

Regional transport of nonsorbing tracer in unsaturated soil: estimation and analysis of block-scale travel time moments

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Abstract Regional simulations of solute transport in soils require the selection of a transport model valid at the scale of a block (map unit) and the estimation of appropriate transport parameters. In this paper, three modelling approaches using different assumptions regarding lateral solute mixing are compared: the convection dispersion equation (CDE) with effective parameters, the parallel soil column (PSC) model and the convective lognormal (CLT) model. Starting from local CDE solutions fitted to measured bromide concentration profiles, the comparison is based on calculated travel time moments at the location of the groundwater table. While mean travel times of the blocks calculated with the different modelling approaches differed only slightly, coefficients of variation (CVs) differed considerably, especially at larger transport distances (deep groundwater table). In regard to regional solute breakthrough this is of minor importance since the block-scale travel time variances contributed at maximum 14% (PSC model) to the total (regional) travel time variance. At a given location, however, the arrival of small quantities of a solute is expected to occur considerably later with the CDE as compared to the other models. For safety reasons, as long as the selection of solute transport models lacks a sound basis, simulations aiming at locally predicting the early arrival of hazardous solutes should therefore be based on soil column models rather than on the CDE with effective parameters.

INTRODUCTION

Regional simulations of solute transport in soils are in general composed of single simulations each describing transport on a block. The selection of a transport model implies an hypothesis on the nature of the transport process at this scale which, in many cases, is roughly equal to the field scale (say, 1 to 10 ha). It is well recognized that the transport process is particularly affected by the extent of lateral solute mixing (Flühler *et al.*, 1996). At present, for convenience rather than for physical reasons, solute transport is most often assumed to be convective-dispersive. Due to soil heterogeneity, however, the assumption of perfect lateral mixing inherent in the convective-dispersive approach is often not justified in view of the typical transport distances. As an alternative, Jury (1982) and Simmons (1982) have put forward the stochastic-convective hypothesis which implies that lateral solute mixing is negligible (Jury & Roth, 1990). An intermediate approach is to map soil heterogeneity into an ensemble of parallel, isolated soil columns with random properties. Assuming convective-dispersive transport in each column, field-averaged concentration profiles are then calculated by the Monte-Carlo method (e.g. Persaud *et al.*, 1985).

At the present state of knowledge, transport parameters have to be determined by experiment, no matter which transport model is selected. Since a direct (field scale) determination will rarely be feasible the parameters have to be derived from point scale measurements. For the transport models introduced above we will present a simple procedure which will be developed using the example of a small catchment in Lower Saxony, Germany, in which extensive transport experiments had been carried out (Kumke *et al.*, 1997).

FIELD EXPERIMENTS

In the winters of 1994/1995 and 1995/1996, bromide transport experiments were conducted in the investigation area of the Special Collaborative Programme (SCP) 179 (Eisenbach catchment). The size of this area is about 10 km². For the present study the area under agricultural use was subdivided into 894 blocks each 100 m × 100 m in size. Geologically, the major part of the investigation area is a glacial basin surrounded by a push terminal moraine. Soils are sandy, in the north being partly interspersed with loamy patches. Predominant soil types are cambisols. In the west they are partly podzolic with gleysols and stagnic gleysols in the north. The groundwater table is situated at about 30 m below surface in the south but its depth decreases northwards to less than 1 m.

In four fields of the investigation area, grids (labelled S2, S3, S4, S5, respectively) each slightly smaller than 1 ha were laid out. Characteristic distances between adjacent points ranged 12–20 m. Winter cereals were cultivated at S2 and S3. S4 and S5 lay bare. In the winter of 1994/1995, 50 kg ha⁻¹ KBr was applied. After 21–66 days, corresponding to a cumulative infiltration of 58–153 mm, bromide displacement was measured by taking 30 soil cores from each grid (fine grid samples). In the winter of 1995/1996, analogous transport experiments were conducted in the whole investigation area. In 74 blocks, 50 kg ha⁻¹ KBr was applied to a 10 m long strip of 12 m width. Bromide displacement was determined for each plot by taking one central soil core 102–122 days after application corresponding to 73–82 mm of infiltration (coarse grid samples). During the experiments most soils lay bare. At 24 experimental sites winter cereals were grown. Unfortunately, the extreme duration of ground frost during the winter of 1995/1996 led to severe crop damage. To enable substitute planting the fields concerned were tilled immediately after thawing and so these sites could not be sampled.

Soil samples were taken with an Edelman screw auger at 0.1 m depth intervals. Sampling was in general to a depth of 1 m, but at some points of the coarse grid to 0.5 or 0.6 m. Before bromide application, and with the final sampling, gravimetric water content distribution with depth was measured at all points. Measured water contents were converted to volumetric water contents using bulk density data from the central database of the SCP 179. Precipitation occurred exclusively by rainfall and snowfall and was measured centrally with an automated Hellmann gauge. For more details of the field experiments see Kumke *et al.* (1997).

The solution of the CDE was fitted to each measured bromide concentration profile. Water fluxes, variable with depth, were calculated by balancing infiltration

with measured water contents. Evaporation was neglected. The CDE was solved numerically using an implicit-explicit (Crank-Nicolson) discretization scheme. Parameters fitted were (a) the applied mass per square metre, m_0 , (b) the dispersion length λ , and (c) a factor ζ which scales the centrally measured infiltration to a local value. Essentially, m_0 determines the area of a concentration curve, λ its spread, and ζ the position of the peak. All three parameters were assumed to be constant with depth. For two coarse grid profiles no reasonable fit could be achieved. Thus, altogether 168 parameter sets were estimated: 120 from the fine grid profiles and 48 from the coarse grid profiles. The coefficient of determination, defined as the proportion of explained variance, was on average 0.93. Table 1 gives some statistical information on the estimates and the measured water content averaged over 1 m depth, θ . The CV of the recovery rate equals the CV of fertilizer application measured in a separate experiment.

Table 1 Means and coefficients of variation (CV) of estimated parameters ζ , λ , and m_0 (relative to mass) applied, m_{app} and measured volumetric water content (θ) averaged over 1 m depth.

Variable	Mean	CV (%)
ζ	1.0	46
λ (cm)	1.8	263
m_0/m_{app}	0.67	44
θ	0.21	40

Within the scope of this paper, we will deal only with ζ , θ and λ , which for simplicity are hereafter referred to as the given parameters. As shown in Fig. 1 the given parameters are approximately lognormally distributed at the fine grids. Point-to-point correlation coefficients between $\ln(\theta)$ and $\ln(\zeta)$, $\ln(\lambda)$ and $\ln(\zeta)$, and $\ln(\lambda)$ and $\ln(\theta)$ are 0.14, -0.46 , and 0.03, respectively. No differences in correlation coefficients were found when coarse and fine grid data were evaluated separately.

The variograms of the logtransformed given parameters are shown in Fig. 2. Spherical models with sills of 0.25 and 0.115 and ranges of 370 and 260 m were fitted to the variograms of $\ln(\zeta)$ and $\ln(\theta)$, respectively. An exponential model with a sill of 1.3 and a range of 200 m was fitted to the variogram of $\ln(\lambda)$. The remarkable increase of scattering with distance may be explained by the fact that fine grid and coarse grid experiments were conducted in two winters with very different weather conditions (see above). As a consequence, the reliability of the variogram models is somewhat limited.

THEORY

Transport models

Assuming a stationary water regime, the one-dimensional convection dispersion equation reads (CDE with effective parameters):

$$\frac{\partial C}{\partial t} = D_{eff} \frac{\partial^2 C}{\partial z^2} - V_{eff} \frac{\partial C}{\partial z} \quad (1)$$

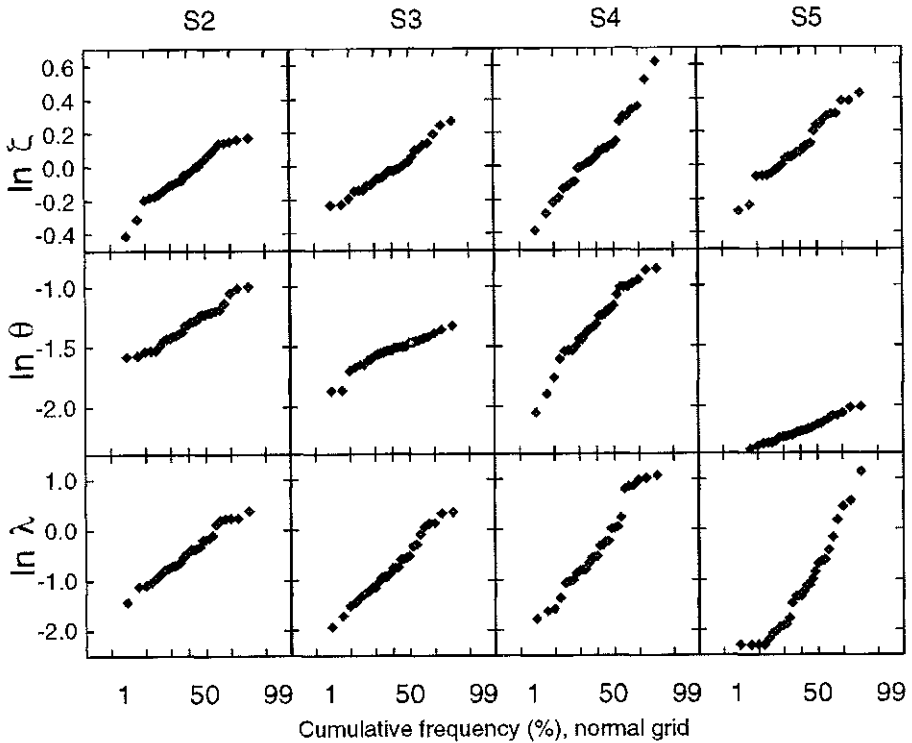


Fig. 1 Distributions of logtransformed given parameters at the four fine grids S2, S3, S4, and S5.

where C denotes the solute concentration in solution (g m^{-3}), V_{eff} (m day^{-1}) the effective pore water velocity and D_{eff} ($\text{m}^2 \text{day}^{-1}$) the effective dispersion coefficient; t (days) and z (m) are time and space coordinates, respectively. Equation (1) assumes that solute transport at the block scale has fully developed to a convective-dispersive process (Butters & Jury, 1989) and can thus be represented by effective transport parameters. According to Salzmann & Richter (1995) V_{eff} and D_{eff} can be calculated from the distributions of local V and D , presuming that both parameters are lognormally distributed and independent. Basic to this approach is to interpret block-averages of local concentrations as solutions of the CDE.

Considering the soil as an ensemble of parallel soil columns the block-averaged solute flux concentration is given by (PSC model):

$$\bar{C}(z,t) = \frac{\langle J_w C(z,t;V,D) \rangle}{\langle J_w \rangle} \quad (2)$$

where $C(z,t;V,D)$ (g m^{-3}) stands for the solute flux concentration as obtained by solving the convection dispersion equation with local parameters V and D . The distribution of V and D is described by their joint probability density function. J_w (m day^{-1}) denotes the water flux density. Here and in the following, angles indicate ensemble averages.

Neglecting the effect of local dispersion, that is, approximating solute transport in a soil column by a piston flow model, yields a special case of the PSC model. In the

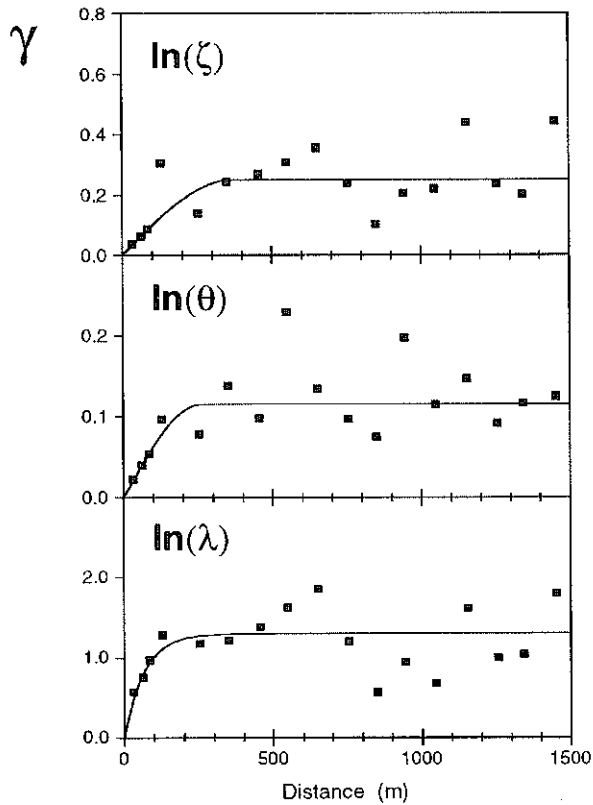


Fig. 2 Experimental variograms of logtransformed given parameters and fitted models.

following this simplified model will be referred to as the CLT model. Although derived from a different starting point, it is equivalent to the Convective Lognormal Transfer function model introduced by Jury (1982) if the pore water velocities are lognormally distributed (Jury & Roth, 1990). In particular, it represents a stochastic-convective transport process.

Travel time moments

The analysis of travel time moments offers a convenient way to compare predictions of different models. Travel time moments are the statistical moments, particularly mean and variance, of a solute breakthrough curve with normalized (unit) area. This curve may be regarded as a probability density function (pdf). It characterizes the probability that a solute particle added to a soil volume at $t = 0$ will leave it between t and $t + \Delta t$ (Jury & Roth, 1990, chap. 1). Travel time moments were evaluated at the block scale.

The travel time moments of the CDE with effective parameters are given by (cf. Jury & Roth, 1990, chap. 2.5):

$$E_z[t] = \frac{z}{V_{eff}} \quad (3)$$

$$VAR_z[t] = \frac{2D_{eff}z}{V_{eff}^3} \quad (4)$$

The travel time moments of the PSC model can be derived analytically from the moments of the CDE assuming that the local parameters V and D form a bivariate lognormal distribution. The straightforward calculation yields (cf. Toride & Leij, 1996):

$$E_z[t] = \frac{z}{\langle V \rangle} \exp(\sigma_{\ln V}^2) \quad (5)$$

$$VAR_z[t] = \frac{2z\langle D \rangle}{\langle V \rangle^3} \exp(6\sigma_{\ln V}^2 - 3\rho_{\ln V, \ln D}\sigma_{\ln V}\sigma_{\ln D}) \\ + \frac{z^2}{\langle V \rangle^2} (\exp(3\sigma_{\ln V}^2) - \exp(2\sigma_{\ln V}^2)) \quad (6)$$

where σ^2 and ρ denote variance and correlation coefficient of the subscript variables, respectively. Since we assumed constant mass input per unit area the formulae are different from those derived recently by Toride & Leij (1996) on the assumption that mass input is proportional to infiltration.

CALCULATION OF TRANSPORT PARAMETERS

The local transport parameters V and D are related to the given parameters ζ , θ , and λ by:

$$V = \frac{\zeta}{\theta} \frac{I}{\Delta t} \quad (7)$$

and, on the common assumption that $D = \lambda V$,

$$D = \lambda \frac{\zeta}{\theta} \frac{I}{\Delta t} \quad (8)$$

where I denotes the local cumulative infiltration during the time span of interest, Δt . In the following calculations, I was set to 300 mm. This value is close to the average annual seepage in the investigation area which is partly due to irrigation. Δt was set to 365 days.

The logtransformed transport parameters $\ln(V)$ and $\ln(D)$ are linear combinations of the logtransformed given parameters which were found to be approximately multinormal at the fine grids (Fig. 1). Since fine grids and blocks have almost the same size, V and D can be assumed to be approximately lognormal within each block. Means and (co-)variances were calculated from the statistical moments of the logtransformed parameters by applying standard formulae (Morrison, 1967, chap. 3.4). The procedure requires the estimation of block means and within-block (co-)variances of $\ln(\zeta)$, $\ln(\theta)$, and $\ln(\lambda)$.

Block means were calculated by block kriging. Within-block variances were approximated by their respective expectations, the dispersion variances (Journel &

Huijbregts, 1978, chap. 2). The latter were calculated from the variogram models shown in Fig. 2. Covariances were calculated using the experimental correlation coefficients as given in the field experiments section. This produces identical covariance matrices for all blocks of the region.

The effective parameters of the CDE were calculated using the procedure of Salzmann & Richter (1995). The condition for employing this, independence of $\ln(V)$ and $\ln(D)$, was found to be satisfied ($r = 0.1$).

RESULTS AND DISCUSSION

The travel time moments of all 894 blocks were calculated with each model for the corresponding groundwater table depths. The calculation presumes that the transport properties of the soil are represented by those found in the uppermost 1 m. At locations with deep groundwater this is of course a gross simplification which, however, will often be unavoidable in practice. This applies particularly to the southern part of the study area. Mean travel times predicted by the CDE with effective parameters are slightly lower (max. 3%) than those predicted by the PSC and CLT models. The average value for all blocks is 325, while that of the other two models is 333 days per metre of transport distance. With either model, the CV of mean travel times is 57%.

Large differences between the models occur with regard to the CVs of the travel time pdfs. Figure 3 shows the CVs of all blocks as a function of the depth of groundwater table. First of all, the plots reflect the well-known difference between the convective-dispersive and the stochastic-convective transport process concerning the dependency of the CV on the transport distance. The CVs predicted by the CLT model are constant. Recalling that block scale variances of the given parameters were approximated by the respective dispersion variances, we can explain this result by the peculiarity of the lognormal distribution the CV of which depends solely on the variance of the logtransformed variable. At locations with shallow groundwater the PSC model predicts much higher CVs than the CLT model. However, the effect of local dispersion dies off rapidly with depth and the CVs approach the constant value predicted by the simple CLT model. In comparison to the soil column models, the CDE predicts much lower CVs at locations deeper than 1–2 m. Accordingly, the

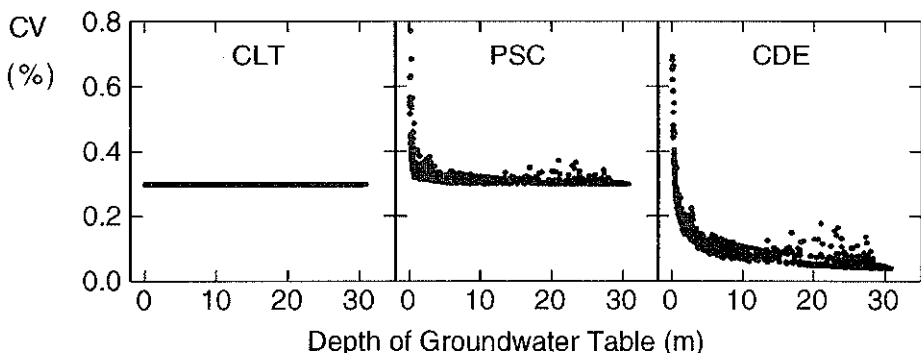


Fig. 3 CVs of travel times of the blocks, as predicted by the different models, as a function of the location of the groundwater table (transport distance).

arrival of small concentrations (“leading edge”) is expected to occur considerably later. As long as the selection of the transport model lacks a sound basis, soil column models should therefore be given preference to the CDE with effective parameters in simulations aiming at the spatially resolved prediction of the first arrival of a solute.

From a regional point of view, however, the block scale travel time variances are less important, irrespective of the model applied. If the travel time pdfs of the blocks are assembled to a regional pdf, it turns out that their variances contribute only 2 (CDE), 13 (CLT) or 14% (PSC) to the total (regional) travel time variance. The major part is due to the variability of the mean travel times between the blocks which in turn is caused to a considerable extent by the large differences in groundwater table depths.

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