Soil Heterogeneity

Soils are known to have heterogeneous physical, chemical, and biological properties. Different properties have different degrees of variability (Mallants et al., 2010). Heterogeneous properties relevant to contaminant transport through soils include hydraulic functions describing the water retention characteristic and the (un)saturated hydraulic conductivity (Tseng and Jury, 1994). Chemical properties such as sorption behaviour also exhibit spatial variability and cause additional spreading of the contaminant plume (Bosma et al., 1993; Jacques et al., 1999).

In the subsequent discussion study the spatial variability is restricted to the physical properties, i.e., the parameters of the water retention relationship and the unsaturated hydraulic conductivity function. The first property, \( \theta(h) \), describes the potential of the soil to retain water and is described here as (van Genuchten, 1980):

\[
\theta(h) = \theta_s + \frac{\theta_r - \theta_s}{(1 + (\alpha |h|)^n)^m}
\]  

(1)

where \( \theta \) is soil water content (cm\(^3\) cm\(^{-3}\)), \( h \) is pressure head (cm), subscripts \( s \) and \( r \) denote saturated and residual water content, \( \alpha \) (cm\(^{-1}\)), \( n \), and \( m \) are curve shape parameters, with \( m = 1-1/n \). The second property, \( K(h) \), is used to represent the capacity of a soil to transmit water (van Genuchten, 1980):

\[
K(h) = K_s \left[ (1 + |ah|^n)^{m-1} |ah|^{m-1} \right]^{2}
\]  

(2)

where \( K_s \) (cm day\(^{-1}\)) is saturated hydraulic conductivity, \( l = 0.5 \) and all other parameters are as defined previously.

Spatial variability in \( \theta(h) \) and \( K(h) \) in a two-dimensional space was described using the theory of microscopic geometric similitude, in which case the field heterogeneity is characterized by a single scaling factor. The local hydraulic properties in each of the nodes of the spatial domain are derived from reference properties defined here by the mean values of the hydraulic functions. The parameters for the mean \( \theta(h) \) and \( K(h) \) were \( \theta_s = 0.4 \) cm\(^3\) cm\(^{-3}\), \( \theta_r = 0.05 \) cm\(^3\) cm\(^{-3}\), \( \alpha = 0.019 \) (cm\(^{-1}\)), \( n = 1.59 \), and \( K_s = 144 \) cm d\(^{-1}\) (Mallants et al., 1997).

Synthetic Heterogeneous Field

Using the turning bands method (Tompson et al., 1989), we constructed a two-dimensional random field of a lognormally distributed scaling factor \( \delta \) representing a 7.5 m wide and 4 m deep hypothetical soil profile. The spatial correlation structure of \( Y = \ln \delta \) was described with an anisotropic exponential correlation function, using a horizontal and vertical correlation
length of $L_x = 0.5$ and $L_z = 0.1$ m, respectively (Figure 1). The variance of $Y$, $\sigma_Y^2$, was chosen to represent a very heterogeneous soil, i.e. $\sigma_Y^2 = 1$. Because the variances of $Y$ and $\ln K_s$ are related through $\sigma_{\ln K_s}^2 = 4\sigma_Y^2$, we impose the variability in $\ln K_s$ as being $\sigma_{\ln K_s}^2 = 4$.

![Figure 1 Theoretical and estimated (from data points generated within the random field of scaling factor $\delta$) correlogram for horizontal and vertical direction.](image)

Soil hydraulic functions (Eq. 1) and (Eq.2) were described at each of the 15 762 grid points making up the uniform grid system with horizontal and vertical spacing of 10 and 2 cm, respectively. Figure 2 shows the synthetic random field of the scaling factor $\delta$. Dark zones correspond to sandy sediments (high permeability) whereas lighter zones represent clayey layers. Note how the clay and sand layers alternate along the vertical direction, which is a direct result of the short vertical correlation length relative to the soil depth and relative to the (five times larger) horizontal correlation length. Estimated correlograms based on data points sampled from the random field of scaling factor $\delta$ compare well with the theoretical ones (Figure 1). This indicates that the imposed geostatistical properties of scaling factor $\delta$ have been correctly implemented in the numerical model.
**Water Flow and Contaminant Transport**

Two-dimensional water flow in a variably-saturated soil profile was described by Richards equation:

\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i} \left[ K_{ij} \left( \frac{\partial h}{\partial x_j} + K_{ij} \right) \right] \quad i = 1, 2
\]  

(3)

where \( x_i \) are spatial coordinates (\( x_2 = z \) is taken positive upward), \( K_{ij} \) are components of the dimensionless anisotropic tensor \( K \), and \( t \) is time.

Solute transport in the heterogeneous vertical cross section is described by the CDE as:

\[
\frac{\partial (\partial C)}{\partial t} = \frac{\partial}{\partial x_i} \left[ \theta D_{ij} \frac{\partial C}{\partial x_j} \right] - J_{w_i} \frac{\partial C}{\partial x_i}
\]  

(4)

where \( C \) is the solute concentration in the fluid phase (g cm\(^{-3}\)), \( D_{ij} \) is the dispersion tensor (cm\(^2\) d\(^{-1}\)), and \( J_{w_i} \) is the \( i \)th component of the water flux.

Figure A2-2 Simulated spatial variability in scaling factor \( \delta \). Dark zones are coarse-textured soil layers, light zones are fine-textured layers.
Flow and transport equations (3) and (4) were solved numerically using the finite element FORTRAN code SWMS-2D (Šimunek et al., 1994). We assumed constant transverse and longitudinal dispersivities of 0.02 and 0.25 cm, respectively. In the numerical experiment we applied a constant water flux \( J_w = 1.44 \text{ cm d}^{-1} \) to the surface of the heterogeneous soil profile until steady-state flow was established. Next, a 0.1 g cm\(^{-3}\) tracer pulse was applied during one day. Following the addition of the solute, water flux \( J_w \) continued to be applied for another 150 days until the solute plume approximately reached the bottom of the profile.

**Concentration Profiles**

Spatial variability in hydraulic properties will generate tortuous, three-dimensional flow patterns of chemicals leaching from the surface to the groundwater. This can be seen from the solute concentration distributions (g cm\(^{-3}\) soil) in a heterogeneous soil at time = 15, 35, and 50 days after tracer application (Figure 3). Such concentration profiles are generally obtained through soil coring or by using the time domain reflectometry (TDR) technique (Mallants et al., 1996). Note that a sufficient number of vertical cores needs to be sampled in a contaminated soil for a proper characterization of the degree of pollution. Also shown in Figure 3 are the first, the last, and the mean breakthrough curve (BTC), where the latter has been averaged over 76 computational nodes for each depth interval. Close to the surface the BTCs are relatively smooth and symmetric. Highly irregular BTCs including the mean curve are seen deeper in the soil profile (time = 50 days) indicating an extreme heterogeneous and complex flow process. A comparison between the first and last arrivals of the peak concentrations at time = 50 days indicates that the former is approximately 100 cm ahead of the latter. These curves give an insight into the heterogeneous nature of flow and transport processes in soils. Moreover, they clearly illustrate that the local heterogeneities cannot be modelled by means of a simple one-dimensional transport model, whose application is necessarily limited to the description of the mean field-scale transport.

**Testing of simple models**

Risk assessment studies dealing with the movement of pollutants through unsaturated soils have mostly been performed using one-dimensional models based on the CDE. Field-scale variability may be included by running a multitude of simulations in parallel using local values of transport parameters followed by averaging the results. Another approach is to use effective or field-scale mean transport parameters and run the model only once. The latter approach was tested here using the detailed set of data from the numerical experiment.
Figure 3 Calculated contaminant plume in a heterogeneous soil profile (left) and mean concentration obtained by horizontal averaging over 76 computational nodes (right).
The macroscopic CDE with effective or macroscopic parameters is given as (Toride and Leij, 1996):

\[
\frac{\partial < C' >}{\partial t} = D_{\text{eff}} \frac{\partial^2 < C' >}{\partial z^2} - v_{\text{eff}} \frac{\partial < C' >}{\partial z}
\]  

(5)

where \( C' \) is resident concentration, \( D_{\text{eff}} \) and \( v_{\text{eff}} \) are effective dispersion (cm\(^2\) d\(^{-1}\)) and pore-water velocity (cm d\(^{-1}\)), respectively. The effective parameters are assumed constant with depth. We tested the predictive capacity of this simple model by calibrating the parameters at a shallow depth (or at early time) using the mean observed BTC, followed by a comparison between predicted and observed mean BTC at greater depths (or later times).

![Figure 4](image_url)

**Figure 4** Comparison between mean observed and CDE-predicted concentration (B-C-D), based on fitting of the CDE after 15 days (A).
Figure 4 shows that the fitted CDE with effective parameters accurately describes the mean observed resident concentration distribution at time = 15 days. Predicted mean BTCs at time = 20, 40, and 50 days together with observed curves are also given. At a depth close to the calibration depth the agreement is still good. Furthermore, the mean arrival time of the solute plume at all depths is well described by means of the macroscopic CDE. However, deeper in the profile the predicted curves overestimate the peak concentration and underestimate the observed tailing. This is the result of using a constant dispersion with depth, which is a requirement of the CDE hypothesis. Solute spreading or dispersion at greater depths is thus underestimated as the true dispersion or dispersivity, $\lambda = D/v$ (cm), keeps on increasing with increasing depth (Figure 5). This behaviour of the dispersion coefficient is known as the dispersion-scale effect and represents the transition of an early time process without lateral solute mixing (stochastic-convective transport) to an infinite time process with complete mixing (convective-dispersive transport).

![Figure 5](image-url) Calculated dispersivity-scale effect.
Although the current analysis did not consider reactive chemicals, sorption and desorption processes, decay, degradation and volatilization can be easily incorporated in the numerical simulation as well as in the macroscopic CDE. In such case spatial variability in chemical properties such as the distribution coefficient will also have to be accounted for.

We demonstrated how spatial variability in soil hydraulic properties can be incorporated in a numerical calculation of flow and transport processes at the field scale. Although such detailed numerical simulations using high-performance computing techniques may be used for location specific risk assessment of disposal sites, they require considerable computational resources in addition to detailed information on the spatial variability of the hydraulic functions. These requirements restrict somewhat the applicability of the sophisticated two- or three-dimensional models for management or regulatory purposes. The alternative is to use simplified one-dimensional models with average properties, such as the macroscopic CDE. The limitations of this transport model were illustrated using hypothetical though realistic data on leaching of chemicals from a contaminated site. The random field represented a very heterogeneous soil profile with a distinct layering illustrative of a mixture of sand and clay sediments. Predictions with the CDE model calibrated at shallow depth overpredicted the solute peak and underpredicted the spreading at greater depths. In other words, the true fieldscale dispersion at greater depths was larger than the dispersion obtained through calibration at the shallow depth. The dispersion-scale effect persisted up to a depth of at least 4 m, which corresponds to 40 vertical correlation lengths of the hydraulic conductivity. Generalization of the results obtained here should be done with care because of the specific flow regime established following the imposed field heterogeneity. Nevertheless, numerical experiments may help improve our understanding of field-scale transport and may be helpful in defining limitations of simple transport models.

References


