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PREDICTION OF SOLUTE BREAKTHROUGH FROM SCALED SOIL PHYSICAL PROPERTIES

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ABSTRACT

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Solute transport in unsaturated soil may be described with a transfer function model in which the travel time distribution for a nonreactive solute depends on the distribution of the flow velocity (V). When the spatial variable V is described with the scaling theory of similar media, the travel time distribution follows from the scaling factor (δ) distribution.

Using an experimentally assessed distribution for δ, the travel time distributions were calculated with Monte Carlo simulation. By comparison of travel time distributions found by assuming that the hydraulic conductivity [$K(\theta)$], the volumetric moisture fraction θ, or both are stochastic variables, we found that the stochastic nature of $K(\theta)$ was the dominant factor in the transport process. Assuming θ constant, an analytical approximation was derived for the travel time distribution in a soil system that is homogeneous with depth. The approach was used to predict the breakthrough of an inert tracer from an unsaturated–saturated system. Comparison of these predictions with the observed breakthrough suggests a relatively fast breakthrough that could not be accounted for by our simplified model.

INTRODUCTION

A quantitative understanding of solute transport under field conditions is needed for predicting field-scale behavior and transport of contaminants and nutrients. At first, the convection–dispersion equation (CDE) was assumed to describe transport adequately, but as experimental information increased it became apparent that the CDE model was unable to accurately quantify transport under field conditions due to, among others, soil heterogeneity (Biggar and Nielsen, 1976; Bowman and Rice, 1986; Richter and Jury, 1986).

To take such heterogeneity into account, Jury (1982) introduced the "transfer function" concept. His approach is based on the expectation that

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processes in soils are too complex to be adequately modeled in a deterministic manner, but that the overall response of a system may be measured. In view of the breakthrough often observed in natural soil systems, the response upon an input impulse is explained by a lognormally distributed residence time of solute in the system. In later work, Jury et al. (1986) gave a physical interpretation of the transfer function representing the field by a macroscopically homogeneous column. White et al. (1986) and Jury et al. (1982) applied the concept to both columns and field plots. Because the CDE model predicts a normally distributed residence time for realistic dispersion coefficients and column lengths, this model is often less adequate than the transfer function model (TFM). The CDE model remains popular moreover, because of the simplicity to evaluate analytical solutions of the CDE, and the simplicity in obtaining a field average flow velocity (from the average moisture content and the net recharge rate), which is necessary as model input. The residence time in the TFM approach varies around an average value which may be very small for solutes transported in macropores, and very large for solutes that enter a stagnant soil water phase. As was shown by Sposito et al. (1986), this may lead to a nonnormal distribution of travel times not accounted for by the CDE.

Both modeling approaches require a parameter which accounts for soil heterogeneity. For the CDE model this is the dispersion coefficient, which becomes very large if the residence time is not normally distributed. In view of the physical background of the dispersion coefficient (Bolt, 1979) there is little inclination to accept such large values (Bresler and Dagan, 1979). On the other hand, the TFM approach lumps heterogeneity into a variance of the residence time without giving a physical meaning to the model parameters. However, due to increased interest by soil physicists and hydrologists to describe flow and transport in spatially variable flow domains, it has now become feasible to give a physical background and a quantification of the residence time distribution.

A promising way to describe water flow, taking into account the spatial variability of soil hydraulic properties, is offered by means of the scaling theory of similar media. The concept of scaling soil hydraulic properties was introduced by Miller and Miller (1955, 1956), and has been later applied successfully by Warrick et al. (1977), Russo and Bresler (1980), and Hopmans (1987). The scaling theory was used by Bresler and Dagan (1979), Dagan and Bresler (1979) to describe field-averaged transport of a nonreactive solute, and by Van der Zee and Van Riemsdijk (1987) for a reactive solute.

In this paper, we present a method to predict the solute residence time distribution from the scaling factor distribution. The method is illustrated by application to a field situation.

THEORY

The scaling technique

The purpose of scaling is to provide a simple mechanistic description of part of the variance of properties of interest. By scaling, the spatial variability of soil hydraulic properties is expressed by the variability of an ensemble of scale factors, δ_i, that relate the soil hydraulic properties at each sampled location, i, to a reference.

The scaling parameter, δ_i, is defined as the ratio of a microscopic characteristic length, λ_i, of a soil at location i, and the characteristic length, λ_m, of a reference soil (Peck et al., 1977):

$$\delta_i = \lambda_i / \lambda_m \tag{1}$$

Scaling theory results in a relation of the soil water retention and hydraulic conductivity curve at any location i, with a mean pressure head h_m and hydraulic conductivity K_m, such that for the soil water pressure head (negative in the unsaturated zone):

$$h_i = h_m / \delta_i \tag{2}$$

and for the unsaturated hydraulic conductivity:

$$K_i = \delta_i^2 K_m \tag{3}$$

For similar media, eqns. (2) and (3) hold for h_i and K_i measured at different water contents. Owing to the fact that soils in general do not have identical values of porosity, h and K are written as a function of degree of saturation S rather than volumetric moisture fraction θ.

Reference soil water retention curves and reference $K(\theta)$ relations, and the corresponding scaling factor distributions can be assessed with techniques as described by Hopmans (1987). In accordance with Rao et al. (1979), a distribution of the scaling factors may be tested for log-normality. If true, the continuous scaling factor distribution may be used for interpolation and extrapolation to other retention functions $\theta(h)$ than those found experimentally. In case there is good agreement between the scale factors determined from conductivity and water retention data, the distribution characteristics of the latter are sufficient to describe the variation of both hydraulic functions. With the probability density functions (PDF's) of δ and the reference curves, the hydraulic properties are fully characterized, and flow may be calculated once initial and boundary conditions are specified.

Derivation of the residence time distribution

To derive the travel time distribution we assume that the following conditions are met: (1) gravity flow, i.e., a unit hydraulic gradient; (2) steady-state water flow; (3) a uniform soil profile with respect to the hydraulic properties; and (4) a purely convective vertical transport. Based on these assumptions, the controlling variable time may be expressed as the amount of water drained (Van Ommen et al., 1988, this volume).

The pore water velocity V [LT^{-1}] under unit gradient follows from $K(\theta)$ and the volumetric content θ:

$$V = K(\theta)/\theta \tag{4}$$

The variability in both the conductivity, $K(\theta)$ and water content $[\theta(h)]$ relations can be expressed in terms of the variability of the scaling parameter, δ [eqns. (2) and (3)]. In a layer of thickness L the residence time, T (T), equals:

$$T = L\theta/K(\theta) \tag{5}$$

Transformation of time T into the equivalent amount of drain discharge T' is done by multiplication of T with the areally averaged flux density, $\bar{K}$, which equals (Bresler and Dagan, 1979):

$$\bar{K} = K_m \exp(2\mu_Y + 2\sigma_Y^2) \tag{6}$$

K_m is defined as in eqn. (3), and the exponential term is the expectation of the log-normally distributed δ^2, where $Y = \ln\delta$, and μ_Y and σ_Y are the mean and standard deviation of Y respectively.

Combination of eqns. (3), (5), and (6) yields the travel time T' [L], now expressed as percolated water depth:

$$T' = L\theta/\delta^2 \exp(2\mu_Y + 2\sigma_Y^2) \tag{7}$$

From the representative soil water pressure head in the field, and the distribution of the scaling parameter δ, the distribution of travel times to a soil depth L, and thus the breakthrough curve for an instantaneous input of unit magnitude, can be constructed using Monte Carlo simulations. However, the statistical properties of the travel time distribution can also be derived analytically if it is assumed that the variability in T' is mainly determined by the variation in downward flux, $K(\theta)$, and to a lesser extent by the variation in θ, i.e., the water content is kept fixed at a "field-average value". It can then easily be shown (see e.g. Van der Zee and Van Riemsdijk, 1987) that:

$$\mu_{\ln T'} = \ln(L\theta) + 2\sigma_Y^2 \tag{8}$$

$$\sigma_{\ln T'} = 2\sigma_Y \tag{9}$$

where $\mu_{\ln T'}$ and $\sigma_{\ln T'}$ are the mean and standard deviation of $\ln(T')$ respectively. The PDF of T' is:

$$\rho(T') = [T'\sigma_{\ln T'}\sqrt{(2\pi)}]^{-1} \cdot \exp[-(\ln T' - \mu_{\ln T'})^2/2\sigma_{\ln T'}^2] \tag{10}$$

which corresponds with the PDF of the transfer function model (Jury, 1982).

APPLICATIONS

The soil hydraulic properties and their variations, pertaining to both applications to follow, were measured on samples taken from an experiment field in the study area "Hupselse Beek" in The Netherlands. The watershed and the soil physical measurement techniques were described by Hopmans and Stricker (1987). In Table 1 we present the scale factor statistics and the parameters of the analytical hydraulic model of Van Genuchten (1980). The data describe the scaled mean hydraulic functions for both the A and BC-horizon.

TABLE 1

Parameter values for description of variability of soil hydraulic functions

Parameter of Van Genuchten model for scaled mean hydraulic functions	Horizon	
	A(25)*	BC(46)
α	0.0282	0.0238
n	1.451	1.669
θ_s	0.403	0.316
θ_r	0.000	0.000
K_s (cm d^{-1})	72.0	60.0
Statistics scale factor values		
μ_Y	−0.3050	−0.1960
σ_Y	0.8531	0.6492

* Number of sampled locations.

Solute breakthrough for the unsaturated soil

For a first illustration we consider a hypothetical soil profile ($L = 1$ m) consisting of a BC-horizon only. The soil water retention curves of the 46 sample locations within the 0.5 ha field before and after scaling are shown in Fig. 1a and b, respectively. The solid line in Fig. 1b represents the scaled mean water retention curve. Clearly, scaling was very successful in explaining the variations in the $h(S)$ relation.

Figure 2 shows four travel time PDF's, three of which are the result of a Monte Carlo (MC) simulation, while the fourth is determined from the analytical solution [eqn. (10)], to check the accuracy of the MC simulation results. The uniform soil water pressure head at which solute transport is assumed to occur was set equal to -100 cm. Three cases with respect to the origin of the travel time variation are shown: (I) contribution of the flux variability only; (II) contribution of the moisture content variability only, as was done by Bresler and Dagan (1979); and (III) contribution from both the moisture content and flux variability. The number of MC replicates, from which the PDF's were determined, was chosen to be 40,000. The travel times on the horizontal axis of Fig. 2 were sorted into 100 classes of 5 mm width.

From Fig. 2 it appears that the results of the MC simulation for case I (variable flux) is in good agreement with the analytically derived PDF. Furthermore, the travel time distributions of cases I and III are not very different. Figure 2 also shows that the travel time distribution based on a uniform flux [$\delta = 1$ in eqn. (7)], and a variable moisture content (case II) is completely different from all other cases. The variation in travel time for case II is far less than those for a variable flux. We therefore conclude that the variability of the residence time is much more affected by the variability of the flux than by the variability of the moisture content.

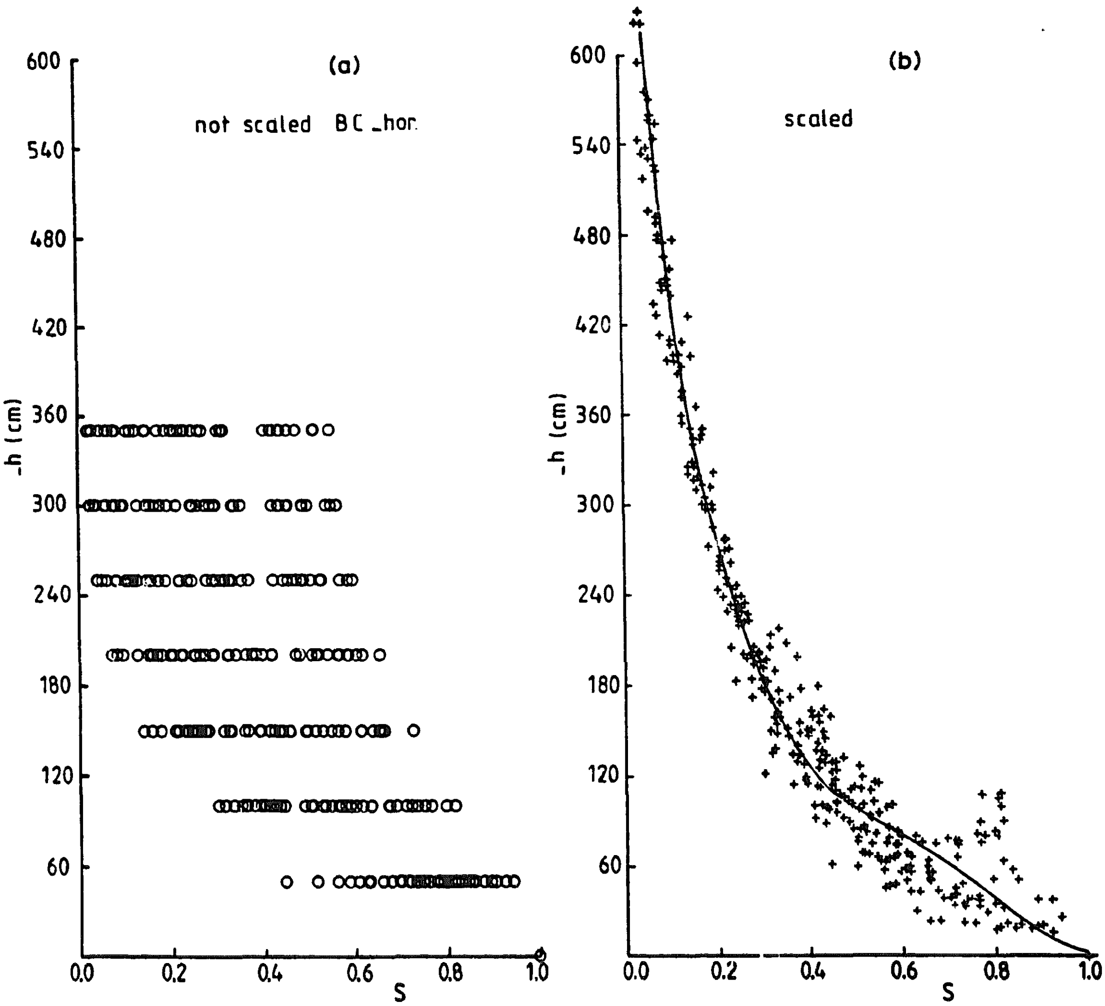

Fig. 1. Unscaled (a) and scaled (b) soil water retention curves of the BC-horizon.

Field experiment

In order to investigate which case would approach the actual solute breakthrough the best in a field soil, we applied the presented theory to a field experiment.

The field experiment involved the study of solute migration in an unsaturated-saturated transport system in the Hupselse Beek catchment area. Bromide tracer solution was uniformly applied to the 260 m long, 11 m wide catchment area of a drain. From the measured bromide concentrations in the drain water, the breakthrough curve from the coupled unsaturated–saturated transport system could be constructed. The experiment is described in detail by Van Ommen et al. (1989, this volume). A study in the same field was also carried out to describe the spatial variability of soil physical properties (Hopmans and Stricker, 1987). Since the variability study discriminated between topsoil (A-

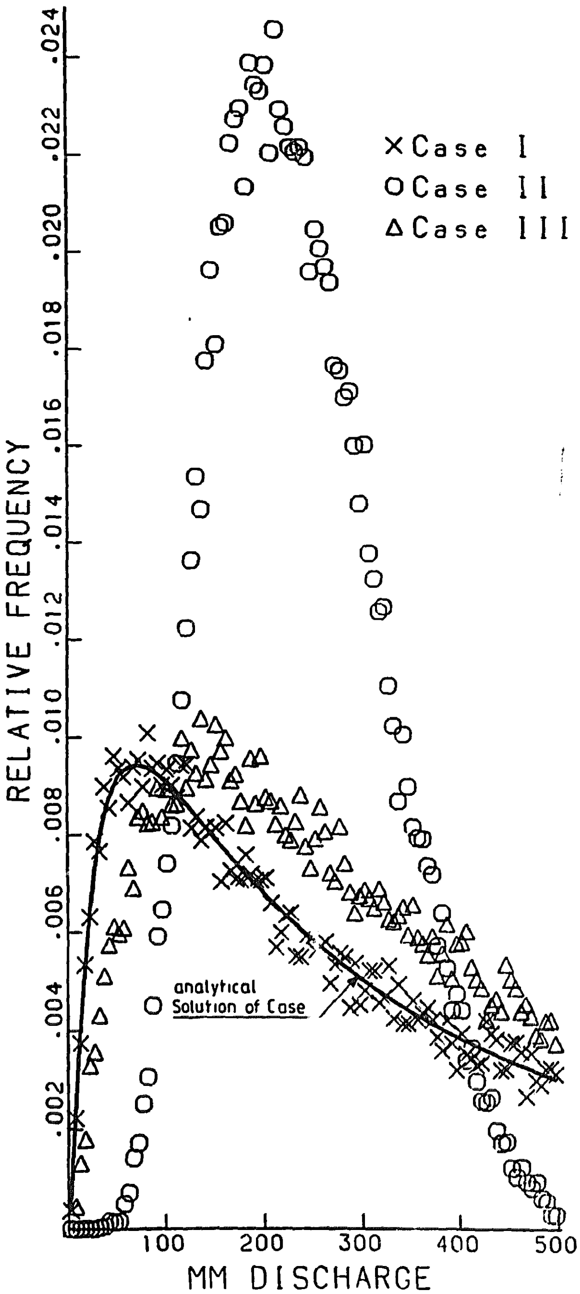

Fig. 2. Travel time distribution functions ($h = -100$ cm) determined from the MC simulations for case I (flux density variable), case II (volumetric water content variable), case III (both flux density and volumetric water content variable), and analytical solution for case I.

horizon) and subsoil (BC-horizon), the simulated flow system was adapted to this situation.

The field transport system is discretized by means of "flow blocks" along the drain. In our case such a flow block consisted of the topsoil, the subsoil, and the saturated zone (Fig. 3). Each block had its own value for the thickness of the

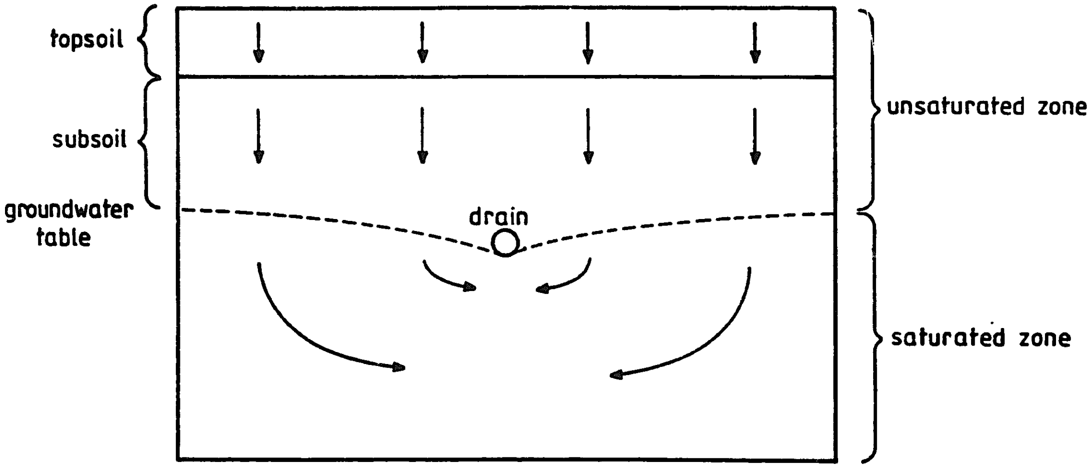

Fig. 3. Flow block of unsaturated–saturated soil water transport system.

subsoil and the thickness of the saturated zone depending on the position along the drain. The thickness of the topsoil was 25 cm.

Transport within a flow block was modeled as follows. Based on MC simulations using eqn. (7), the impulse response for the topsoil transport system was determined. The breakthrough curve at a depth of 25 cm served as input for the second transport system, of which the impulse response could be determined in a similar way. Convolution of the impulse response of the subsoil with the input from the topsoil resulted in a breakthrough curve at the groundwater level. Finally, the concentration in the drainage water of one flow block was calculated from convolution of the concentration at the groundwater level with the impulse response of the saturated transport system. This last procedure is described in detail by Van Ommen et al. (1989, this volume). After averaging of the flow block concentrations, the concentration of the drain water at the outlet of the coupled transport system was determined as a function of the amount of drainage (mm).

Figure 4 shows drain effluent breakthrough curves assuming a variable flux and a fixed moisture content (case I) for various standard deviations in Y. The measured variability of soil physical parameters, expressed in the standard deviations of the scale factor, appears to result in a variation of travel times which is much larger than that derived from the measured solute breakthrough curve. For values of σ_Y smaller than measured (Table 1), calculated solute breakthrough curves were in better agreement with the experimentally determined curve. Although the fit improved at lower variabilities, the measured breakthrough curve still begins sooner than predicted. The value of the soil water pressure head used in this simulation was equal to -100 cm while decreasing this value to -500 cm (not shown) did result in slightly higher concentration values; it did not affect $\sigma_{\ln T}$ [eqn. (9)].

Figure 5 shows the breakthrough curves for a fixed flux and a variable moisture content (case II). The calculated breakthroughs are for soil water pressure head values of -100 cm and -500 cm. We emphasize that the period

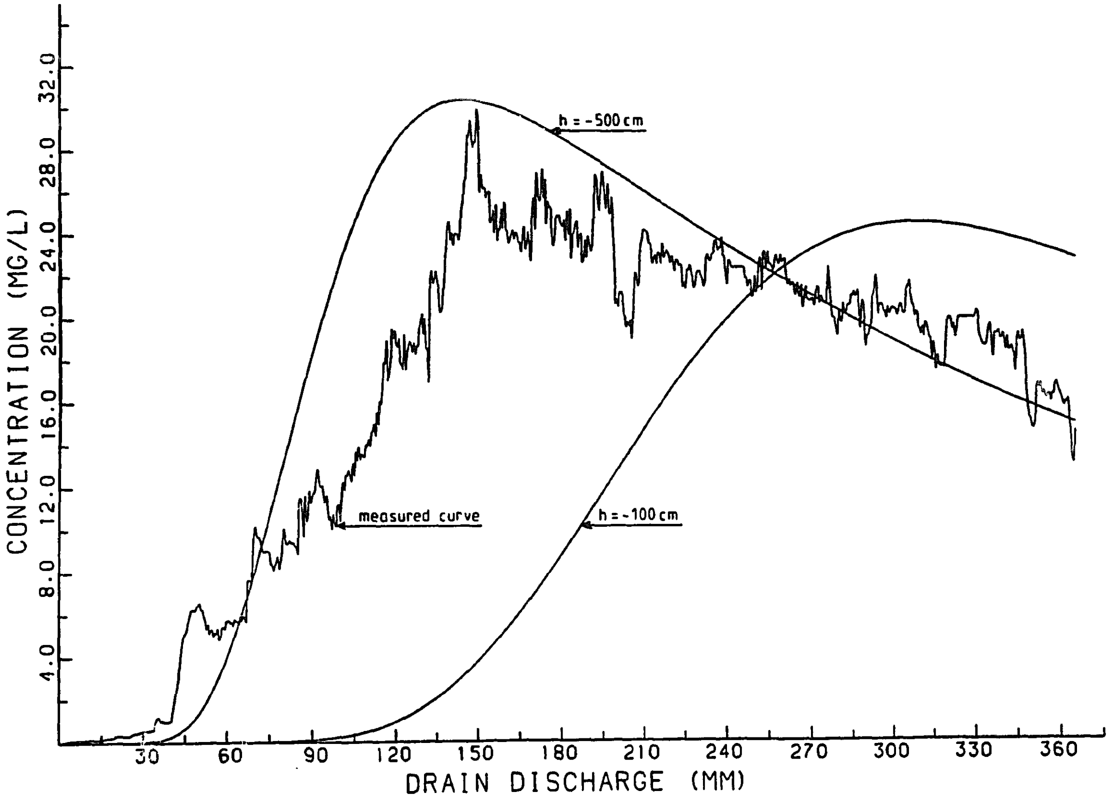

Fig. 4. Observed field breakthrough curve and predicted breakthrough curves (h = − 100 cm) with variable fluxes only (case I) and for different values of σ_Y for the top- and subsoil, respectively. The lowest curve is based on measured variability of scale factors.

of drain discharge up to 250 mm coincides with the winter and spring percolation season, during which the discharge rates are high and transpiration low. Therefore, a representative soil water pressure head of − 100 cm should much closely mimic the actual field situation than a value of − 500 cm, which produced a reasonable fit. From Figs. 4 and 5 it appears that in this case the measured variability of travel times seems to be more determined by the variability of moisture contents than by variable fluxes. This statement must be made cautiously since preferential flow in the subsoil caused an accelerated breakthrough to the groundwater table from the transport system (Van Ommen et al., 1988, this volume). If the experiment had been carried out under ponded infiltration conditions, the variability of fluxes might have been in far better agreement with the predicted breakthrough based on flux variability only.

CONCLUSIONS

We presented a simple model to predict solute breakthrough for an unsaturated soil. The residence time distribution was expressed by means of the statistical properties of the scale factors, and a value for the effective soil water pressure head at which transport presumably occurred. A simple analytical solution could be presented if the water content is uniform in the system.

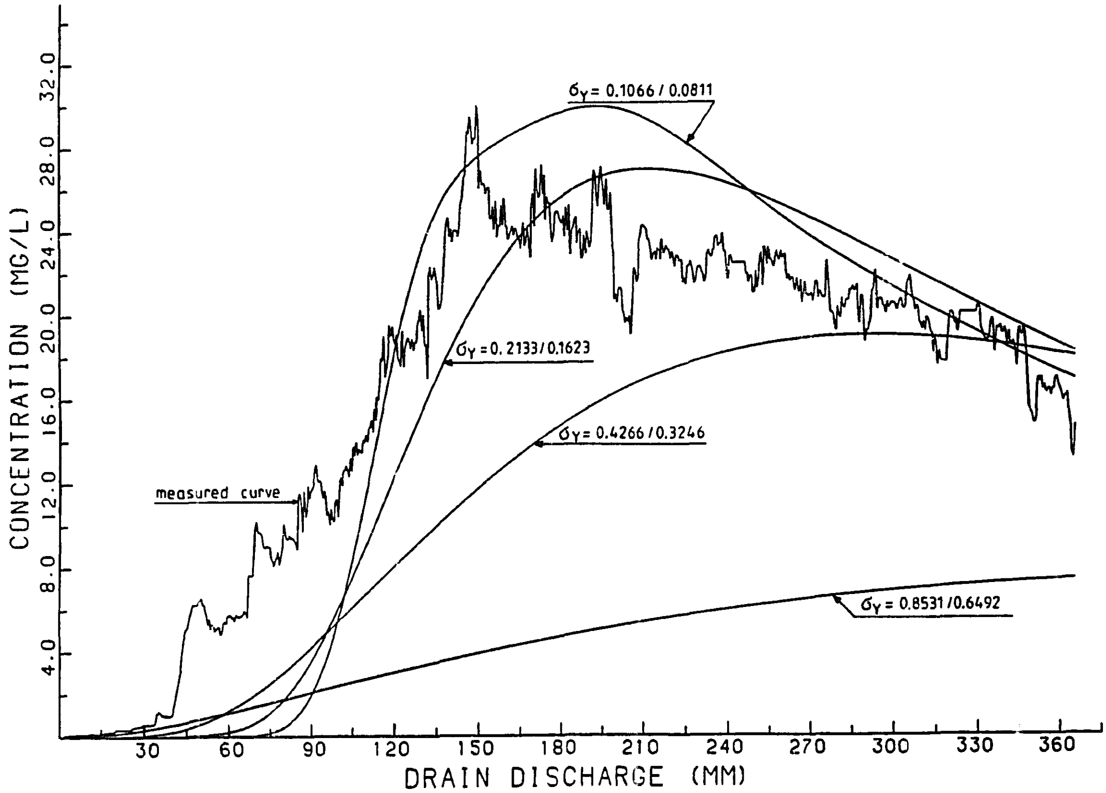

Fig. 5. Observed and predicted drain water breakthrough curves with variable volumetric moisture content only (case II) and for different values for the uniform soil water pressure head.

Application of the model showed that the variability in solute travel times is dominated by the variability in fluxes rather than the variability in volumetric water content.

The model was verified with a field experiment involving the application of bromide to the intake area of a drain, and the measurement of concentrations the drain water. Model results did not agree with the measured breakthrough curve when the measured variability in scale factors and a realistic soil water pressure head were substituted in the model.

We believe that the negative outcome of the field verification experiment does not necessarily prove that the presented model is invalid. However, the simple physically-based expression that translates the parameters of the transfer function concept into measurable quantities, might be more successful under different experimental conditions.

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