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# Moving through scales of flow and transport in soil

H.-J. Vogel*, K. Roth

*Institute of Environmental Physics, University of Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg, Germany*

**Abstract**

Flow and transport in soil is governed by the binary geometry of solid and void. This may be described at typical length scales of some millimeters, and even less. In contrast, the problems which are supposed to be solved in soil physics are related to a scale of some meters, the typical distance between soil surface and groundwater. A quantitative understanding of flow and transport, based on measurements of hydraulic properties and transport parameter at a given scale, requires the transfer of information in space, time, and across scales. This is the major challenge in heterogeneous soils and this has motivated many concepts for the organization of heterogeneities, including macroscopic homogeneity, discrete hierarchy and fractal geometry. We propose a conceptual approach termed 'the scaleway' to predict flow and transport in structured materials, whatever the scale, and whatever the specific type of structural organization. This is based on the explicit consideration of structure that is assumed to be present at the scale of interest, while the microscopic heterogeneities are replaced by averaged, effective descriptions. The three ingredients needed are: a representation of the structure, a process model at the scale of interest, and corresponding effective material properties. We demonstrate the scaleway for one example of solute transport in a soil column and discuss implications for future research.


*Keywords:* Structure; Solute transport; Water flow; Upscaling; Modeling

## 1. Introduction

Water flow and solute transport through structured soil is still far from being understood quantitatively. It is a challenge to develop models having predictive power, and which concern phenomena such as fast transport through macropores, preferential flow due to the spatial variability of hydraulic properties, or the instability of wetting fronts which results in fingering flow. On the other hand, models are highly required for a sustainable management of the environment including the pollution of groundwater by agrichemicals, the construction of waste disposal sites or the remediation of contaminated soils.

Despite several decades of intense research on flow and transport in porous media, and the considerable knowledge on the physical processes, there is no simple answer to the problem: given some specific site and some specific distribution of solutes, what can presently be said of the distribution at some later time? The answer to this question is highly sensitive to the structure of the porous medium which is not typically homogeneous, irrespective of the scale of observation. The importance of heterogeneity of soil, and variation in its physical properties have been clearly recognized by Nielsen et al. (1973). Since then, this topic has moved to the center of research in the field of soil physics.

On one hand essential information on hydraulic material properties and transport parameters can be measured at fixed points for a certain set of boundary

* Corresponding author.
*E-mail address:* hjvogel@iup.uni-heidelberg.de (H.-J. Vogel).

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conditions. On the other hand the continuous heterogeneous structure of these properties for the range of possible boundary conditions is required as soon as the soil is not homogeneous. This demands the necessity to transfer information in space, time, and across scales and forms the major difficulty for a predictive modeling of flow and transport.

In this paper we start by describing a few examples of spatial heterogeneity in soil, and we define the related terms. Then, we briefly discuss different approaches to incorporate the phenomenon of spatial heterogeneity to modeling flow and transport. Next we propose a concept we term ‘the scaleway’, which is based on the explicit consideration of spatial structure. We suggest it is a promising tool for predictive modeling of flow and transport in the subsurface, at any scale. This concept is demonstrated for the prediction of a breakthrough curve in an undisturbed soil column using structural information from two different scales. Finally, we discuss the implications for the application of our approach at larger scales.

## 2. Spatial heterogeneity—direct observations and experimental evidence

Fig. 1 shows the visual appearance of a silty soil (Orthic Luvisol) obtained with different instruments at different scales of observation. The size of the different fields-of-view differ by about one order of magnitude. The variable measured at the largest scale using an optical camera is color, for the smaller scales it is the density of electrons as measured by X-ray tomography. From the example of Fig. 1, it is obvious that there may be some sort of structure at any scale of observation. Fig. 1 may be extended in both directions. At the larger scale we may detect patterns of different soil types which themselves are part of regional soil associations, and so forth. The same is true towards smaller scales where we may detect the structure of intra-aggregate pores and the arrangement of mineral grains. Such a structural organization seems to be typical for terrestrial systems, and this has been described for both aquifers (Anderson, 1997) and soils (Wagenet, 1998).

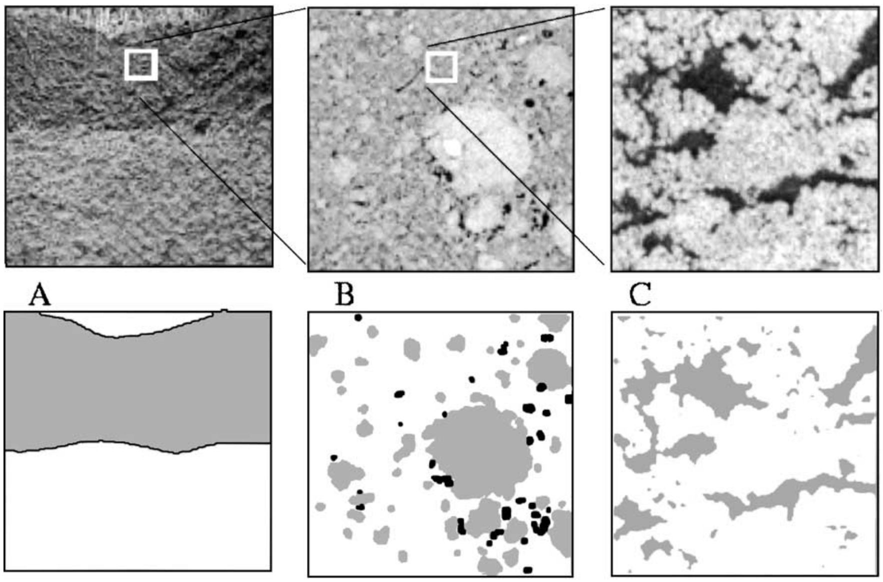


Fig. 1. Structure at different scales in a silty soil obtained with different instruments. Top left: photograph of a vertical profile, width ≈ 1 m. Top middle: X-ray tomography of the A-horizon, width ≈ 0.1 m, resolution 0.5 mm/pixel, gray values are proportional to bulk density (pores are dark). Top right: X-ray micro-tomograph, width ≈ 0.01 m, resolution 0.04 mm/pixel (pores are dark). Below, the images are segmented into the structural units at the corresponding scales. Bottom left: two different horizons. Bottom middle: dense aggregates (gray) within a loose matrix (white) and a few macropores (black). Bottom right: pores (gray) within a porous matrix.

At this point we wish to introduce a few terms which are used to describe the characteristic lengths and the features of spatial heterogeneity at different scales.

The linear extent of the entire investigated region is denoted as the *scale of observation*. The notion of *macroscopic* and *microscopic* is that macroscopic means 'of similar size' and microscopic means 'very much smaller' compared to the scale of observation. By analogy, we distinguish between *structure* and *texture*, where the structure is composed of form-elements comparable in size with the scale of observation, while the textural elements are very much smaller. In that way the terminology used is independent of the scale considered. The notion of structure and texture is used here in a broader sense than in common textbooks of soil science where texture refers to the size distribution of soil particles, and structure to their aggregation into larger units.

Some examples are given in Fig. 1 where the structural elements for the three different scales of observation are shown (Fig. 1, lower row). The macroscopic structural elements may be of different origins which, for the specific cases in Fig. 1, are indicated by different levels of gray. Accordingly we may distinguish different *structural units*. At the intermediate scale in Fig. 1 (middle), these structural units are 'dense aggregates' (gray), 'loose matrix' (white), and 'macropores' (black). Different structural units can be distinguished according to their texture.

It is worthwhile to note that the transition between structure and texture, or macroscopic and microscopic, can either be very clear as in the case of the structural units of soil horizons in Fig. 1 (left), or it can be somewhat fuzzy as for the dense aggregates and the loose matrix in Fig. 1 (middle). This problem is discussed in detail below.

It is assumed that the structural units are also different in terms of the relevant physical properties that govern flow and transport—namely, the soil water characteristic and the hydraulic conductivity—thus, the dominating impact of structure on the phenomenology of flow and transport is clear. As a consequence, for structured materials we observe spatial variability in replicated measurements of the soils' physical properties at different locations within a given material. This is true because, by definition, the structural units are not captured representatively in the sense of a representative elementary volume (REV). Moreover, the outcome of any measurement depends not only on the location, but also on the scale of observation.

To that point, these conclusions are only based on purely structural observations. On the other hand, they are corroborated by flow and transport experiments reported in the literature. Gomez-Hernandez and Gorelick (1989) could not find a unique value for the effective hydraulic conductivity of an aquifer based on various well positions and pumping rates. Desbarats and Bachu (1994) found a steady increase in the spatial variability of transmissivities obtained over increasing scales of observation which covered more than two orders of magnitude. Transport experiments in groundwater indicated that the dispersivity increases approximately with a power of the observation scale (Gelhar, 1986; Neuman, 1990). Similar results have been reviewed by Gelhar et al. (1992). By visualizing transport patterns in soil, Flury et al. (1994) demonstrated for a large variety of soils that structural units are critical. At the pore scale, Vogel et al. (2002) analyzed geometric properties of the pore space together with measures of gas diffusion, as a function of the scale of observation. They could find a characteristic length of an REV, but only after separating the pore space into structural units.

That soils and aquifers are structured at any scale seems to be the rule. The existence of a macroscopically homogeneous medium seems to be the exception. In Section 3 we discuss different approaches to tackle this kind of spatial heterogeneity.

## 3. Modeling spatial heterogeneity

One step towards modeling spatial heterogeneity is to apply stochastic continuum theory. Thereby, the relevant material properties, such as the hydraulic conductivity $K$, are considered to be stationary random variables that can be described by its mean value and autocovariance function. Pioneering work in that field was done by Gelhar (1974, 1986) and Dagan (1984, 1989) who modeled heterogeneous groundwater systems. Applying perturbation methods they showed, amongst other things, that the apparent longitudinal dispersion coefficient increases with transport distance, and that it asymptotically reaches a value that depends on variance and correlation length of the logarithmic conductivity field. This result depends crucially on the correlation length being finite. Furthermore, the approach to the asymptotic limit is on a length scale that is very much larger than the correlation length, and depends on details of the conductivity field, and on the initial solute distribution. The stochastic continuum approach may be useful for studying some heterogeneous media with discrete hierarchies, or for estimating material properties of the texture.

There are other models of spatial heterogeneity that account for the fact that structure may be present at all scales. Cushman (1990) considered there may be a discrete hierarchy of structural units when moving through various scales of observation. In this case, as shown in Fig. 2, the result of some kind of measurement has a well-defined value only when sampling a single hierarchical level. This value becomes unstable in the transition zone between two different hierarchical levels. A discrete hierarchy implies a clear disparity of scales where the statement of the REV is a local property related to a single structural unit. This concept is

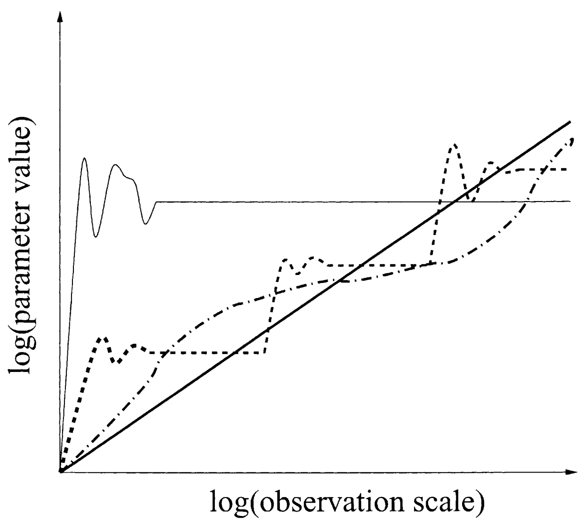


Fig. 2. Dependency of an imaginary parameter value on the scale of observation assuming different concepts of spatial heterogeneity: macroscopic homogeneity (thin line), discrete hierarchy (dashed line), continuous hierarchy (dashed dotted line), and fractal (thick line).

successfully applied at very-large scales where discrete geological facies are distinguished (Anderson, 1997), and also in the field of hydrological modeling (Blöschl and Sivapalan, 1995) where the structure may be represented by hydrological response units (Flügel, 1995). Also in soil science where different soil horizons are considered to be functional entities with internal heterogeneity, the system can be treated as a discrete hierarchy.

However, there may be no clear disparity in scales. This means the structural units are interlaced and nested at different scales, so we cannot expect any meaningful material property that is independent of the scale of observation. Hence, no REV exists even for a limited fraction of scale. In that case, material properties are expected to change continuously with scale (Fig. 2). This type of structural organization may be referred to as a continuous hierarchy (Cushman, 1990), or evolving heterogeneities (Wheatcraft and Cushman, 1991). The experimental findings of continuously evolving properties, as cited above, point into that direction.

Fractals can be considered as a special case of continuous hierarchy where the structural units at different scales are self-similar. As a consequence, a well-defined relation between material properties and the scale of observation can be expected (Fig. 2). This approach is appealing since information obtained at a given scale can be easily transferred to another scale. Neuman (1990) suggested a universal scaling law for longitudinal dispersivities $a_L = 0.017s^{1.5}$, where $s$ is the mean travel distance. His analysis was averaged over a broad variety of geologic media and a broad variety of flows and transport conditions. As argued by Anderson (1991), similar results may be obtained for a discrete hierarchical organization of geological facies. The potential of fractal models to predict transport properties at a specific site still remains to be demonstrated. Soil structure and related material properties have been suggested to be fractal (Wheatcraft and Tyler, 1999; Rieu and Sposito, 1991; Perrier et al., 1995; Baveye and Boast, 1998), yet it is not obvious that soil should exhibit fractal properties. The self-similarity of the structure would suggest some self-similarity in the generation processes of the structure. While this may be the case in some aquifers due to their alluvial origin, we do not expect this for all soils. Here, quite disparate processes are responsible for structure formation, and each of them may actually introduce a scale of its own. Examples for such processes are formation of organo-clay complexes, desiccation cracking, borrowing animals, or the formation of soil patterns due to the topography.

## 4. The scaleway

In the following we introduce the scaleway as a concept that is able to handle multi-scale heterogeneities to predict flow and transport at a specific site and at a given scale. The proposed concept is in contrast to effective models and classical perturbation theories that are based on macroscopic homogeneity and the existence of a finite correlation length.

Most simply, the scaleway can be demonstrated for discrete hierarchical structures, for which at each scale of observation the structural units can be clearly distinguished. This corresponds to the consideration of discrete geological facies as discussed above. However, as described below, the scaleway is also applicable to continuous hierarchies and fractal structures.

We start from the knowledge that many processes in soil are dissipative in the sense that microscopic details average out at the macroscopic scale and hence, only the macroscopic structure is relevant. This is obvious at least for those processes described by linear diffusion (Hammel and Roth, 1998), but it may not be obvious and actually it may not be true for others. A notorious example of a non-dissipative process is invasion of air into water-saturated soil where structural features at the microscopic scale may control the macroscopic behavior.

For the class of dissipative processes, we may choose an arbitrary scale for separating structure, which is to be represented explicitly, from texture, which is to be described by material properties. The scheme of this concept is shown in Fig. 3. At any particular scale we observe some sort of structure, where the different structural units are labeled by a certain texture. The structure is, at least in principle, directly observable by appropriate instruments irrespective the scale of observation. We assume further that the detected structural units are associated with specific material properties that govern flow and transport. Consequently, we associate the texture of the different structural units with a set of material properties. At the scale of a small plot this would for instance be the soil water characteristic and the hydraulic conductivity function. For the remaining

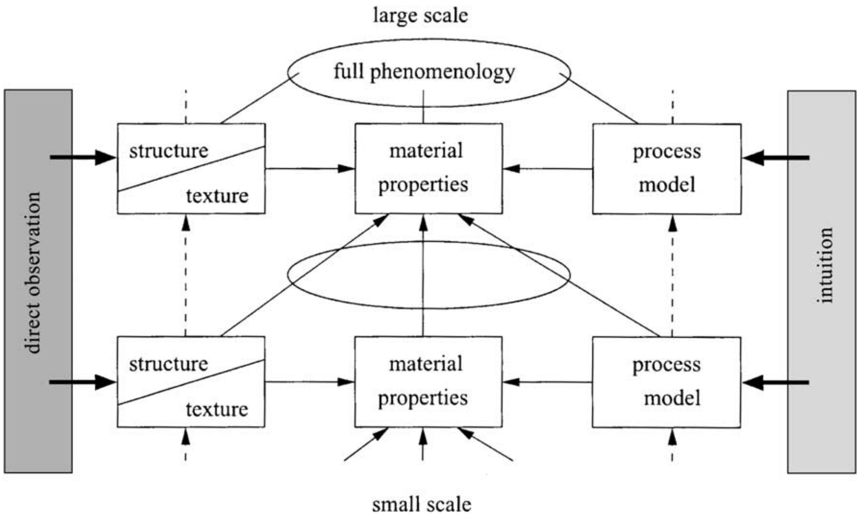


Fig. 3. Sketch of the scaleway from small scale (bottom) to larger scales (top). At each scale we observe structural units distinguished by their texture which is associated with a set of material properties. The structure of material properties together with an appropriate process model are necessary but sufficient ingredients to calculate the full phenomenology at the next larger scale and effective material properties at this larger scale.

ingredient at a given scale we need an appropriate process model, for instance Stokes' equation at the pore scale, or Richards' equation at the continuum scale. Then, the effective properties at a given observation scale can be calculated. These effective properties may represent the material properties of a structural unit at the next larger scale, while the structure at the actual scale translates into texture and so forth.

Note that we do not only get some effective parameters at the scale of observation. Additionally, the complete phenomenology without invoking effective processes is available at the scale of observation provided that the underlying process model is correct. This is the base that allows one to predict the effective behavior. It is possible because the continuous structure of the relevant material properties is available.

To enter the scaleway at some point, the structure must be known. Typically, the instruments used to measure the structure do not directly measure the variables required by the process model like for instance hydraulic parameters. Hence, we aspire to measure the structure of some property that is correlated with the variables of interest and we use such proxy variables to distinguish between different structural units. The material properties for each structural unit, i.e. the variables of interest, are directly measured whenever feasible. If this is not the case, they must be calculated from the next smaller scale as a convolute of structure, material properties and process model. The fundamental input comes from the observation of the structure and our understanding of the processes. The process models are typically ad hoc formulations based on experiences and our intuition.

Obviously, the scaleway is not restricted by the type of forms, be they uniform, regularly structured, fractal or irregularly structured. The price for this generality is the inability to predict anything beyond the scale of observation. Since such predictions appear rather useless in light of the multi-scale nature of natural forms, we do not perceive this as a severe restriction. An example for a continuous hierarchical structure is shown in Fig. 1 (middle). Here, the separation of the soil material into structural units, which are dense aggregates and loose matrix, is not obvious. The hierarchy may be considered to be continuous. There is no clear lower limit for the size of aggregates and therefore, it is not clear which aggregates should be considered explicitly as part of the structural unit dense aggregates and which aggregates are small enough to be part of the texture of the loose matrix. With respect to solute transport, this problem may not be very severe because the processes are dissipative. This means that the effective behavior, such as the breakthrough curve of a solute pulse, is mainly affected by the coarse structural elements, while the effect of tiny details is smeared out.

## 5. Example

As an application of the scaleway we consider solute transport within an undisturbed soil column taken from the top horizon of an arable soil (Orthic Luvisol). The goal was to predict the breakthrough curve of a conservative tracer that was transported by a stationary water flow. This problem is described in the context of the scaleway in Fig. 4. The different steps required are only summarized here since they have already been published elsewhere (Vogel and Roth, 1998; Kasteel et al., 2000).

The cylindrical column had a diameter of 160 mm and a height of 90 mm. After establishing a stationary water flux of 11.4 mm $h^{-1}$, the tracer, $Br^-$, was applied as a step input and a classical breakthrough curve was measured.

To predict the result, the structure of bulk density was measured for the complete column by X-ray tomography at a resolution of 0.4 mm. Then, the three-dimensional image was segmented into dense aggregates and loose matrix, and coarse-grained to a resolution of 3 mm (Fig. 5) in order to run the subsequent numerical simulation of flow and transport more efficiently.

At this scale, we assume that the measured bulk density can be used as a proxy for hydraulic properties, i.e. soil water characteristic $\theta(\psi_m)$ and hydraulic conductivity function $K(\theta)$ where $\theta$ denotes the water content and $\psi_m$ the matric potential of water. Once these material properties are known, we apply Richards' equation

$$\partial_t \theta - \nabla \cdot [K(\theta)\nabla\psi] = 0, \quad (1)$$

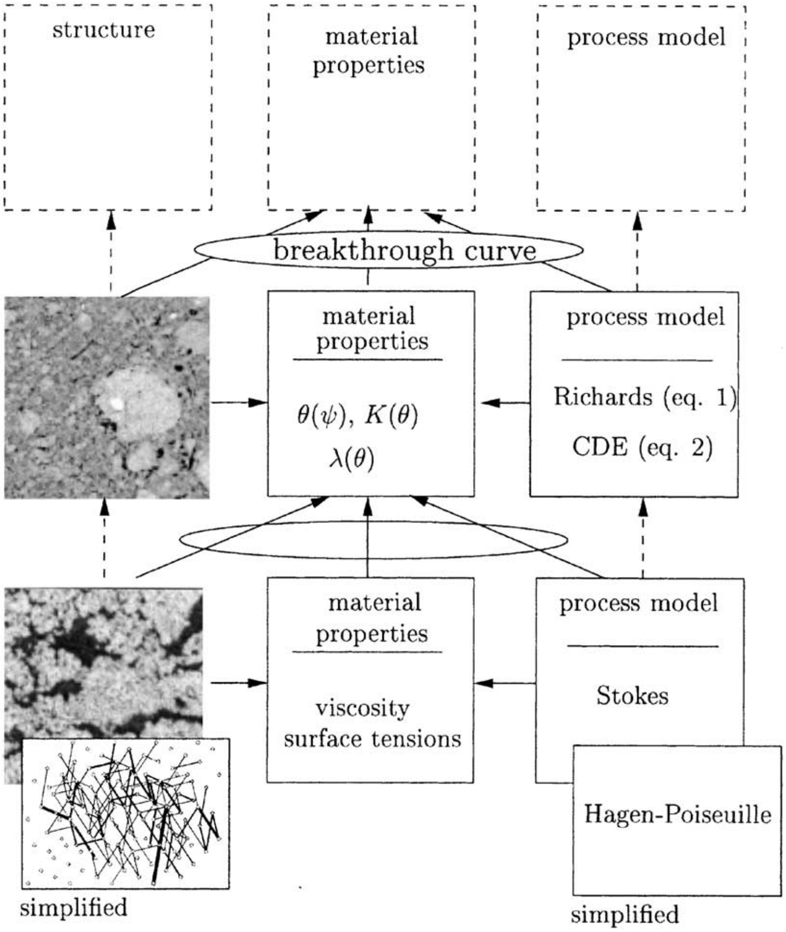


Fig. 4. Prediction of the breakthrough curve of a conservative tracer for a undisturbed soil column following the scaleway.

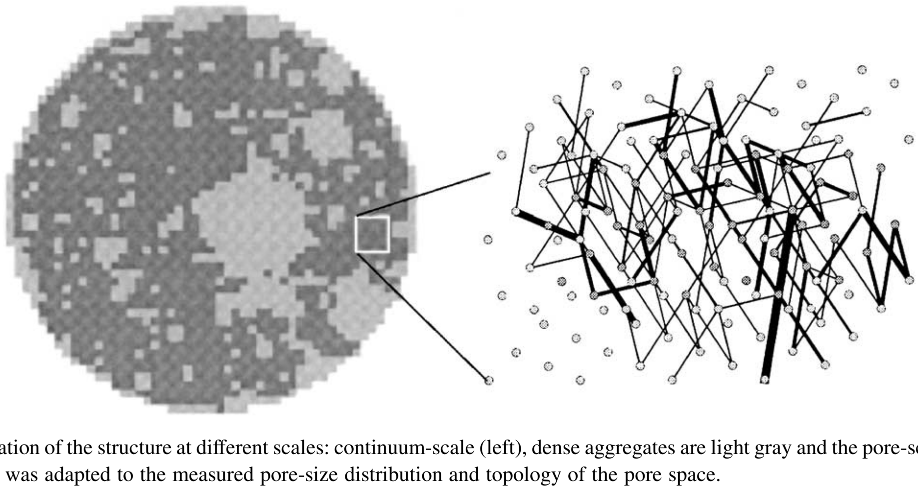

Fig. 5. Representation of the structure at different scales: continuum-scale (left), dense aggregates are light gray and the pore-scale (right) where a network model was adapted to the measured pore-size distribution and topology of the pore space.

where $\psi$ is the total soil water potential, as a process model to describe the water dynamics.

The dynamics of the transport of a conservative tracer is modeled by the convection dispersion equation (CDE)

$$\partial_t[\theta C_\mathrm{w}] + \nabla\cdot[\theta V C_\mathrm{w}] - \nabla\cdot[\theta D \nabla C_\mathrm{w}] = 0, \quad (2)$$

where $C_\mathrm{w}$ denotes solute concentration in the water phase, $V$ pore water velocity, and $D$ dispersion tensor. Consequently additional parameters are required: the velocity field $V$ and $D$ which are functions of the water content and the water flux. These functions are generally not well known however. For our experiment $V$ is obtained from the solution of Eq. (1) and we add the dispersivity $\lambda = D/V$ as another material property which was kept constant. For a detailed derivation of the models (1) and (2) the reader is referred to some textbook on soil physics (Jury et al., 1991).

The remaining question is how to get the material properties $\theta(\psi)$ and $K(\theta)$ for the two different structural units. Direct measurements using subsamples of some 10 mm are not feasible. Hence, with the scaleway in mind, we move to the smaller scale, since $\theta(\psi)$ and $K(\theta)$ can be considered to be effective descriptions of the underlying pore structure. Subsamples were impregnated with a polyester resin and the three-dimensional geometry of the pore space was obtained by serial sections at a resolution of 0.013 mm. Details are given by Vogel (1997). We now enter the scaleway. Given the three-dimensional pore structure, the hydraulic properties may be calculated using Stokes' equation with viscosity of water and surface tensions water/air and water/solid as material properties at this scale. However, to solve numerically that problem for a complex structure is a monumental task, and therefore we chose a simpler approach.

The complex pore geometry was quantified in terms of pore size distribution and pore topology. These two properties are expected to govern the hydraulic properties. To obtain the pore size distribution we applied morphological erosion followed by dilation using spherical structuring elements of different radii $r$ (Serra, 1982). This procedure filters all pores smaller than $r$. Hence, each point within the pore space can be attributed to a pore size class. Additionally, the spatial connectivity of the different pore size classes is known to be critical for the hydraulic behavior of porous media. A quantitative description of the pores' topology was obtained by the connectivity function, which is defined as the Euler number in dependency of the pore size (Vogel, 1997). These morphological results were used to represent the pore structure by an equivalent network model. Thereby, the complex pore structure is idealized by a network of cylindrical tubes of different radii. Fig. 5 shows a small cutout ($4^3$ nodes) of a network with $64^3$ nodes which was used for the simulations. The model was constructed such that its pore size distribution and connectivity function corresponds to the measured values.

For such network models $\theta(\psi)$ can be directly calculated using the Young–Laplace relation, essentially $\psi_\mathrm{m} \propto 1/r$ and taking into account the continuity of the gaseous phase. Additionally, the hydraulic conductivity function can be obtained by simulating a pressure gradient over the network and using Hagen–Poiseuille's law, essentially $K \propto r^2$, to calculate the effective conductivity. Details are given by Vogel and Roth (1998).

In this way we obtained an estimation for the hydraulic properties of the two structural units as a convolute of structure and process model at the subscale. Vogel and Roth (1998) compared the results with direct multi-step outflow experiments and found a reasonable agreement. Together with the three-dimensional image measured by X-ray tomography, the complete three-dimensional structure of hydraulic properties was available. Given the hydraulic properties, solution of Eq. (1) using SWMS_3D (Šimůnek et al., 1995) yielded the flow field $j_\mathrm{w}$. Transport properties $V$ and $D$ were estimated by (i) presuming that the entire water phase was active in transport, hence $V = j_\mathrm{w}/\theta$, and (ii) by choosing 1 mm for the longitudinal dispersivity and 0.5 mm for the transversal dispersivity which is smaller than the spatial discretization of 3 mm. The transport problem (2) was solved by a random-walk algorithm (Roth and Hammel, 1996).

Fig. 6 shows some horizontal sections of the simulated tracer distribution after 28.5 mm of infiltration. It should be noted that a tensiometer was installed in a depth of 20 mm which led to some compaction of the soil material. Consequently there

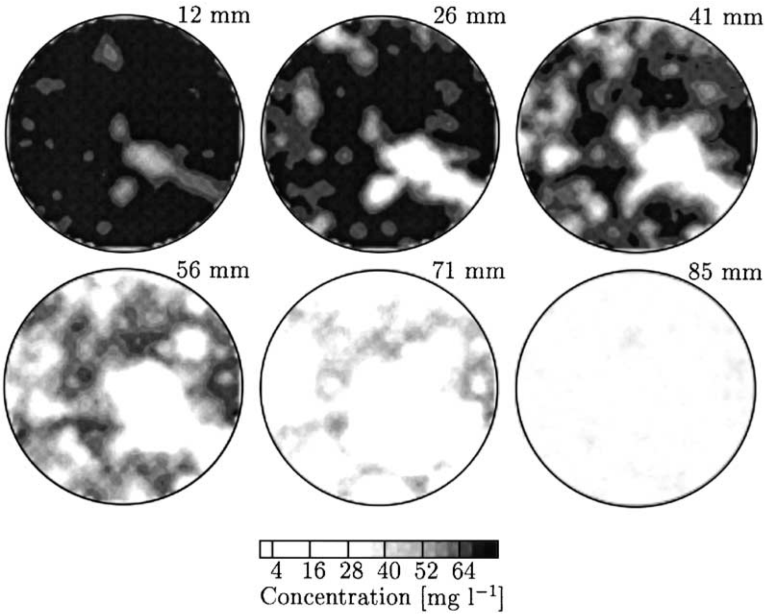


Fig. 6. Simulated concentration distribution of a conservative tracer at various depths of a soil column after an infiltration of 28.5 mm.

was a dense aggregate in the surroundings of that instrument and the effect on tracer distribution is clearly visible. This also demonstrates that the physical reality of the experiment is faithfully represented.

The comparison between measured and simulated breakthrough curves is shown in Fig. 7. Although the long tail of the measured curve is not represented well in the simulation, the agreement between the two curves was reasonable which demonstrates the predictive power of our approach. This is especially true considering the fact that we have not used any information from the experiment itself. This is in contrast to the mobile–immobile model (van Genuchten and Wierenga, 1976) which yields a much better description of the measured data but is only a retrospective description of the specific experiment. This is because the partitioning into mobile and immobile water and the exchange term between theses compartments is fitted to the measured data, and the physical meaning of the introduced parameters is not clear. Our prediction based on the structure of material properties emulates the physical reality. It reproduces the observed phenomenology without a heuristic partitioning into mobile and immobile fractions of the water phase.

## 6. Implications and extension to larger scales

The example presented in Section 5 operates on the relatively small scale of a soil column while the scale of typical problems in solute transport is much larger. It is in the order of some meters, the distance from the soil surface to the groundwater. When moving to

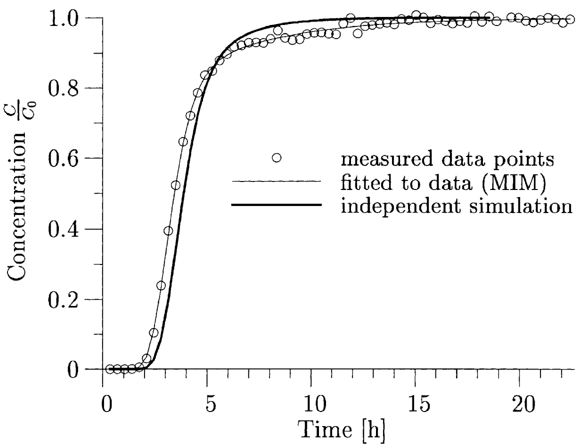


Fig. 7. Breakthrough curve of a conservative tracer: measured (symbols), independently predicted (thick line) and mobile–immobile-model fitted to the data (thin line).

larger scales, the instruments to measure the relevant structure may change. The same is true for the process model and for the material properties.

Irrespective of the techniques used, the structure must be measured continuously at a resolution that allows to represent the structural units including their topology. The latter describes the connectivity which is a critical property for any kind of transport process and requires a continuous measurement. Thereby, more specifically, we need the structure of the relevant material properties.

However, in most cases, the material properties cannot be measured directly. As already mentioned above, we have to rely on surrogates that are suitable proxies for the required material properties and that can be measured efficiently and continuously. In the example presented above we used bulk density which could easily be measured by X-ray tomography as a proxy for hydraulic properties. In catchment hydrology topography is widely used as proxy for hydraulic variables, since this information is continuous in space and readily available.

Measuring technologies at the field scale and beyond are not as developed as at the lab scale. However there are a number of geophysical methods that have originally been invented for exploring deeper layers of the earth, but may be adapted to near-surface measurements. One example is ground-penetrating radar (GPR) which can be used to map the dielectric structure of the subsurface. This is an excellent proxy for the pore size distribution which can be linked to hydraulic properties. While this link does not yield the hydraulic properties themselves, probably not even a useful estimate for its value, we believe that it yields the spatial structure of the corresponding fields. This suffices for entering the scaleway. In contrast to pedotransfer functions, where the variables of interest are directly calculated from the proxy variables after some kind of regression analysis, we suggest to use the proxy variable merely to identify the structural units.

By using proxy variables to describe the structure, the measurement error is increased due to the imperfect correlation between proxy and the required material properties. However, there is some evidence, that a relatively coarse description of the three components—structure, material properties, and process model—may be sufficient to predict the effective behavior reasonably well. This is corroborated by the small scale example (Fig. 4) where all these components are represented by rather coarse approximations. Obviously, if one of these components is missing, prediction would not be possible at all.

These coarse approximations, however, must encompass all significant properties. Considering the pore geometry, the significant properties are the size distribution of pores and their topology which both are represented in the network model. It was demonstrated by Vogel (2000) for the same data set, that ignoring the topological characteristics of the pore space leads to completely different results for both, the hydraulic properties and the transport parameters.

The topology or connectivity of the structure may be a critical point at any scale of observation. Clearly, topology of structural units plays a crucial role for any kind of transport process. On the other hand, in terrestrial systems we often face structural units that are extremely anisotropic. At the small scale the most notorious structures of this kind are earthworm burrows, root channels and cracks. Examples at the large scale are river networks, their remnants in the subsurface, and thin sedimentary layers. To represent the topology of structural units the ratio between field of view and resolution, which is a characteristic of the instrument used to measure the structure, should be much larger than the anisotropy ratio of the structural units. In some cases this condition may be hard to meet. Photographic techniques and X-ray tomography have a relatively high ratio between field of view and resolution of some $10^3$. For near-surface geophysical methods, such as GPR, this ratio is more like $10^1$.

Another tool to get a continuous description of the spatial structure is provided by geostatistics where point measurements are extrapolated using different methods of kriging (Chilès and Delfiner, 1999). Thereby, however, the extrapolation is based on critical assumptions on the structure, such as isotropy, and topological characteristics are typically lost completely. Hess et al. (1992) found that a very large number of points of measurement are required to come up with a conductivity field that is able to predict the macroscopic dispersivity. Using proxy information seems to be much more efficient. This was also proposed by Sivapalan (1993) who used information on topography, climate and vegetation cover to identify structural units at the subscale. Viney and Sivapalan (2001) termed it the disaggregation–aggregation approach. Thereby, in a first step, the results obtained at the large scale are disaggregated, i.e. distributed in space, using appropriate proxy information. Then, in an aggregation step, the effective behavior at the observation scale is obtained based on the spatially distributed parameter field.

In summary, concerning the measurement of structure, there are promising perspectives also for the larger scale. But what about the process model? Is Richards' equation still applicable at the regional scale? We should comment that such qualitatively new knowledge cannot be expected to result from some mechanistic operation, but only comes out of some new vision of the matter. Of course, the scaleway may serve as a base to produce such a vision and to verify it. Given the structure of material properties, the full phenomenology at a given (large) observation scale can be calculated as a result of the chosen model and herewith the model prediction can be compared to the reality.

## 7. Conclusions

Geologic materials like soils and aquifers are almost always heterogeneous and they are often so across many scales. Many important processes in such media, for instance groundwater flow or solute transport in soil, are dissipative in the sense that the details of small-scale features are immaterial at a larger scale. For that kind of process we arrive at the following conclusions.

1. The explicit consideration of structure in modeling flow and transport, here referred to as the scaleway, is a predictive tool to quantify the phenomenon of solute transport. By introducing the structure of the material, we do not have to prejudice any 'effective' process model at the scale of observation. The effective phenomenon of solute transport is implicit in the structure and the microscopic process model.
2. Once the structure, the related material properties, and the process model are known, a relatively coarse description of these ingredients may be sufficient to come up with a reliable prediction. On the other hand if one of those is qualitatively wrong, the effective behavior cannot be predicted.
3. As a consequence of (2) we should focus more on measuring structure rather than on measuring hydraulic properties with more and more precision. Moving the location of the sample by a short distance would change the result anyway, if the material is structured. The identification of suitable proxy variables is crucial in this context, because direct measurement of the relevant variables is typically not possible.

We demonstrated the concept of the 'scaleway' for a simple example which we already know in much detail. While a lot of experimental and theoretical work will be required to make the proposed concept operational at larger scales, we believe that it allows a consistent transition from one scale to the next.

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## References

Anderson, M.P., 1991. Comment on 'Universal scaling of hydraulic conductivities and dispersivities in geologic media' by S.P. Neuman. Water Resour. Res. 27, 1381–1382.

Anderson, M.P., 1997. Characterization of geological heterogeneity. In: Dagan, G., Neumann, S.P. (Eds.), Subsurface Flow and Transport: A Stochastic Approach, International Hydrology Series, University Press, Cambridge, pp. 23–43.

Baveye, P., Boast, C., 1998. Fractal geometry, fragmentation processes and the physics of scale-invariance: an introduction. In: Baveye, P., Parlange, J., Stewart, B. (Eds.), Fractals in Soil Science, Advances in Soil Science, CRC Press, Boca Raton, pp. 1–54.

Blöschl, G., Sivapalan, M., 1995. Scale issues in hydrological modelling: a review. Hydrol. Process. 9, 251–290.

Chilès, J.-P., Delfiner, P., 1999. Geostatistics, Modeling Spatial Uncertainty, Wiley, New York.

Cushman, J.H., 1990. An introduction to hierarchical porous media. In: Cushman, J.H., (Ed.), Dynamics of Fluids in Hierarchical Porous Media, Academic Press, London, pp. 1–6.

Dagan, G., 1984. Solute transport in heterogeneous porous formations. J. Fluid Mech. 145, 151–177.

Dagan, G., 1989. Flow and Transport in Porous Formations, Springer, Berlin.
Desbarats, A.J., Bachu, S., 1994. Geostatistical analysis of aquifer heterogeneity from the core scale to the basin scale: a case study. Water Resour. Res. 30 (3), 673–684.
Flügel, W.-A., 1995. Delenating hydrological response units by geographical information system analysis for regional hydrological modelling using PRMS/MMS in the drainage basin of the river Bröl, Germany. In: Kalma, J.D., Sivapalan, M. (Eds.), Scale Issues in Hydrological Modelling, Wiley, New York, pp. 181–194.
Flury, M., Flühler, H., Jury, W.A., Leuenberger, J., 1994. Susceptibility of soils to preferential flow of water: a field study. Water Resour. Res. 30, 1945–1954.
Gelhar, L.W., 1974. Stochastic analysis of phreatic aquifers. Water Resour. Res. 10, 539–545.
Gelhar, L.W., 1986. Stochastic subsurface hydrology. From theory to applications. Water Resour. Res. 22, 135S–145S.
Gelhar, L.W., Welty, C., Rehfeldt, K.R., 1992. A critical review of data on field-scale dispersion in aquifers. Water Resour. Res. 28, 1955–1974.
van Genuchten, M.T., Wierenga, P.J., 1976. Mass transfer studies in sorbing porous media. I. Analytical solutions. Soil Sci. Soc. Am. J. 40, 473–480.
Gomez-Hernandez, J.J., Gorelick, S.M., 1989. Effective groundwater model parameter values: influence of spatial variability of hydraulic conductivity, leakance, and recharge. Water Resour. Res. 25, 405–419.
Hammel, K., Roth, K., 1998. Approximation of asymptotic dispersivity of conservative solute in unsaturated heterogeneous media with steady state flow. Water Resour. Res. 34, 709–715.
Hess, K.M., Wolf, S.H., Celia, M.A., 1992. Large-scale natural gradient tracer test in sand and gravel, Cape Cod, Massachusetts. 3. Hydraulic conductivity variability and calculated macrodispersivities. Water Resour. Res. 28, 2011–2027.
Jury, W.A., Gardner, W.A., Gardner, W.H., 1991. Soil Physics, Wiley, New York.
Kasteel, R., Vogel, H., Roth, K., 2000. From local hydraulic properties to effective transport. Eur. J. Soil Sci. 51, 81–91.
Neuman, S.P., 1990. Universal scaling of hydraulic conductivities and dispersivities in geologic media. Water Resour. Res. 26, 1749–1758.
Nielsen, D.R., Biggar, J.W., Erh, K.T., 1973. Spatial variability of field-measured soil-water properties. Hilgardia 42, 215–259.
Perrier, E., Mullon, C., Rieu, M., de Marsily, G., 1995. Computer construction of fractal soil structures: simulation of their hydraulic and shrinkage properties. Water Resour. Res. 31, 2927–2943.
Rieu, M., Sposito, G., 1991. Fractal fragmentation, soil porosity and soil water properties: I. Theory. Soil Sci. Soc. Am. J. 55, 1231–1238.
Roth, K., Hammel, K., 1996. Transport of conservative chemical through an unsaturated two-dimensional miller-similar medium with steady flow. Water Resour. Res. 32, 1653–1663.
Serra, J., 1982. Image Analysis and Mathematical Morphology, Academic Press, London.
Šimůnek, J., Huang, K., van Genuchten, M.T., 1995. The SWMS_3D code for simulating water flow and solute transport in three-dimensional variably-saturated media. Research Report 139, US Salinity Laboratory, USDA/ARS, Riverside, CA.
Sivapalan, M., 1993. Linking hydrologic parametrizations across a range of spatial scales: hillslope to catchment to region. In: Bolle, H.-J., Feddes, R.A., Kalma, J.D. (Eds.), Exchange Processes at the Land Surface for a Range of Space and Time Scales, Proceedings of the Yukohama Symposium, IAHS Publication No. 212, pp. 115–123.
Viney, N.R., Sivapalan, M., 2001. Scaling of hydrologic conceptualizations: approaches to handling subgrid variability. Proceedings of MODSIM 2001, International Congress on Modelling and Simulation, Canberra, Australia 2001, 383–388.
Vogel, H.J., 1997. Morphological determination of pore connectivity as a function of pore size using serial sections. Eur. J. Soil Sci. 48, 365–377.
Vogel, H.J., 2000. A numerical experiment on pore size, pore connectivity, water retention, permeability, and solute transport using network models. Eur. J. Soil Sci. 51, 99–105.
Vogel, H.J., Roth, K., 1998. A new approach for determining effective soil hydraulic functions. Eur. J. Soil Sci. 49, 547–556.
Vogel, H.J., Cousin, I., Roth, K., 2002. Quantification of pore structure and gas diffusion as a function of scale. Eur. J. Soil Sci. 53, 465–473.
Wagenet, R.J., 1998. Scale issues in agroecological research chains. Nutrient Cycling Agroecosyst. 50, 23–34.
Wheatcraft, S.W., Cushman, J.H., 1991. Hierarcical approaches to transport in heterogeneous porous media. Rev. Geophys., Suppl., March 1991, 263–269.
Wheatcraft, S.W., Tyler, S.W., 1999. An explanation of scale-dependent dispersivity in heterogeneous aquifers using concepts of fractal geometry. Water Resour. Res. 24, 566–578.