Using bulk density measured by x-ray tomography to estimate the hydraulic structure of soil

VOGEL Hans-Jorg (1), **ROTH Kurt** (1) **and BASTIAN Peter** (2)

(1) Institute of Environmental Physics, University of Heidelberg, INF 229, 69120 Heidelberg, Germany
(2) Interdisciplinary Center for Scientific Computing, INF 368, 69120 Heidelberg, Ger many

Abstract

Many phenomena of flow and transport are governed by the heterogeneous structure of the material. A notorious problem in soil physics is to predict preferential flow along highly conductive regions. In many cases, the key for a quantitative understanding of such processes is the spatial structure of hydraulic properties which lead to complex flow fields of water. Direct measurements of the hydraulic structure at the scale of a soil column of some 10-30 cm in diameter are difficult. As an alternative, we assume that the soil bulk density within a given soil can be used as a suitable proxy.

First, based on a multistep-outflow experiment we estimate effective hydraulic parameters for a soil column. Then, we measure soil bulk density within that column at a resolution of 1.0 mm using x-ray tomography, and we separate different density classes which are presumed to represent different hydraulic properties. Finally we estimate the hydraulic parameters of the different density classes by suitable assumptions and a non-linear regression using the effective measurements and the known structure.

To verify the consistency of our approach we simulate the multi-step outflow experiment using the resulting three-dimensional heterogeneous parameter field. The simulation results are in reasonable agreement with the experiment. The presented approach has the potential to predict the hydraulic structure and herewith the phenomenology of solute transport while no effective transport model has to be postulated.

Keywords: solute transport, hydraulic properties, x-ray tomography

Introduction

The prediction of water flow and solute transport in heterogeneous structured soil is still one of the major challenges in the field of soil physics.

The common approach which often fails to predict the experimental reality is to consider soil to be a macroscopically homogeneous porous medium having well defined effective properties as the water retention characteristic, hydraulic conductivity function and dispersivity of solute transport. All these attributes are thought to apply for a representative elementary volume (REV) (Bear, 1972) and are considered to be constant material properties. However, critical phenomena as preferential flow cannot be modeled based on that approach.

This led to the formulation of effective models for flow and transport which allow to discriminate different flow domains as the mobile-immobile model (van Genuchten and Wierenga, 1976) or the dual-porosity model (Gerke and van Genuchten, 1993). Although such models are in the position to quantitatively describe an early break-through and a long tailing of a solute pulse, their predictive power is limited because the physical meaning of the lump parameters for the size of the domains and the exchange between the domains is unclear and hence, the required parameters have to be fitted to experimental data.

In the last decades, many experiments on solute transport in soil clearly demon-strates the dominant effect of the heterogeneous structure of the material on the phenomenology of flow and transport. This is true for a wide range of scales ranging from soil columns in the laboratory (Kasteel *et al.,* 2000) to soil profiles (Flury *et al.,* 1994) and solute dispersion in aquifers (Gelhar, 1986). Thereby, the morphology of different hydraulic regions is critical, i.e. their variance, correlation length and connectivity. The latter is the main difficulty in following a morphological path to predict physical properties, because the measurement of connectivity requires a continuous representation of the structure within all relevant spatial dimensions at a resolution which is able to detect the relevant structural units. This is true irrespective of the scale of observation.

Clearly, it is not feasible to meet this condition for the direct measurement of hydraulic functions. However, there are other properties which may be used as surrogates that are suitable proxies for the required material properties and which can be measured continuously and efficiently. One such proxy variable is the soil bulk density. At the typical scale of a soil column, some 15 cm in diameter, the structure of bulk density can be measured at a resolution of some 0.5 mm using x-ray tomography (Anderson *et al.,* 1988).

Hence, presuming that bulk density is a suitable proxy for hydraulic properties the continuous hydraulic structure is measured efficiently by x-ray tomography which is appealing. The remaining question is: how to get the related parameters? Kasteel *et al.* (2000) estimated the hydraulic properties of different density classes within a soil column using a network model which was based on quantitative analysis of the underlying pore structure. The resulting three-dimensional parameter field was used to successfully simulate the breakthrough curve of a conservative tracer. In this paper we follow the same idea as Kasteel *et al.* (2000) but circumvent the elaborate analysis at the pore scale. We present an efficient approach to estimate the heterogeneous field of hydraulic parameters within a soil column. It is based on two relatively simple measurements: i) x-ray tomography to obtain the structure of bulk density and ii) the effective hydraulic functions measured for the entire column. We demonstrate the proposed approach for one soil column taken from the top horizon of a Loess soil.

Measurement of Effective Hydraulic Properties

As a first step of our approach we need to measure effective hydraulic properties for the entire soil column, i.e. the water retention characteristic $\theta(\psi)$ and the hydraulic conductivity function $K(\theta)$ where θ denotes the volumetric water content and ~ the matric potential of soil water.

This was done using a classical multi-step-outflow experiment (Van Dam *et al.,* 1994). The sample was saturated with water and mounted on a ceramic plate where the water potential could be adjusted. The sample was desaturated by stepwise decreasing the water potential at the lower boundary. The resulting outflow was measured with high temporal resolution.

Then, the hydraulic parameters were estimated by solving the inverse problem of the Richards equation for the corresponding initial and boundary conditions:

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

with $C(\psi) = \partial\theta/\partial\psi$. The required parametric descriptions of the water retention characteristic 0(~) and the hydraulic conductivity function $K(\Theta)$ were chosen according to van Genuchten (1980):

$$\Theta(\psi) = [1 + [\alpha\psi]^n]^{-1+1/n} \qquad (2)$$

$$K(\Theta) = K_s\Theta^{0.5}\left[1 - \left[1 - \Theta^{n/[n-1]}\right]^{1-1/n}\right]^2 \qquad (3)$$

where $\Theta = (\theta - \theta_r)(\theta_s - \theta_r)^{-1}$ is the water saturation, θ the volumetric water content, 08 the volumetric water content at saturation, θ_r, the residual water content, K_s the hydraulic conductivity at water saturation and n and α are fitting parameters. This leads to a parameter vector $\hat{\vartheta}(\hat{\theta}_s, \hat{\theta}_r, \hat{n}, \hat{\alpha}, \hat{K}_s)$ where the hat over the symbols indicates that these parameters are effective parameters averaged over the heterogeneous structure of the entire column. The saturated water content $\hat{\theta}_s$ corresponds to the mean porosity $\hat{\phi}$ and was obtained from the bulk density of the column.

Measurement of Local Porosity by X-Ray Tomography

The next step is to measure the spatial structure of bulk density or porosity within the entire soil column.

From x-ray tomography we get a measure of the local attenuation coefficient μ_x at each location x at a resolution of 0.5 mm in the horizontal plane and 1.0 mm in the vertical (Figure 1). We assume that the attenuation coefficient of the solid material μ_s as well as the attenuation coefficient of water μ_w, is constant. Prior to x-ray tomography the column was saturated with water so that only the two phases solid and water were present. Then, the measured local attenuation coefficient μ_x depends only on the local porosity ϕ_x

$$\mu_x = [1 - \phi_x]\mu_s + \phi_x\mu_w \qquad (4)$$

The grey level g_x obtained for each voxel in the x-ray images is a measure of the local attenuation coefficient, $g_x \propto \mu_x$. To calculate the local porosities according to relation (4) the attenuation coefficients μ_s and μ_w are required. The latter corresponds to the grey level g_w measured within the large water filled pores and hence, is directly available. To calculate $\mu_s \propto g_s$ we use the measured mean porosity of the entire column $\hat{\bar{\phi}}$ which is related to the measured mean grey level *gm* of the column:

$$g_m = \hat{\phi} g_w + [1 - \hat{\phi}] g_s \tag{5}$$

This equation is solved for g_s which is a measure of μ_s and then, the local porosity is obtained by

$$\phi_x = \frac{g_s - g_x}{g_s - g_w} \tag{6}$$

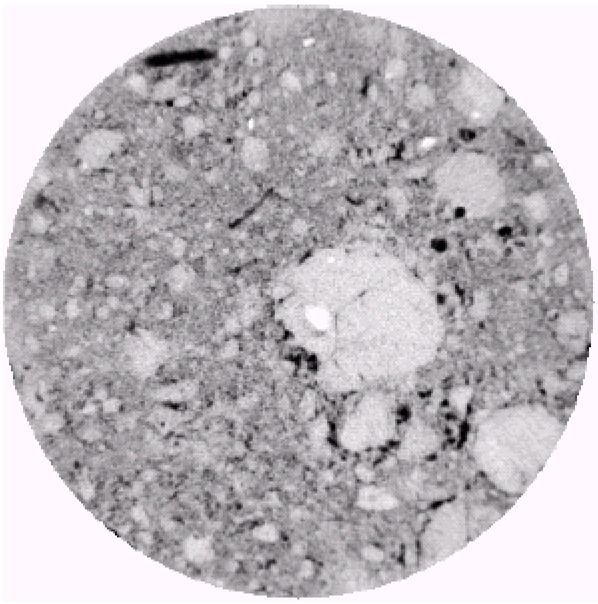

Figure 1 Horizontal section through the water saturated soil column obtained by x-ray tomography, diameter is 16 cm. The grey levels are proportional to the x-ray attenuation and serve as a measure of local porosity.

Estimating Local Hydraulic Properties

Following the hypothesis that the local porosities ϕ_x can be used as a proxy for the local hydraulic properties $\theta_x(\psi)$ and $K_x(\theta)$, the next step is to relate each grey level $g_i \in [0, 255]$ to a corresponding parameter vector $\vartheta_i(\theta_{s,i}, \theta_{r,i}, n_i, \alpha_i, K_{s,i})$ which describes the specific hydraulic properties for the different density classes. Thereby, the subscript i corresponds to the different bulk densities, i.e. the different grey values in the x-ray image of the column.

Specific water characteristic

While $\theta_{s,i} = \phi_i$ is directly obtained from the x-ray images using equation (6) the other parameters, n_i, α_i and $\theta_{r,i}$ were estimated based on different simplifying assumptions.

First we presume that the measured effective water retention characteristic $\hat{\Theta}(\psi)$ can be expressed as a weighted sum of the local properties:

$$\hat{\Theta}(\psi) = \sum_i \omega_i \Theta_i(\psi) \tag{7}$$

where ω_i, with $\sum_i \omega_i = 1$, represents the frequency of grey levels or density classes i and thus can be directly obtained from the grey level histogram of the x-ray image. Equation (7) implies that the local water characteristic is independent of the macroscopic structure. It should be noted that this may be critical near water saturation where a reduced mobility of the air phase within the surrounding material affects the local hydraulic behavior.

As a further simplification we assume that the shape of the pore size distribution is the same for the different density classes. This means that the parameter n which determines the shape of the water characteristic does not change. In contrary, the residual water content θ_r is expected to vary with bulk density. It is considered to be a certain proportion c of the saturated water content $\theta_{s,i}$. This proportion is expected to increases with bulk density because of the increasing ratio between pore surface and pore volume. This considerations lead to the relation

$$\theta_{r,i} = \theta_{s,i}\, c\, (1 - \theta_{s,i}) \tag{8}$$

Herewith we obtain the plausible value $\theta_{r,i} = 0$ for macropores $(\theta_{s,i} = 1)$ as well as for solid mineral grains $(\theta_{s,i} = 0)$ and a maximum value between these extremities. The constant c is chosen such that the measured effective porosity $\hat{\theta}_s$ leads to the measured effective residual water content $\hat{\theta}_r$.

The parameter α which can be considered to be a measure of the mean pore size is also expected to vary with bulk density. At this point α_i is the only missing component of the parameter vector describing the specific water characteristic. Hence, according to equation (7), we determine the specific α_i in a way that the relation is fulfilled. This was done by non-linear regression using the Levenberg-Marquardt Algorithm (Press *et al.,* 1992) with the additional condition that $\alpha_i > \alpha_{i+1}$. This condition ensures that the pores become smaller with increasing bulk density.

$$\hat{\theta}(\psi) = \sum_i \omega_i (\theta_{s,i} - \theta_{r,i}) \left[1 + (\alpha_i \psi)^n\right]^{-1+1/n} + \theta_{r,i} \tag{9}$$

Specific hydraulic conductivity

The effective hydraulic conductivity of a heterogeneous material lies between the extremities of the harmonic and the arithmetic mean of the local conductivities (e.g. Dagan, 1989). These bounds are valid for the extreme cases of flow parallel or perpendicular to layers of different conductivities. Journel *et al.* (1986) proposed a power average which we apply to the saturated hydraulic conductivity of the different density classes i.

$$\hat{K}_s^{\,p} = \sum_i \omega_i K_{s,i}^p \tag{10}$$

with an exponent p in the interval between between -1 and 1. Note that these bonds correspond to the harmonic and the arithmetic mean respectively. For a statistically homogeneous and isotropic three-dimensional media one obtains $p = 1/3$ (Ncetinger, 1994). The structure of our soil column is characterized by dense aggregates lying in a continuous loose porous matrix and therefore we raise this exponent and chose $p = 0.5$.

To estimate the specific saturated hydraulic conductivity $K_{s,i}$ for the different density classes, we use its proportionality to the squared pore radius according to Poiseuille's law, $K_{s,i} \propto r_i^2$. Based on the known water retention characteristic $\Theta_i(\psi)$ we define a mean water potential $\bar{\psi}_i$ for which $\Theta_i(\bar{\psi}_i) = 0.5$ which is related to a mean pore radius by rice $\bar{r}_i \propto \bar{\psi}_i^{-1}$ according to the Young-Laplace Equation. Then, we obtain the specific saturated hydraulic conductivity by

$$K_{s,i} = c\,\bar{r}_i^2 \tag{11}$$

where the constant c is determined to meet the condition

$$\hat{K}_s = \left[\sqrt{c}\sum_i \omega_i \bar{r}_i\right]^2 \tag{12}$$

At this point the specific parameter vector ϑ_i for the different density classes is complete.

Results and Discussion

The set of hydraulic parameters can now be plotted as a function of bulk density (Figure 2). By definition, the saturated water content is directly related to bulk density and the residual water content follows Equation (8). The parameter α decreases with bulk density so that the effective water characteristic is recovered using Equation (7) and the saturated conductivity is directly related to α through (11). The minimum and maximum values of the different parameters are given in Table 1 together with the effective parameters measured in the multi-step outflow experiment.

Table 1 Effective hydraulic parameters obtained from the multistep outflow experiment and minimum and maximum values for the specific parameter vectors.

	fixed	estimated			
	n	$\alpha\,[cm^{-1}]$	θ_r	θ_s	$K_s[cmh^{-1}]$
effective		**0.0445**	**0.250**	**0.503**	**9.28**
minimum	1.7262	0.0041	0.000	0.099	0.0942
maximum		0.2053	0.251	1.000	228.0

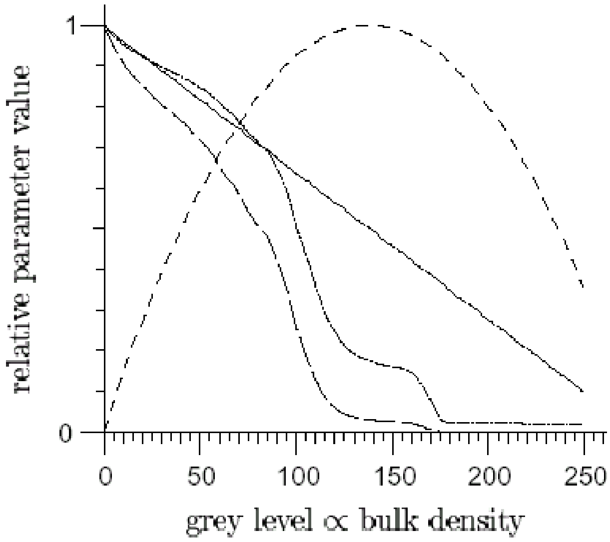

Figure 2 Relative parameter values as a function of bulk density indicated by the grey level of the x-ray image: *Os* (line), 0r (short dashed line), a (dashed dotted line) and *Ks* (long dashed line).

Altogether 48 density classes were distinguished within the soil column. The corresponding specific water characteristic and hydraulic conductivity functions are shown in Figure 3 together with the effective results measured by the multistep out- flow experiment. Clearly, the saturated water content and the saturated hydraulic conductivity decrease with bulk density. With decreasing water potential, the water content and hydraulic conductivity decreases more rapidly for low bulk densities which has to be expected. Although the size distribution of pores was considered to be constant (n = const), our approach seems to retain enough flexibility for a plausible description of the system.

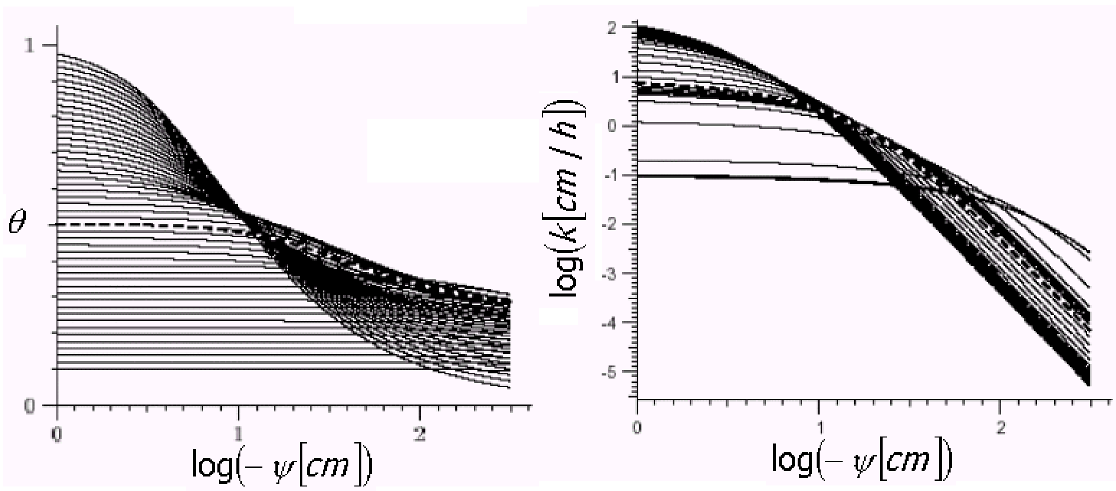

Figure 3 Band of water retention characteristics (left) and hydraulic conductivity functions estimated for the different density classes.

To verify the consistency of our approach we simulate the multi-step outflow exper-iment based on the three-dimensional heterogeneous parameter field using Richards Equation. Thereby the parameter field is immediately given by the x-ray data. The results are shown in Figure 4.

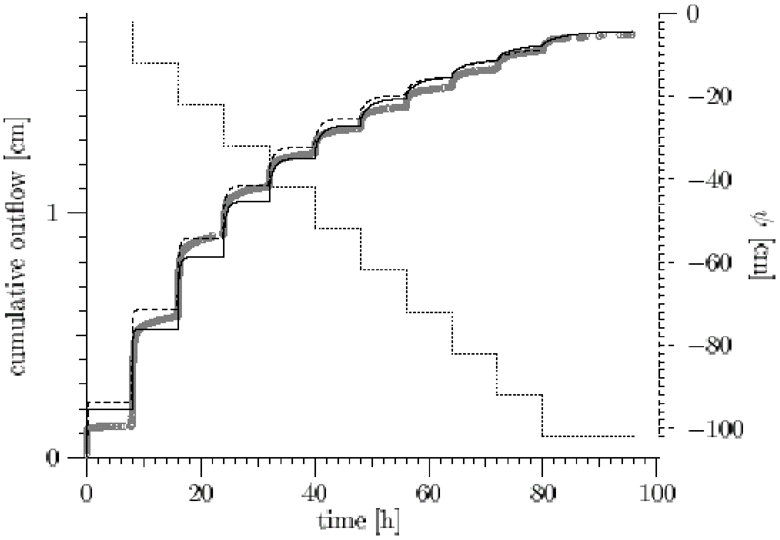

Figure 4 Experimental and simulated results of the multi-step outflow experiment with stepwise decreasing water potential ψ at the lower boundary (dotted line): measured cumulative outflow (symbols), result of 1D Richards Equation for optimized effective hydraulic parameters (line) and simulation result of 3D Pdchards Equation based on the heterogeneous parameter field.

First it should be noted that the optimized result of the 1D Richards equation based on fitted hydraulic parameters does not perfectly reflect the experimental data. However this blemish is not important in our context.

For the heterogeneous simulation it could be expected that it reproduces the results of the optimized 1D-Richards equation with respect to the volume of water that leaves the column at each pressure step. This is true because the heterogeneous description of the water retention characteristics is in accordance with relation (7) and the macroscopic structure has no influence on the effective behavior. This is implicit for the chosen model, since Richards Equation does not consider the gaseous phase explicitely. Hence, the effective retention curve is just the sum of the local ones. Actually the heterogeneous simulation is close to the 1D-model but not identical. The discrepancy is due to the fact that the spatial discretization of the 3D-simulation was reduced by a factor of 7 compared to the original resolution of the x-ray image to reduce the computational effort.

In contrast to the water retention characteristics, there may be differences in the dynamics of the water phase due to the macroscopic structure of the hydraulic conductivities which differ by 3 orders of magnitude (Table 1). The shape of the cumulative outflow as a result of the different pressure steps should be sensitive to the dynamics of the water phase. However, there is no noticeable difference between the 3D-simulation and the 1D-model. In contrary, the shape of the outflow steps measured in the experiment is clearly different from both models. After each pressure step a fast outflow is followed by period of much slower outflow in the experiment. This phenomena is not reproduced by the model where the equilibrium is reached much faster. A possible reason may be the assumption that the conductivity of the gaseous phase is in any case very much higher compared to the conductivity of water. This is implicit when using Richards equation.

The simulated multi-step outflow experiment based on the estimated parameter field is in reasonable agreement with the experimental data. The presented approach has the potential to predict the hydraulic structure within a soil sample based on simple and efficient measurements. This opens perspectives to predict the phenomenology of solute transport which will be the issue of future studies.

References

Anderson, S.H., C.J. Gantzer, J.M. Boone and R.J. Tully. 1988. Rapid nondestructive bulk density and soil-water content determination by computed tomography. Soil Sci. Soc. Am. J. 52:35-40.

Bear, J. 1972. Dynamics of Ttuids in Porous Media. American Elsevier Pub. Co., New York.

Dagan, G. 1989. Flow and Transport in Porous Formations. Springer, Berlin.

Flury, M., H. Fliihler, W.A. Jury and J. Leuenberger. 1994. Susceptibility of soils to preferential flow of water: a field study. Water Resources Res. 30:1945-1954.

Gelhar, L.W. 1986. Stochastic subsurface hydrology. From theory to applications. Water Resour. Res. 22:135S-145S.

Gerke, H.H. and M.T. van Genuchten. 1993. A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media. Water Resour. Res. 29(1):305-319.

Journel, A.G., C.V. Deutsch and A.J. Desbarats. 1986. Power averaging for block effective permeability. Society of Petivleum Engineers, SPE. 15128.

Kasteel, R., H. Vogel and K. Roth. 2000. From local hydraulic properties to effective transport. Europ. J. Soil Sci. 51:81-91.

Noetinger, B. 1994. The effective permeability of a heerogeneous porous medium. 15:99-127.

Press, W.H., S.A. Teukolsky, W.T. Vetterling and B.P. Flannery. 1992. Numerical Recipez in C. The Art of Scientitic Computing. 2nd ed. Cambridge University Press.

van Dam, J.C., J.N.M. Stricker and P. Droogers. 1994. Inverse method to determine soil hydraulic functions from multistep outflow experiments. Soil Sci. Soc. Am. J. 58:647-652.

van Genuchten, M.T. and P.J. Wierenga. 1976. Mass transfer studies in sorbing porous media. I. Analytical solutions. Soil Sci. Soc. Am. J. 40:473-480.

van Genuchten, M.T. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44892-898.