How Useful are Small-Scale Soil Hydraulic Property Measurements for Large-Scale Vadose Zone Modeling?

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A major challenge that recurs throughout the geophysical sciences is the downscaling (disaggregation) and upscaling (aggregation) of flow or transport processes and their measurement across a range of spatial or temporal scales. Such needs arise, for example, when field-scale behavior must be determined from soil hydraulic data collected from a limited number of in situ field measurements or analysis of small soil cores in the laboratory. The scaling problem cannot be solved by simple consideration of the differences in space or time scale, for several reasons. First, spatial and temporal variability in soil properties create uncertainties when changing between scales. Second, flow and transport processes in geophysics and vadose zone hydrology are highly nonlinear. We present a historical overview of the theory of scaling procedures, and demonstrate the application of various aggregation techniques, such as scaling and inverse modeling, to aggregate laboratory-scale soil hydraulic properties to larger scale effective soil hydraulic properties. Examples of application of these aggregation techniques from the pore scale to the watershed scale are demonstrated. We conclude that the development of new instrumentation to characterize soil properties and their variation across spatial scales is crucial. Moreover, the inherent complexity of flow in heterogeneous soils, or soil-like materials, and the need to integrate theory with experiment, requires innovative and multidisciplinary research efforts to overcome limitations imposed by current understanding of scale-dependent soil flow and transport processes.

INTRODUCTION

For the past few decades, soil scientists have applied soil hydraulic data to characterize flow and transport processes in large-scale heterogeneous vadose zones, using measurement scales that are typically much smaller. For example, prediction of soil-water dynamics at the field-scale is derived from the measurement of soil hydraulic properties from laboratory cores, collected from a limited number of sampling sites across large spatial extents, often using large sampling spacings. Typically, the measurement scale for soil hydraulic characterization is in the order of 10 cm, with a sample spacing of 100 m or larger.

This scale-transfer question is being asked more frequently than ever, mostly because of water quality issues resulting from chemical contamination of soil, groundwater, and surface water systems worldwide. Appropriate answers are expected, requiring the estimation of appropriate soil hydraulic parameters for use in describing the behavior of pollutant plumes at field or landscape scales. In 1991, the U.S. National Research Council [*NRC*, 1991] identified the scaling of dynamic nonlinear behavior of hydrologic processes as one of the priority research areas that offer the greatest expected contribution to a more complete understanding of hydrologic sciences. Simultaneously, with the increasing awareness of the crucial role of the soil and the vadose zone in the management of chemical loadings to groundwater and surface waters, soil hydraulic characterization is needed to predict transport and fate of agricultural and industrial chemicals at the regional or landscape scale. Routine measurement of soil hydraulic properties are usually conducted in the laboratory [*Dane and Hopmans,* 2002], using small-size soil cores, collected in-situ from a few representative or many random locations within the region of interest, or is done in the field on small field plots at the meter-scale [*Green et al*., 1986] using either direct or inverse methods [*Hopmans et al*., 2002]. Soil parameters obtained from cm-scale measurements (laboratory scale) are included in numerical models with a grid or element size ten times as large or larger, with the numerical results extrapolated to field-scale conditions. A critical analysis of the assumptions made when applying small-scale (subgrid) parameters to the model grid scale, was presented by *Beven* [1989].

Irrespective of scale, transient isothermal unsaturated water flow in non-swelling soils is described by the so-called Richards' equation,

$$C(h_m)\frac{\partial h_m}{\partial t} = \nabla \cdot \left[\mathbf{K}(h_m)\nabla\left(h_m - z\right)\right] \qquad (1)$$

which provides the soil water matric potential (h_m), water content (θ) and water flux density as a function of time and space, using one-, two-, or three-dimensional flow models (e.g.,*Šimůnek et al*., 1995]. In (1), $\mathbf{K}$ is the unsaturated hydraulic conductivity tensor (L T^{-1}), and z denotes the gravitational head (L) to be included for the vertical flow component only. The function $C(h_m)$ in (1) is the so-called soil water capacity, and represents the slope of the soil water retention curve. Both the soil water retention and unsaturated hydraulic conductivity functions are highly nonlinear, with both h_m and K varying many orders of magnitude over the water content range of significant water flow. These nonlinearities make the application of (1) across spatial scales inherently problematic. Specifically, the averaging of processes determined from discrete small-scale samples may not describe the true soil behavior involving larger spatial structures. Moreover, the dominant physical flow processes may vary between spatial scales. For example, *Dooge* [1997] discussed the hypothesis that the mathematical model represented by Eq (1) may not be applicable to describe unsaturated water flow at the watershed scale. Because their measurement is time-consuming, the number of measured hydraulic data is usually limited, and is usually far less than statistically required to fully characterize soil heterogeneity. As a result, data assimilation techniques, such as linear regression analysis, pedotransfer functions and neural networks [*Pachepski et al*., 1999, *Schaap et al*., 1998] have been developed to derive soil hydraulic functions from other, easier-to-obtain soil properties. Considering that soil hydraulic measurements are typically conducted for small measurement volumes and that the natural variability of soils is enormous, the main question asked, is how small-scale measurements can provide information about large-scale flow and transport behavior [*Gelhar*, 1986].

Field experiments have confirmed that soil heterogeneity controls flow and transport, including preferential flow. Initial attempts of the prediction of large-scale flow problems used deterministic modeling. Although studies such as those of *Hills et al*. [1991] showed a qualitatively acceptable comparison between field-measured and predicted water contents using a deterministic approach, other studies have shown the need for either distributed physically-based modeling [*Loague and Kyriakidis*, 1997] or stochastic modeling [*Famiglietti and Wood*, 1994] at the watershed scale, mostly because it will require an enormous amount of data to accurately represent the multi-dimensional soil heterogeneity. Similarly, stochastic approaches have been developed to characterize field-scale soil water flow, e.g. by using scaling and Monte-Carlo analysis [*Hopmans et al.,* 1988; *Hopmans and Stricker*, 1989], stochastic modeling [*Mantoglou and Gelhar*, 1987] and geostatistical methods [*Yeh and Zhang*, 1996; *Rockhold,* 1999].

Alternatively, the conceptual characterization of the flow system may be simplified by modeling the key flow mechanisms for representative elementary areas (REA) only, and for which effective hydrological parameters can be defined [*Duffy*, 1996; *Famiglietti and Wood*, 1994], assuming that variability within a REA is statistically homogeneous. Although partially successful in surface hydrology, it has been determined that the size of the REA is event-dependent, controlled by initial conditions and rainfall intensity [*Blőschl et al., 1995; Grayson et al*., 1997]. Surface hydrological modeling at watershed scales has also demonstrated that the spatial distribution of hydrological processes is controlled by the spatial organization of key soil properties (*Blőschl and Sivapalan*, 1995; *Merz and Plate*, 1997]. The need to incorporate the spatial organization of these key soil properties, such as the soil hydraulic functions, is also recognized in soil science. Specifically, we refer to the treatise by *Roth et al.* [1999], outlining a conceptualization of the control of soil heterogeneity on soil flow and transport processes, using the so-called scaleway approach. In this approach, the soil is conceptualized by a hierarchical heterogeneous medium with discrete spatial scales, that each may require different effective process models with distinct effective material properties.

Assuming that soils are statistically heterogeneous, *Freeze* [1975] questioned the existence of a uniquely defined equivalent saturated hydraulic conductivity, and concluded that its value is likely a function of the boundary conditions and soil geometry. In his review of some basic issues of the consequences of natural soil variability for prediction of soil hydraulic properties, *Philip* [1980] extended the work of *Freeze* [1975] to unsaturated, scale-heterogeneous soils, to hypothesize that the field application of theory of heterogeneous soil systems might lead to "trans-science." Although his conclusion appears bleak at first reading, Philip ends this remarkably insightful paper with a plea to 'not abandon the task of seeking to understand as much about these systems as we possibly can.' It is in this spirit that many soil scientists have continued their analysis of theories, both deterministic and stochastic, and soils, both at the field and landscape scale, to increasingly elucidate the control of small-scale processes on larger-scale flow behavior.

The following was partly presented at the joint 'Soil Science Society of America-German Soil Science Society' meeting in Osnabrueck [*Hopmans and Bristow*, 2000], and specifically asks whether routine soil hydraulic measurements conducted in the laboratory can successfully be applied to larger-scale flow and transport problems.

We will make an attempt to answer this question, while adopting the relativist concept of *Baveye and Sposito* [1984], assuming that soil property values are dependent on the scale of the measurement that can vary between soil properties. We also agree with *Baveye and Sposito* [1984] and *Beven* [2001] that the physical laws of the model scale must be consistent with the measurement scale. Hence, laboratory-measured soil hydraulic properties are appropriate input for laboratory-scale columns studies and simulation models. When applied to larger spatial scales, we offer two alternatives. First, the laboratory-scale soil hydraulic properties may be spatially distributed across the larger spatial scale of interest, assuming that the integrated flow behavior can be determined from aggregation of many individual, soil column-like flow processes. Second, laboratory-measured soil hydraulic functions can be used as initial estimates, and improved by using inverse modeling (IM), conditioned by scale-appropriate boundary conditions and flow measurements. Hence, we concur that prediction of hydraulic behavior of heterogeneous soils is likely impossible from the a priori knowledge of the homogeneous soil components that make up the heterogeneous soil, and that its estimation can only be accomplished using scale-appropriate measurements.

SCALE-DEPENDENCY OF SOIL PROPERTIES AND PROCESSES

Upscaling requires integration and aggregation of spatial information into larger spatial units, e.g., as in the estimation of an effective field soil water retention or conductivity curve from small-scale laboratory core measurements. As clearly pointed out by *Baveye and Boast* [1999], *Darcy*'s experiment [1856] can in effect be interpreted as yielding an upscaled, effective saturated hydraulic conductivity. In contrast, the downscaling requires the disaggregating of scale information to smaller scales, e.g., by discerning the contribution of different soil structures to the effective soil hydraulic conductivity function (*Kasteel et al*., 2000). In a statistical sense, one may refer to scale as the spatial correlation length or integral scale of the measurement, property, or process [*Dagan*, 1986]. In his classic treatise, Dagan distinguishes between the laboratory core scale, local scale, and regional scale. He defines the laboratory scale as equal to the representative elementary volume (REV), for which the mean is a constant deterministic quantity, and the variance approaches zero [*Bear,* 1972]. It is this scale, for which the Darcy equation can be used as the equation of motion, as derived from the volume averaging of the Stokes equations [*Whitaker*, 1986]. At the next, larger scale, *Dagan* [1986] defines the local scale, where the soil is heterogeneous, but stationary in the mean and variance. We interpret the regional scale as the spatial dimension at which the relevant soil properties become nonstationary.

Nonstationary Soil Properties

When increasing spatial scales, soil properties typically become nonstationary [*Russo and Jury*, 1987a], as evidenced by the delineation of soil map units in a soil survey. Much of the early soil spatial analysis, specifically geostatistics, was based on the intrinsic hypothesis of stationarity (stationarity of spatial differences), however, it is questionable whether this stationary model is realistic [*Webster*, 2000]. Nevertheless, as was pointed out by *Kavvas* [1999], the averaging of hydrologic observations or aliasing at a larger observation scale may remove nonstationary trends at the smaller observation scale. Specifically, as one moves through a hierarchical sequence of increasing sampling scales, nonstationarities at smaller spatial scales may be eliminated. An ideal instrument, such as the mathematical tool by *Cushman* [1984], will work similarly and filter out the high frequency variability component of a spatial signal to yield a scale-specific measurement. The remaining nonstationary trends of the natural variability or process scales [*Blőschl and Sivapalan,* 1995] may be determined from the power spectrum, covariance analysis, and by wavelet analysis [*Lark and Webster*, 1999].

As an example, a model of evolving heterogeneity [*Sposito,* 1986], assuming fractal heterogeneous soil properties, was presented by *Wheatcraft and Tyler* [1986], showing a pattern of heterogeneity that is scale-independent across a large range of scales (Figure 1).

Natural patterns of soil variability may show embedded, organizational structures as in Figure 1, that are not necessarily fractal, but that lead to nonstationary soil properties or processes. However, as pointed out by *Cushman* [1990], spatial patterns of soil properties within and between scales (structural hierarchy) might be different from the organization of the soil hydrological processes (functional hierarchy) across spatial scales. As different flow processes may be dominant at each scale, different mathematical relationships may be required to describe the underpinning physical process at each scale [*Klemeš*, 1983]. As one moves towards a larger spatial scale, soil properties may change from deterministic to random, with the smaller-scale variations filtered out by the larger-scale process, thereby eliminating nonstationary trends at the smaller spatial scales.

The spatial organization and its evolvement across spatial scales can be defined in various ways. The example of Figure 1 shows a discrete and a continuous variation pattern between and within the main spatial units, respectively. As noted by *Gelhar* [1986], at each field-of-view, the large-scale variation, which causes the nonstationairity of the specific soil variable or process, can be regarded as deterministic, whereas the smaller scale variations within each main unit can be treated stochastically. Alternatively, one can define the types of variability as ordered (between main units) and disordered (within main units), or as macroscopic and microscopic variations. Most appropriately, the hierarchical heterogeneous soil medium can be described by the structural and textural definitions or the scaleway approach of *Roth et al.* [1999], with the structural elements describing the dominating soil patterns that affect the physical mechanisms operating at the a priori defined field-of-view. In contrast, the textural patterns within the structural units are merely perturbations of the main processes, and can be described statistically. Thus, when characterizing soil hydraulic variability for the prediction of soil hydrologic processes, it is assumed that the occurrence and location of these structural elements are dominating, and must be accurately determined. We conclude that stationarity of a soil hydrological process or parameter is dependent on the scale of observation.

Analysis of process scales

Scale-dependent, nonstationary processes exhibit statistical properties that are different than what is usually assumed in geostatistical analysis. Specifically, the REV [*Bear*, 1972] cannot be defined, as the soil property changes value, when increasing the scale of observation. Moreover, the spatial correlation structure of nonstationary fields will depend on the spatial extent or sampling area of the data, resulting in variograms with multiple sills (see Figure 2) that occur at correlation lengths of the multiple process scales [*Gelhar*, 1986]. In addition, *Rodriquez-Iturbe et al.* [1995] demonstrated that nonstationary properties will show a power law decay of the variance, resulting in a linear relation between variance and observation scale, when plotted on a log scale.

The power spectrum is determined from the Fourier transform of the autocovariance functions and represents the partitioning of the sample variance into spatial frequency components [*Greminger* et al., 1985]. Process scales occur at spectral peaks, whereas spectral gaps represent spatial scales with minimum spectral variance. An example of a hypothetical power spectrum is demonstrated in Figure 3, with a small-scale (core scale) component, superimposed on two large-scale components (local and regional scale).

The Nyquist frequency of the power spectrum determines that the smallest process scale that can be examined is twice the sampling scale [*Cushman*, 1984]. In other words, if the sampling distance is d (spatial frequency is 1/d), then no fluctuations in processes with size smaller than 2d (or larger than 1/2d) can be observed. Using measurement scales larger than defined by the Nyquist frequency would merely show noise, rather than describing spatial trends. Analogously, *Russo and Jury* [1987b] demonstrated for stationary fields that the correlation length of the process scale could only be accurately estimated if the sampling distance is smaller than half of the range of the underlying process. This constraint is usually not an issue for most soil hydraulic measurements, as the soil sampling scale (about 10 cm) is usually smaller than the natural process scale.

According to the scaleway or nested approach of Roth et al. [1999], subsequent aggregation of information and the modeling of flow and transport at one specific scale, provides the required information at the next, larger scale level. However, rather than implying that this type of analysis is needed across many spatial scales, we argue that likely only two scale levels need to be considered within the spatial domain of interest. For example, if the scale of interest is an agricultural field, one defines the structural elements based on the dominant physical mechanism that causes the major differences in soil water regime between the structural units. Most recently, *Becker and Braun* [1999] defined these units as hydrotopes or hydrological response units, based on differences between vegetation types, shallow groundwater presence, soil type or hillslope. *Wood* [1995] and *Famiglietti and Wood* [1994] described the aggregated watershed response by aggregation of total watershed runoff using area-weighted average runoff values of REA's with different topography indices. Likewise, in his review on scale issues in hydrological models, Beven [1995] introduced the simple patch model for scale-dependent modeling, with a patch defined as any area of the landscape that has broadly similar hydrological response in terms of the quantities of interest. In soil hydrological studies, soil map units may define the structural units across the landscape [*Ferguson and Hergert*, 1999] or may be indicative of geologic hydrofacies as identified using the transition probability geostatistical method [*Weizmann et al*., 1999]. The smaller spatial scale level of the textural information within structural units is distributed either deterministically or stochastically, e.g. using scaling of soil hydraulic properties from laboratory soil cores [*Hopmans and Stricker*, 1989]. The upscaling from the textural to the structural scale level may result in effective, scale-appropriate soil hydraulic functions that may differ in form and parameter values between scales, but serve a similar function across scales. The subsequent distribution of the structural units is deterministic (distributed modeling) and their aggregation to the scale of interest may be possible by simple mass conservation principles, e.g by the fractional area approach (addition or averaging). It is important to realize that the spatial organization of structures might be caused by different soil processes at different spatial scales.

SCALING ACROSS SPATIAL SCALES

Whereas we have presented a general framework to measure and model flow and transport processes across spatial scales, various mathematical and analytical tools are needed to aggregate soil hydraulic information across spatial scales. Specifically, we review scaling and inverse modeling.

Scaling and Monte Carlo Analysis

Most of the uncertainty in the assessment of water flow in unsaturated soils at the field scale can be attributed to soil spatial variability caused by soil heterogeneity. The knowledge of constitutive relationships for the unsaturated hydraulic conductivity, water saturation, and soil water matric potential are essential in using (1). The exact nature of the functional dependence of these flow variables with water content differs among soil types with different particle size compositions and pore size geometry within a heterogeneous field soil. The scaling approach has been extensively used to characterize soil hydraulic spatial variability and to develop a standard methodology to assess the variability of soil hydraulic functions and their parameters. The single objective of scaling is to coalesce a set of functional relationships into a single curve using scaling factors that describe the set as a whole (e.g. structural unit). The concept of this approach has been developed principally from the theory of microscopic geometric similitude as proposed by *Miller and Miller* [1956]. The procedure consists of using scaling factors to relate the hydraulic properties in a given location to the mean properties at an arbitrary reference point. *Philip* [1967] designated this type of variability scale-heterogeneity, emphasizing that the spatial variation of soil properties is fully embodied in the spatial variability of the scaling factor. Instead of using pore radius as the microscopic characteristic length, similarity of pore size distribution [*Kosugi and Hopmans*, 1998] was used to scale soil water retention curves for soils that exhibit a lognormal pore-size distribution. In this study, the physically based scale factors were computed directly from the physically based parameters describing the individual soil water retention [*Kosugi*, 1996] and unsaturated hydraulic conductivity [*Tuli et al*., 2001] functions. The physically based scaling concept provides for the simultaneous scaling of the soil water retention and unsaturated hydraulic conductivity functions, assuming that all soils within a structural unit are characterized by a lognormal pore-size distribution. This approach leads to scaled-mean soil hydraulic functions for each structural unit that may serve as effective soil hydraulic functions. In addition, physically based scaling results in a set of lognormally distributed scaling factors, from which the textural distribution within a structural unit can be characterized. Using Monte Carlo analysis, stochastic soil water flow modeling can be conducted, with scaling factors generated from a known probability density function [*Hopmans and Stricker*, 1989].

Inverse Modeling

The inverse method offers a powerful procedure to estimate flow properties across spatial and temporal scales. As numerical models have become increasingly sophisticated and powerful, inverse methods are applicable to laboratory and field data, no longer limited by the physical dimensions of the soil domain, or type of imposed boundary conditions. Inverse methods might be especially appropriate for estimating regional-scale effective soil hydraulic parameters, from boundary condition measurements. For example, *Eching et al.* [1994] estimated field-representative hydraulic functions using inverse modeling of Eq. (1) with field drainage flow rate serving as the lower boundary condition for the Richards' flow equation applied at the field-scale. The application of inverse modeling to estimate soil hydraulic functions for laboratory soil cores has been extensively reviewed by *Hopmans et al*. [2002].

The inverse modeling approach mandates the combination of experimentation with numerical modeling. Since the optimized hydraulic functions are needed as input to numerical flow and transport models for prediction purposes, it is an added advantage that the hydraulic parameters are estimated using similar numerical models as used for predictive forward modeling, with similar grid sizes so that the estimated effective hydraulic properties include the within grid integration of real soil variability. Although application of inverse methodology may suffer from non-uniqueness (e.g., *Beven*, 2001], the application of inverse methods in general to estimate soil hydraulic functions across spatial scales is very promising. This technique has demonstrated potential as an excellent new tool for a wide spectrum of transient laboratory and field experiments, yielding effective or lumped hydraulic properties that pertain to the scale of interest. We will demonstrate various applications in the following examples.

EXAMPLES OF SCALING APPLICATONS ACROSS SPATIAL SCALES

We demonstrate the application of the various aggregation techniques, to estimate effective large-scale soil hydraulic properties from small-scale laboratory measurements on soil cores. We start with the measurement of REV of porosity at the pore-scale, and present scaling applications at the soil core, field plot, field, and watershed scale, respectively. As the examples will show, the conceptualization of separating soil heterogeneity into textural and structural elements allows the integration of small-scale soil hydraulic properties to larger spatial scales, possibly resulting in scale-dependent soil hydraulic properties.

Pore Scale

Although (1) is not applicable at the pore scale, this example is shown to demonstrate the existence of a REV for porosity, for the first time as we know [*Clausnitzer and Hopmans,* 1999], using x-ray computed tomography (CT). Using the three-dimensional spatial distribution of x-ray attenuation as a proxy, porosity measurements for a glass bead medium were conducted for increasing measurement volumes. X-ray CT measurements were conducted in a random pack of uniform glass beads within a vertical Plexiglas cylinder of 4.76 mm inner diameter. The bead diameter, d_p, was 0.5 mm and the spatial resolution was 18.4 micrometer, resulting in $(18.4\ \mu m)^3$ voxel volumes (see Fig. 4a). In this example, the single structural unit is represented by the glass beads pack, and textural variations are defined by porosity changes at a measurement scale larger than the REV. Starting from the original three-dimensional data set of attenuation values, increasingly larger volumes were extracted, all centered at the same location, beginning with 8x8x8 voxels and incrementing the cube side length, L, of the averaging volume by 4 voxel lengths (0.0736 mm) in each step. The sequence of porosity calculations with increasing volume size was conducted twice, first with the initial 8x8x8 averaging volume centered in the air phase, and subsequently with the averaging volume centered in the glass phase. The resulting curves are presented in Fig. 4b, suggesting a REV of about 3 to 5 times the bead diameter. In an independent, modeling study, *Zhang et al*., [2000] showed that the REV may depend on the quantity being represented, as suggested by *Baveye and Sposito* [1984]. Thus, the REV for porosity may be different than for the Darcy scale at which (1) may be applicable, and for which soil hydraulic properties can be defined.

Soil Core Scale

Both *Roth et al.* [1999] and *Kasteel et al*. [2000] have shown that the spatial structure of soil hydraulic properties at the core-scale must be known, to accurately predict solute transport through the soil core. Using soil bulk density, as measured by x-ray CT, to proxy for soil hydraulic properties, two distinct soils were characterized within a 16-cm diameter soil core. The resulting image of the dense (light) and less dense soil matrix (dark) is shown in Figure 5, delineating the high and low-conductive soil materials or structural elements within the core. In this example, no textural variations within the structural elements were assumed.

The hydraulic properties of the more-conductive soil material were determined using a network model from independently measured pore geometry. Assuming a trial value for the conductivity of the low-conductivity structure, an effective saturated conductivity for the whole soil core was estimated from a composite conductivity, with weighting factors determined by the volume fraction of each soil material. Subsequently, it was demonstrated using a three-dimensional flow and transport code, that the simulated breakthrough of a chloride solution in the unsaturated soil core could be matched reasonably well with breakthrough measurements, if the ratio of saturated conductivity between the two soil materials was optimized, while maintaining the spatial structure of soil variation in the three-dimensional flow and transport code. Specifically, different conductivity ratios affected solute spreading, with preferential water flow through the higher-conductive soil structure dominating transport. The study showed that nonstationarity of the hydraulic properties can have a large effect on solute transport. Moreover, this study demonstrated a successful application of inverse modeling, to estimate a core-scale effective hydraulic conductivity functions with structural contraints.

Field Plot and Field Scale

The next larger scale level was investigated by *Wildenschild and Jensen* [1999a and b] to study the effective water flow behavior in heterogeneous, two-dimensional soil slabs. Experiments consisted of a series of infiltration experiments with varying application rates, in a two-dimensional 100x100x3 cm, heterogeneous soil slab, consisting of various realizations of packings with 5 different sands, using 5x5x8 cm unit cells. The soil hydraulic properties for each sand type were measured in the laboratory first, and represented the structural units. The soil tank was instrumented with strategically placed tensiometers and TDR probes, to estimate local soil hydraulic properties and their spatial distribution, from measurements during various steady state flow regimes, with water flux rates determined by a rain application device. After incorporating the distributed soil heterogeneity deterministically, using the laboratory-measured soil hydraulic functions for the individual sand types, a two-dimensional flow and transport model [*Simunek et al*, 1999] was able to predict the measured spatial variability of soil water flow in the soil slab. In addition, effective soil hydraulic properties for the whole slab were determined using simple statistical averages (geometric and arithmetic), as well as by inverse modeling using the measurements of water content and matric potential in the transient stages between the steady state experiments. In either case, effective hydraulic properties were able to describe the average transient soil water behavior for the heterogeneous soil system, as determined from two-dimensional transient water flow modeling.

In the field experiment by *de Vos et al*. [2000], nine soil horizons were classified into four different hydrologic zones, each determined by different soil hydraulic functions, representing the functional soil structural elements. The tile-drained field was 62.5 by 12 m with a center drain at about the 1 m soil depth. Soil water matric potential, groundwater level, piezometric heads, at various locations within the experimental field, and field discharge rate and nitrate concentrations were measured during the 1991-92 leaching period. Soil water retention, saturated and unsaturated hydraulic conductivity data for the 4 characteristic zones were measured from laboratory soil cores. The HYDRUS-2D model [*Simunek et al*., 1999] was used to simulate the two-dimensional flow regime and nitrate transport in the field, and the drainage rate and nitrate concentration in the drain outlet. Field-effective soil water retention and hydraulic conductivity functions were estimated using an inverse modeling approach, by adjusting the hydraulic parameters that were measured from the laboratory soil cores. Regarding the calibration of the field-representative hydraulic conductivity function, the saturated hydraulic conductivity for each of the four functional soil layers was adjusted, so that the simulated groundwater level-drainage rate relationship matched the measured data, using the constraint that effective saturated hydraulic conductivity values were within their laboratory-measured ranges. Laboratory-measured soil water retention curves were adjusted to match simulated with measured groundwater level and drainage rate during the monitoring period.

Watershed scale

At the watershed scale, *Hopmans and Stricker* [1989] used a stochastic-deterministic model to simulate soil water flow in the spatially heterogeneous Hupsel watershed. Using various laboratory techniques, soil water retention and unsaturated hydraulic conductivity functions were measured for each of 3 hydrologically-distinct soil layers that were widely present in the 650 ha watershed. Simultaneous scaling was used to model the spatial variability of the soil hydraulic data, yielding reference curves and a set of scaling factors for each of the 3 identified soil layers. The objective of this experimental study was to quantify the impact of soil spatial variability on the water balance of the watershed.

The spatial organization of the various soil types was selected based on the starting depth of a clay layer, since it largely controlled spatial variations in groundwater level and drainage rate within the watershed. The influence of small-scale local variations in soil hydraulic properties on water flow within each structural unit was simulated stochastically, using Monte-Carlo simulations, from random generation of scale factors for each of the 3 distinct soil layers. Computer simulations with SWAP [*van Dam et al*., 1997] were conducted for a dry (1976) and a wet year (1982), yielding mean and variance of evapotranspiration, groundwater level, and drain discharge for each structural unit. Subsequently, the same hydrological variables were either simply averaged or added, to yield watershed-representative values. Without any further calibration, independently-measured and simulated groundwater level and watershed discharge were close for both years. This last example shows how the proposed deterministic-stochastic approach using the structure-texture concept was successfully applied at the watershed scale, using laboratory-core soil hydraulic functions.

Using the laboratory-measured soil hydraulic functions as a starting point, *Feddes et al.* [1993a] subsequently demonstrated that almost equally good agreement was found, by using a single set of effective soil hydraulic functions, representative for the whole watershed. Their numerical exercise demonstrated that an area-average, effective parameterization of the soil hydraulic functions can be applied to (1). Results obtained by using the scaled reference hydraulic functions were almost as close as using an inverse approach, by optimization of the hydraulic functions via minimization of the residuals between measured and simulated soil hydrological variables. In a later study, *Kabat et al.* [1997] concluded that effective soil hydraulic properties could successfully describe area-average evaporative and soil moisture fluxes at the 10-100 km^2 scale, provided that the averaged area contained a single soil type only. This was concluded with the understanding that the estimated effective properties are merely calibration parameters, which do not necessarily have the physical meaning implied by application of the Darcy flow equation.

CONCLUDING REMARKS

Although most of the presented examples show that some kind of fitting is needed along the way, the estimated soil hydraulic properties using small-scale laboratory soil cores can be effective in estimating large-scale, effective soil hydraulic properties. We are also convinced that significant progress in the understanding of fundamental flow processes in heterogeneous soils is possible only if scale-appropriate measurement technologies are available. Innovative examples of such instruments that are explored to characterize subsurface flows across spatial scales include the application of noninvasive techniques [*Hopmans et al*., 1999], such as x-ray tomography, electromagnetic induction, electrical resistivity, seismic reflection, and microwave remote sensing [*Jackson et al.,* 1999; *Hollenbeck et al*., 1996; *Mattikalli et al*., 1998]. Present theory and applications of remote sensing may potentially help improve the understanding of large-scale hydrological processes such as runoff, infiltration and evapotranspiration, including their spatial distribution and scale-dependency. The monitoring of transient soil moisture changes by remote sensing may provide the essential information to estimate up-scaled soil hydraulic parameters such as the saturated hydraulic conductivity or unsaturated hydraulic parameters, using the inverse modeling approach. An excellent example of such an application was presented by *Feddes et al*. (1993b), who demonstrated that remote sensing of soil surface temperature and soil moisture combined may provide the essential information to estimate effective soil hydraulic parameters at the catchment scale. The work of *Ahuja et al.* (1993) support this potential application of remote sensing, and showed that spatial variations in surface soil moisture can be related to spatial variations in effective values of soil profile saturated hydraulic conductivity. In their review of scaling field soil-water behavior, *Nielsen et al*. [1998] suggested that increased efforts to measure field-based soil hydraulic data are needed to extend the application of (1) to the landscape-scale.

In his analysis, *Philip* [1980] used the analytical solution of a simple one-dimensional sorptivity experiment to determine whether a sample-mean sorptivity value could be predicted from sorptivity values of the individual soil components that made up a deterministic heterogeneous soil. His results indicated that the averaging of spatially-variable soil parameters does not necessarily result in an average soil water flow behavior. Even now, after a further two decades of dedicated research in soil physics and vadose hydrology, we must agree with *Philip'*s [1980] final statement, 'that our adventures into trans-science will be least likely to lead to disaster if we are as well informed as possible about stochastic heterogeneous systems.' Hence, we conclude that the development of new instrumentation to characterize soil properties and their variation across spatial scales is crucial. Moreover, the inherent complexity of flow in heterogeneous soils or soil-like materials and the need to integrate theory with experiment, requires innovative and multidisciplinary research efforts to break the deadlock, imposed by current understanding of scale-dependent soil flow and transport processes.

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LEFT RUNNING HEAD:
SMALL-SCALE SOIL HYDRAULIC PROPERTY MEASUREMENTS

RIGHT RUNNING HEAD:
HOPMANS ET AL.

FIGURE CAPTIONS

Figure 1. Conceptual model of evolving hetereogeneity [after Wheatcraft and Tyler, 1988].

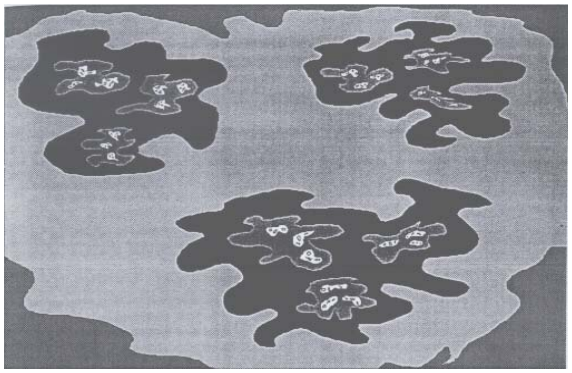
Figure 2. Hypothetical variogram for scale-dependent hydraulic conductivity. Adapted from *Gelhar*, [1986].

Figure 3. Schematic presentation of power spectrum, showing various process scales (d = sampling spacing).

Figure 4a. Three-dimensional image of dry glass beads (light gray) and pore space (dark grey) [after *Clausnitzer and Hopmans,* 1999].

Figure 4b. Estimated porosity for a cubic domain with increasing size within the glass-bead pack [after *Clausnitzer and Hopmans,* 1999].

Figure 5. Illustration of two soil density classes in one specific cross-section of a 16-cm soil core [after *Kasteel et al*., 2000].



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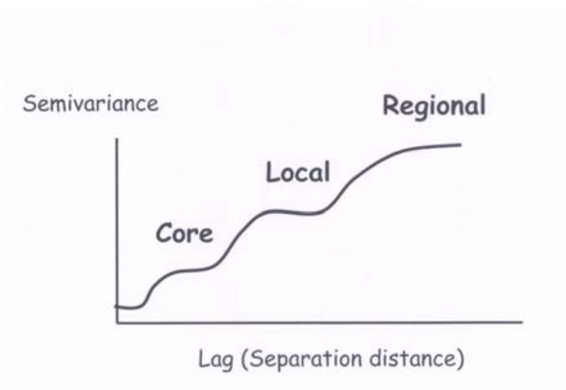

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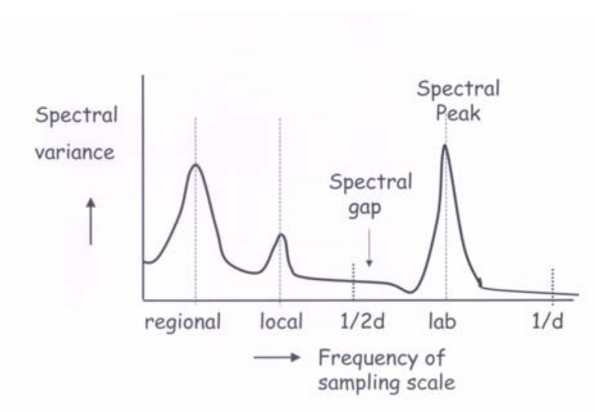

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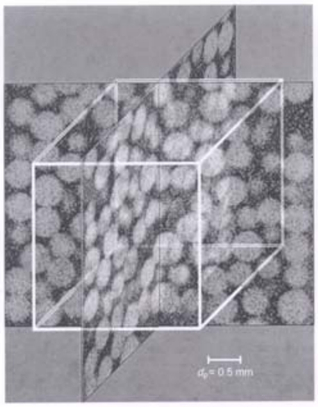

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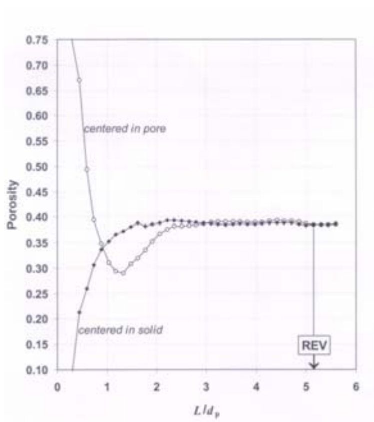

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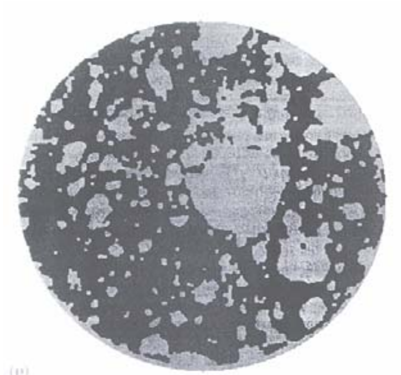

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