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# The Effect of Heterogeneity on Large Scale Solute Transport in the Unsaturated Zone

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The effect of natural heterogeneity on large scale solute transport in the unsaturated zone is investigated using stochastic methods. Several of the physical parameters that control flow and solute transport in the unsaturated zone are regarded as random fields. Specifically, the influence of spatial variability in recharge applied on the surface, saturated hydraulic conductivity, water content at saturation and depth to the groundwater table, on solute flux into the groundwater, is illustrated. It is shown that the prediction of solute penetration into the groundwater through the unsaturated zone is significantly affected by the natural variability in the physical parameters. A simple stochastic model for the estimation of large scale solute flux through the unsaturated zone, is provided.

## Introduction

The unsaturated zone in the upper part of the soil is the link between the soil surface and the groundwater table. It is therefore an important factor in certain aspects of hydrology, such as infiltration and groundwater recharge and quality. The most common approach to modelling flow and transport in the unsaturated zone has been to formulate the mass and momentum balance equations and solve them subject to boundary and initial conditions. The hydraulic parameters that appear in these equations are usually assumed to be uniform over the domain of interest. In other words, the field has been commonly regarded as homogeneous, where the hydraulic parameters are determined by sampling over a few locations and averaging.

Because natural fields exhibit a large variability in their physical properties (*i.e.* they are heterogeneous), it has been recognized by several investigators that accurate field scale modelling of flow and solute transport must account for this heterogeneity (Bresler and Dagan 1981; Nielsen *et al.* 1986; Jensen and Butts 1986). The distribution of the physical properties throughout the field, however, is very difficult to describe deterministically. Furthermore, the variability in these properties has been recognized as essentially random, implying that statistical methods are most appropriate in describing the field scale heterogeneity; thereby, the hydraulic parameters may be regarded as random fields and quantified by probability density functions and correlation structures (Bresler and Dagan 1981).

In this study, the effect of spatial variability in different physical parameters on solute flux into the groundwater through the unsaturated zone, is investigated. Because our interest is to estimate the field scale penetration of solute into the groundwater, we wish to quantify gross (average) values of the solute flux for the entire field, rather than the solute flux at individual points. Thus a simplified flow model and statistical averaging is used, similar to that proposed by Bresler and Dagan (1981). The influence of the spatial variability in the following physical parameters on solute movement in the unsaturated zone is considered: recharge applied on the surface, saturated hydraulic conductivity, water content at saturation and depth from the surface to the groundwater table.

## Deterministic Model for Flow and Solute Flux

### Fluid Flow

We consider a soil extending in the horizontal $x$, $y$ plane with the mean surface at $z = 0$ and $z$ positive downwards. Water flow takes place due to application of recharge $R$ on the surface, at the soil moisture content $\theta$, and at the pore water velocity $V$. We make the same assumptions as Bresler and Dagan (1981), *i.e.*: (1) the flow is vertical, (2) the water flow is steady, implying that the vertical specific discharge, $q$, does not depend on the depth, $z$, or the time, $t$, *i.e.* it is constant in each profile but varies in the $x$, $y$ plane and (3) we neglect soil heterogeneity in the vertical direction as compared to variability in the $x$, $y$ plane. The pore water velocity $V$, is then related to the soil hydraulic properties and the recharge boundary conditions in the following way (Bresler and Dagan 1981):

1) The steady flow is caused by the recharge applied on the surface, $R$, (rainfall, snowmelt, irrigation).

2) If $R<K_s$, where $K_s$ is the saturated hydraulic conductivity, the flow is unsaturated and for gravitational steady flow

$$V = \frac{K(\theta)}{\theta} \doteq \frac{R}{\theta} \tag{1}$$

where $K(\theta)$ is the unsaturated hydraulic conductivity.

3) If $R \geqslant K_s$ ponding occurs and the profile is assumed to be saturated with gravitational flow, *i.e.*

$$V = \frac{K_s}{\theta_s} \tag{2}$$

where $\theta_s$ is the water content at saturation.

4) The relationship $K(\theta)$ adopted here is

$$K(\theta) \equiv K_s \left( \frac{\theta - \theta_{ir}}{\theta_s - \theta_{ir}} \right)^{1/\beta} \tag{3}$$

where $\theta_{ir}$ is the irreducible water content. Although various values have been suggested for the coefficent ß, we assume ß = 0.14, which has been found as a best fit for many soils (Bresler and Dagan 1981).

With regard to the assumption of steady-state flow, a study by Wierenga (1977) shows that solute transport based on a steady-state flow model is comparable with that based on a transient flow model. This implies that even a simple steady-state flow model can provide realistic predictions of field-scale solute transport, which has also been recognized by other investigators (Bresler and Dagan 1981; Nielsen *et al.* 1986; Small and Mular 1987).

**Solute Flux**

Based on the flow assumptions made above, the advection-dispersion equation may be applied in each profile with the pore water velocity $V$, and the dispersion coefficient $D$, independent of $z$, *i.e.*

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial z} \tag{4}$$

where $C$ is the concentration, flux or resident. The definition of resident concentration expresses the mass of solute per unit volume of fluid contained in an elementary volume of the system at a given instant, while the definition of flux concentration expresses the mass of solute per unit volume of fluid passing through a given cross section at an elementary time interval, *i.e.* the flux concentration is the ratio of the solute flux to the volumetric fluid flux. Whenever there are flow paths with different velocities it is in general important to distinguish between these two concentrations (Kreft and Zuber 1978; Parker and van Genuchten 1984).

The solution of Eq. (4) for an instantaneous injection in a semi-infinite domain, with both injection and detection in flux (*i.e.* flux concentration) is (Kreft and Zuber 1978)

$$c_f \equiv \frac{mz}{Q\sqrt{[4\pi Dt^3]}} \exp[-\frac{(z-Vt)^2}{4Dt}] \quad (5)$$

where $m$ is the mass of solute injected in the profile and $Q$ is the volumetric flow rate in the profile. Neglecting molecular diffusion, $D$ is the coefficient of hydrodynamic dispersion, *i.e.* $D = \lambda V$, with $\lambda$ defined as the dispersivity. Regarding the assumption of vertical homogeneity it should be noted that adopting a large field value of $\lambda$, instead of a laboratory measured one, will reflect the heterogeneity of the profile (Bresler and Dagan 1981). The value of $\lambda$ typically ranges from about 0.005 m or less for laboratory scale experiments involving disturbed soils, to about 0.1 m or more for field scale experiments (Nielsen *et. al.* 1986).

An expression for the mass flux of solute into the groundwater, $s$, can now be derived from Eq. (5) for each profile

$$s = \frac{mZ}{\sqrt{[4\pi\lambda Vt^3]}} \exp[-\frac{(Z-Vt)^2}{4\lambda Vt}] \quad (6)$$

where $Z$ is the depth from the surface to the groundwater table in the profile.

## Stochastic Model for Solute Flux

Each profile in the actual field is regarded as a realization of an ensemble of all possible profiles, that are statistically equivalent on the regional scale but locally different. The physical parameters that are regarded as random are: the recharge applied on the surface, the saturated hydraulic conductivity, the water content at saturation and the depth from the surface to the groundwater table. Thus, the solute mass flux in each profile, $s$, becomes a random function of the random variables $R$, $K_s$, $\theta_s$ and $Z$ and depends deterministrically only upon time, $t$.

The probability density functions (pdf) of the investigated parameters are assumed to be statistically stationary and under appropriate ergodic assumptions the ensemble averaging and the space averaging over the horizontal plane in the actual field, are equivalent (Bresler and Dagan 1981). For the sake of simplicity $R$, $K_s$ and $Z$ are regarded as independent random variables; $K_s$ and $\theta_s$ are investigated both as independent and fully correlated.

Because $s$ is a function of the mutually independent parameters, $R$, $K_s$, $\theta_s$ and $Z$ (except for the case when $K_s$ and $\theta_s$ are perfectly correlated, which is discussed below) we can formally express the pdf for $s$ as

$$f(s)ds = f(R)f(K_s)f(\theta_s)f(Z)dRdK_sd\theta_sdZ \quad (7)$$

and the expected solute mass flux is

$$\bar{s} = \int_R \int_{K_s} \int_{\theta_s} \int_Z s(t,R,K_s,\theta_s,Z) f(R) f(K_s) f(\theta_s) f(Z)\, dR\, dK_s\, d\theta_s\, dZ \quad (8)$$

the pdfs for $R$ and $Z$ are assumed to be uniform, while the pdfs for $K_s$ and $\theta_s$ are assumed to be lognormal, *i.e.*

$$f(R) = 0 \quad \text{for} \quad R < \bar{R}(1-\delta_R)\ , \quad R > \bar{R}(1+\delta_R)$$
$$f(R) = \frac{1}{2\bar{R}\delta_R} \quad \text{for} \quad \bar{R}(1-\delta_R) < R < \bar{R}(1+\delta_R) \quad (9)$$

and analogous for $Z$, and

$$f(K_s) = 0 \quad \text{for} \quad K_s < 0$$
$$f(K_s) = \frac{1}{K_s \sigma_k \sqrt{[2\pi]}} \exp\left[-\frac{1}{2}\left(\frac{\ln K_s - \mu}{\sigma_k}\right)^2\right] \quad \text{for} \quad K_s \geq 0 \quad (10)$$

where $\mu$ is the mean of $\ln K_s$ and $\sigma_k$ the standard deviation of $\ln K_s$; analogous pdf to Eq. (10) is assumed for $\theta_s$.

In Eq. (8), $\bar{s}$ is the expected value of $s$, the solute mass flux in each profile; our interest however, is in the expected field value, $\bar{S}$. Assuming that the ergodic hypothesis is satisfied for the given field conditions, we assume that almost all states available to the ensemble of profiles are available in the given field; thus, $\bar{S} \approx \bar{s}$ provided that in Eq. (6) $m$ (the mass injected in each profile) is exchanged with $M$ (the total mass injected over the whole field).

For the case when $K_s$ and $\theta_s$ are fully correlated, the relationship between $K_s$ and $\theta_s$ is based on investigations where the relationship between the porosity (which is approximately equal to $\theta_s$) and the permeability in consolidated deposits has been experimentally identified (see *e.g.* Archie 1950; Griffiths 1958; Bredehoeft 1964). In many of these investigations, the porosity is related to the logarithm of the permeability. Such a relationship can intuitively be anticipated since large changes in the hydraulic conductivity translate into relatively small changes in the porosity. A similar type of relationship can also be intuitively expected in unconsolidated formations. In this investigation the water content at saturation and $\ln K_s$ are related by the following expression

$$\theta_s = \varepsilon \ln K_s + \omega \quad (11)$$

where $\varepsilon$ and $\omega$ are regression parameters that are assumed to be constant. Typical values of $\varepsilon$ may range from 0.01 to 0.05 (see *e.g.* Archie 1950; Griffiths 1958; Bredehoeft 1964). The value of $\theta_s$ can be defined as the sum of a mean value $\bar{\theta}_s$ and a spatial deviation. The definition of the mean $\theta_s$ is then obtained as

$$\overline{\theta_s} = \varepsilon \ln \overline{K_s} + \omega \tag{12}$$

and the variance of $\theta_s$ is defined as

$$\sigma_\theta^2 = \varepsilon^2 \sigma_k^2 \tag{13}$$

which implies that the variance in $\theta_s$ is several orders of magnitude less than the variance in $\ln K_s$.

## Discussion of Results

The transport of the solute through the unsaturated zone is represented by the cumulative breakthrough curve, depicting the fraction of added solute which has leached into the groundwater as a function of time and determined as the integral of the average solute mass flux. Figs. 1-4 show the cumulative breakthrough curves for cases where only one of the investigated parameters varies. Different magnitudes of variability are considered; when $\delta$ or $\sigma$ equals zero the field is regarded as homogeneous. The mean values used to illustrate the effects are $\overline{R}$ = 1.0 cm/h, $\overline{K_s}$ = 10.0 cm/h, $\overline{\theta_s}$ = 0.4 and $\overline{Z}$ = 1.0 m and the deterministic values are $\lambda$ = 0.1 cm and $\theta_{ir}$ = 0. The ratio $r = \overline{R}/\overline{K_s}$ = 0.1 implies that there is almost only unsaturated flow, in view of Eq. (1). The investigated variances of $\ln\theta_s$ (Fig. 3) are selected so small due to the fact that the variance in $\ln\theta_s$ is several orders of magnitude less than the variance in $\ln K_s$ (see Eq. (13) and *e.g.* Jensen and Butts 1986).

Figs. 1-4 show that $R$ and $Z$ have the most significant effect on solute transport through the unsaturated zone and only the impact of $\theta_s$ appears to be negligible. For small variabilities even the impact of $K_s$ is small enough to be neglected, but field measurements show that even the largest variability investigated here ($\sigma_s$ = 1.0) is common in the field (see *e.g.* Bresler and Dagan 1981; Jensen and Butts 1986). Furthermore, when $r$ increases saturated flow becomes more important and

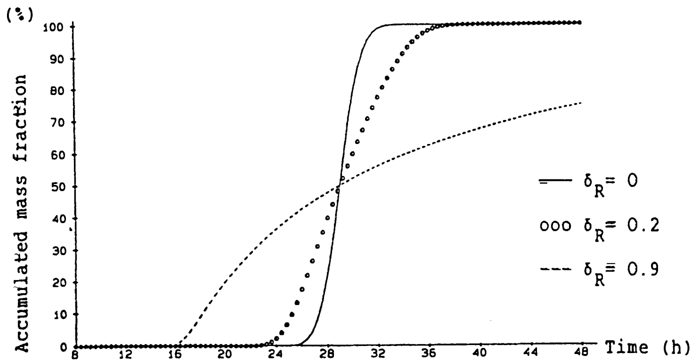


Fig. 1. Cumulative breakthrough curve when only $R$ varies.

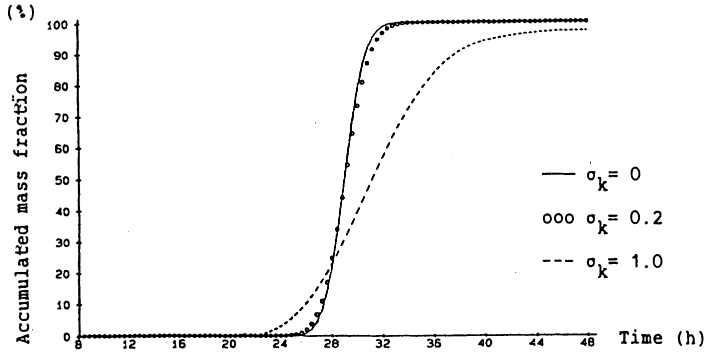


Fig. 2. Cumulative breakthrough curve when only $K_s$ varies.

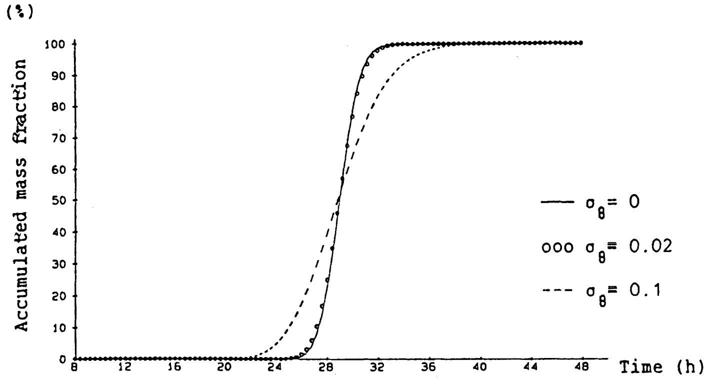


Fig. 3. Cumulative breakthrough curve when only $\theta_s$ varies.

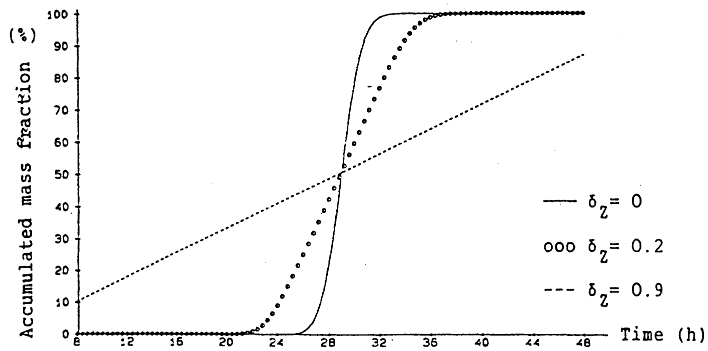


Fig. 4. Cumulative breakthrough curve when only $Z$ varies.

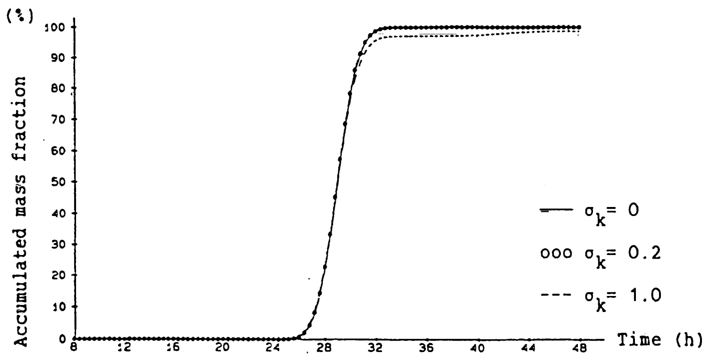


Fig. 5. Cumulative breakthrough curve when $K_s$ and $\theta_s$ vary, fully correlated.

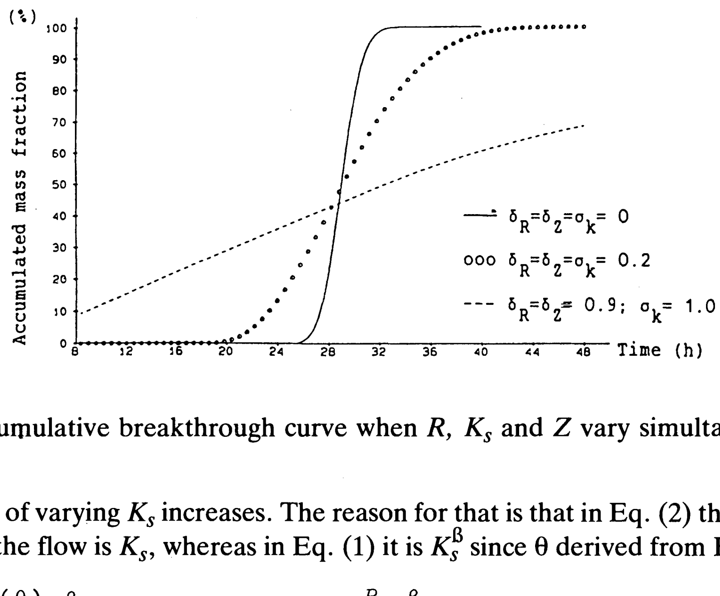


Fig. 6. Cumulative breakthrough curve when $R$, $K_s$ and $Z$ vary simultaneously.

the impact of varying $K_s$ increases. The reason for that is that in Eq. (2) the limiting factor for the flow is $K_s$, whereas in Eq. (1) it is $K_s^\beta$ since $\theta$ derived from Eq. (3) is

$$\theta = \left(\frac{K(\theta)}{K_s}\right)^\beta (\theta_s - \theta_{ir}) + \theta_{ir} = \left(\frac{R}{K_s}\right)^\beta (\theta_s - \theta_{ir}) + \theta_{ir} \qquad (14)$$

with $\beta = 0.14$.

Fig. 5 shows the breakthrough curve for the case where $K_s$ and $\theta_s$ vary, related by Eq. (11), with $\varepsilon = 0.05$.The variation in $\theta_s$ neutralizes in this case the effect of the variation in $K_s$. This is a consequence of the ratio $\theta_s/K_s^\beta$ remaining essentially unchanged in Eq. (14); thus, $\theta$ and $V$ are almost constant in Eq. (1) since $R$ does not vary in this case. Finally, Fig. 6 shows the breakthrough curve when $R$, $K_s$ and $Z$ vary simultaneously. The effect of spatial heterogeneity is here apparent even for small variabilities.

## Conclusions

The spatial variability in the recharge applied on the surface, $R$, and in the depth to the groundwater table, $Z$, appear to have the most significant effect on solute transport through the unsaturated zone. In comparison, the effect of the variability in the water content at saturation (porosity), $\theta_s$, is negligible, if $\theta_s$ is assumed to be an independent random variable. If, however, $\theta_s$ is assumed perfectly correlated with the saturated hydraulic conductivity, $K_s'$, through Eq. (11), it influences the solute movement more notably, by neutralizing the variability in $K_s'$, provided that the unsaturated flow is dominant, *i.e.* the ratio $\overline{R}/\overline{K_s}$ is small. Specifically, the increase of $\overline{R}/\overline{K_s'}$, *i.e.* more saturated flow, increases the impact of spatially varying $K_s'$, while more unsaturated conditions imply that the variability in $K_s$ is less significant.

Although the present analysis is based on a relatively simple flow model, it clearly indicates that natural spatial variability in the physical parameters may have the most significant effect, and should therefore be taken into account for obtaining accurate estimates of solute flux through the unsaturated zone. Furthermore, the present results indicate which of the parameters have a more dominant effect; this may aid in formulating sampling procedures. However, assessing the applicability of the present model to specific field conditions requires further numerical and field experimentation.

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