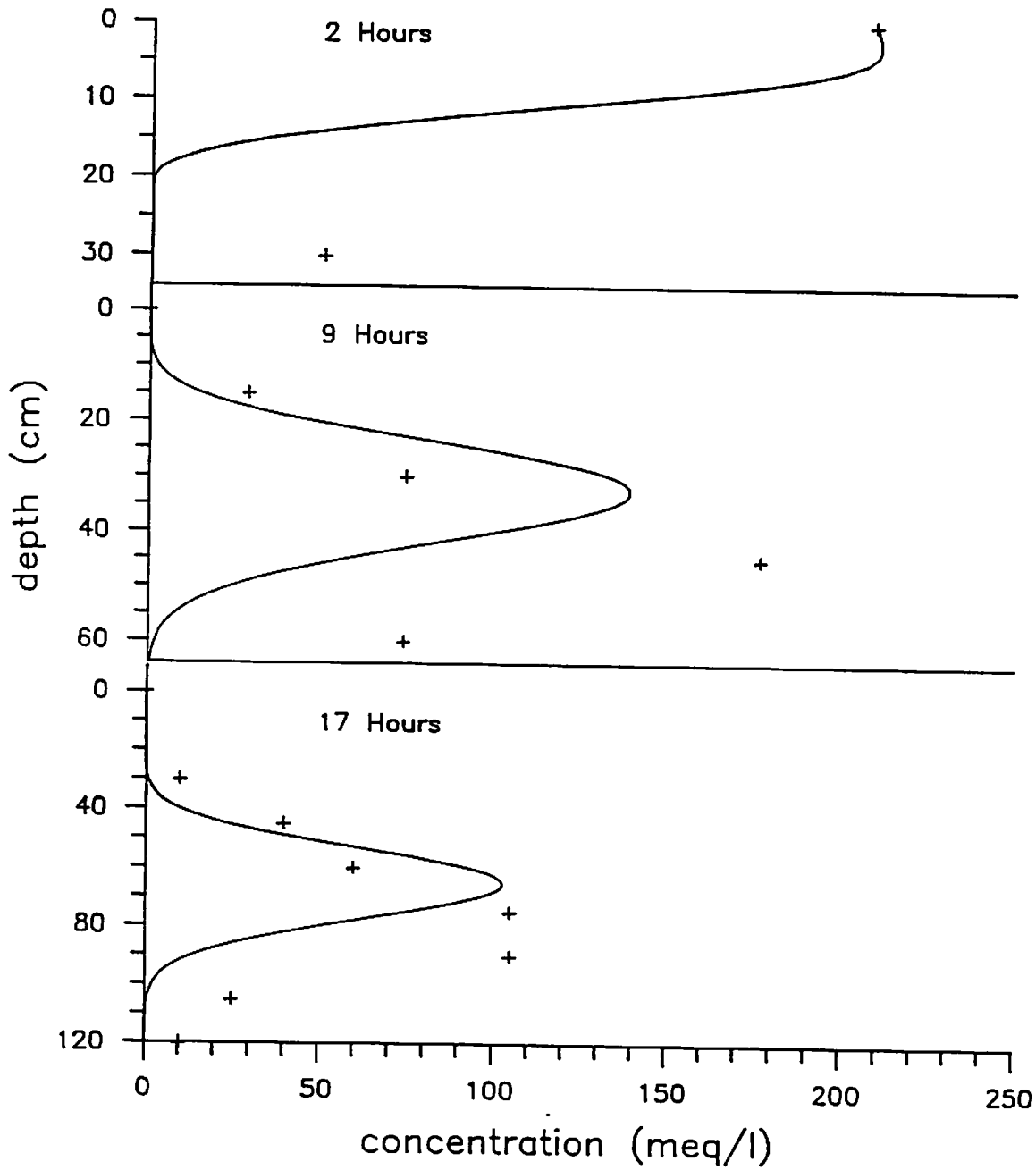
Figure 7. Calculated (lines) and observed (+) concentration distributions for the Panoche silt loam soil.

portion of the model are compounded in the solute transport calculations.

Future efforts will be concentrated on developing better methods for characterizing the K-ψ relation of soils in the vadose zone and on evaluating better methods to incorporate vertical spatial variability into the model. In addition, a sensitivity analysis will be performed in an attempt to reduce the number of parameters required by the current model structure. Additional testing is required to determine the accuracy of the complete root-vadose zone model and the effects of the constant time step on the stability of the solute transport solution.

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LIST OF SYMBOLS

Symbol	Description
C	Specific moisture capacity (1/L)
C_1	Mass of chemical per volume of soil solution (M/L^3)
Cr	Courant number
C_s	Mass of chemical adsorbed per mass of soil (M/M)

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C_T Total chemical mass per total soil volume (M/L^3)

D_e Effective diffusion/dispersion coefficient (L^2/T)

D_o Molecular diffusion coefficient (L^2/T)

h Matric suction (L)

J_T Total solute flux ($M/L^2/T$)

k_d Adsorption coefficient (L^3/M)

k_{oc} Organic carbon adsorption coefficient (L^3/M)

K Unsaturated hydraulic conductivity (L/T)

K_s Saturated hydraulic conductivity (L/T)

m Soil moisture coefficient

n Soil moisture coefficient

OC   Percent organic carbon in the soil (%)

Pe   Peclet number

q Moisture flux (L/T)

R   Retardation coefficient

S_s Solute source (+) or sink (-) ($M/L^3/T$)

t Time (T)

$t_{1/2}$ Chemical half-life (T)

z Vertical coordinate (L)

α Soil moisture coefficient

β First order rate constant for solid phase solute generation (1/T)

γ Zero-order rate constant for liquid phase solute generation ($M/L^3/T$)

θ Volumetric moisture content (L^3/L^3)

θ_r Residual moisture content (L^3/L^3)

θ_s Saturated moisture content (L^3/L^3)

λ Soil dispersivity (L)

μ_e Effective first-order decay coefficient (1/T)

ν First-order rate constant for liquid phase solute generation (1/T)

ρ_b Soil bulk density (M/L^3)

τ Soil tortuosity factor

ψ Matric pressure (L)

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