74: Soil Water Flow at Different Spatial Scales

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A major challenge in hydrological sciences is the modeling of flow and transport processes and their measurement across a range of spatial or temporal scales. Such needs arise, for example, when watershed processes must be determined from soil hydrological 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 timescale, for several reasons. First, spatial and temporal variability in soil hydrological properties create uncertainties when changing between scales. Second, flow and transport processes in vadose zone hydrology are highly nonlinear. As a result, vadose zone properties are nonunique and scale-dependent, resulting in effective properties that vary across spatial scales and merely serve as calibration parameters in hydrologic models. Therefore, their estimation for heterogeneous materials can only be accomplished using scale-appropriate measurements and models. We present examples of soil water flow at the pore, local, and regional scales. The inherent complexity of flow in heterogeneous soils, 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 water flow and transport processes.

INTRODUCTION

The unsaturated zone is bounded by the soil surface at one end and merges with the groundwater in the capillary fringe at the lower end. The distinction between groundwater and the unsaturated zone is usually made within a hydrologic context, emphasizing water as the agent of change of the subsurface and the main driver for transport of chemicals between the atmosphere and groundwater. To emphasize the profound influence of soil chemical and biological processes on water flow and chemical transport, one may generally refer to the unsaturated flow domain as the vadose zone.

The upper part of the vadose zone is the most dynamic, and changes occur at increasingly smaller time and spatial scales when moving from the groundwater towards the soil surface. The most upper part of the vadose zone is subject to fluctuations in water and chemical content by infiltration and leaching, water uptake by plant roots (transpiration), and evaporation from the soil surface. Water is the main ingredient leading to soil formation from the weathering of parent material such as rock or transported deposits, with additional factors, such as climate, vegetation, topography, and parent material, determining soil physical properties. Generally, the soil depth is controlled by the maximum rooting depth (generally within a few meters from the soil surface). However, the vadose zone can extend much deeper than the surficial soil layer and includes unsaturated rock formations and alluvial materials to depths of 100 m or more, determined by hydrologic, topographic, and lithographic characteristics. In the last few decades, research interest in the deeper vadose zones has increased, instignated by the need to sustain quality of groundwater and resources for drinking water and ecological purposes. Scientists are becoming increasingly aware that soil is a critically important component of the earth's biosphere, not only because of its food production function, but also as the safekeeper of local, regional, and global environmental quality. For example, it is believed that management strategies in the unsaturated soil zone will offer the best opportunities for preventing or limiting pollution, or for remediation of ongoing pollution problems. Because chemical residence times in groundwater aquifers can range from years to thousands of years, pollution is often essentially irreversible. Prevention or remediation of

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soil and groundwater contamination starts, therefore, with proper management of the vadose zone.

Transient isothermal unsaturated soil water flow is generally described by the so-called Richards' equation,

$$\frac{\partial\theta}{\partial t} = \nabla \cdot [K(\theta)\nabla(h_{\mathrm{m}} + z)] + S(t) \qquad (1)$$

which solves for 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. In equation (1), $S(t)$ represents a sink/source term that is routinely used to describe plant root water uptake, 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 relationship between h_{m} and θ is determined by the soil water retention function, of which the slope, $C(h_{\mathrm{m}})$, is the so-called soil water capacity. Boundary conditions must be included to allow for specified soil water potentials and fluxes at all boundaries of the soil domain, whereas user-specified initial conditions and time-varying source/sink terms need be specified. Both the soil water retention and unsaturated hydraulic conductivity relations (in combination referred to as soil hydraulic functions) are highly nonlinear, with both h_{m} and K varying many orders of magnitude over the water content range of significant water flow.

Many analytical and numerical mechanistic flow models have been developed to solve equation (1), for specific agricultural or environmental applications. In short, the dynamic water flow equation is a combination of the steady state Darcy expression and a mass balance formulation. Using various solution algorithms, the soil region of interest is discretized in finite-size elements that can be one, two, or three-dimensional. Numerical solution requires that mass balance be maintained within each small volume element within the soil domain at all times. Richards equation is typically a highly nonlinear partial differential equation, and is therefore extremely difficult to solve numerically because of the largely nonlinear dependencies of both water content and unsaturated hydraulic conductivity on the soil water matric potential (h_{m}). Both the soil water retention and unsaturated hydraulic conductivity relationships must be known *a priori* to solve the unsaturated water flow equation. Although soil water retention measurements are time-consuming (Dane and Hopmans, 2002; *see* **Chapter 81, Measuring Soil Hydraulic Properties, Volume 1**), unsaturated hydraulic conductivity data are even much more difficult to obtain from measurements (Klute and Dirksen, 1986). Functional unsaturated hydraulic conductivity models, based on pore size distribution, pore geometry, and connectivity, require integration of soil water retention models to obtain analytical expressions for the unsaturated hydraulic conductivity. The resulting expressions relate the relative hydraulic conductivity K_r, which is defined as the ratio of the unsaturated hydraulic conductivity K to the saturated hydraulic conductivity K_s, to the effective saturation to yield a macroscopic hydraulic conductivity expression. Pedotransfer function models (*see* **Chapter 83, Models for Indirect Estimation of Soil Hydraulic Properties, Volume 1**) have been developed to estimate soil hydraulic parameters for various functional models (`http://www.usyd.edu.au/su/agric/acpa/software/multistep.htm`).

Soil hydraulic functions that characterize flow and transport processes at larger spatial scales are mostly obtained from relatively small measurement scales. For example, prediction of soil water dynamics at the field scale is routinely 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. Soil hydrological parameters obtained from these centimeter-scale measurements are subsequently 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. Because of the high nonlinearity of the soil hydraulic functions, their application across spatial scales is inherently problematic. Specifically, the averaging of processes determined from discrete small-scale samples may not describe the true soil behavior involving larger spatial domains. In addition, the dominant hydrological flow processes may vary between spatial scales, so that potentially different models need to be used to describe water flow at the soil pedon, field scale, or watershed scale. In 1991, the US 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.

Many field experiments have confirmed that soil heterogeneity controls the hydrology of flow and transport, including preferential flow such as through cracks by soil shrinkage (*see* **Chapter 75, Hydrology of Heavy Clay Soils, Volume 1**). Although some hydrological studies successfully applied a deterministic approach, other studies showed the need for either distributed physically based modeling or stochastic modeling at the watershed scale, mostly because deterministic models require an enormous amount of data to accurately represent the multidimensional soil heterogeneity. Alternatively, the conceptual characterization of flow at the large scale may be simplified by modeling the key flow mechanisms for representative elementary areas (REA's) within the larger domain, using REA-appropriate effective hydrological parameters (Blöschl *et al.*, 1995). The need to incorporate the spatial organization of these key properties, such as the soil hydraulic functions, is now 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 and its spatial organization on soil flow and transport processes, using the so-called scaleway approach. In this approach, the three-dimensional field domain is defined by structural and textural elements. The various identified structural elements describe the dominating physical features that affect the hydrological mechanisms operating at the larger spatial scale, whereas the textural patterns within the structural units merely cause perturbations of these main hydrological processes. This hierarchical notation of structure and texture within a hydrological context should not be confused with soil texture and soil structure, although it can be argued that soil properties such as soil structure and texture may have a dominant control on soil hydrology. Thus, characterizing soil hydraulic variability is predicated on identifying those soil hydrological units that cause major differences in soil water regime at the spatial scale of interest. In soil hydrological studies, these structural units across the landscape may be defined by soil map units (Ferguson and Hergert, 1999). The smaller spatial scale level of textural information within the larger structural units can be determined either deterministically or stochastically, for example, through 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 spatial scales, but serve a similar function in equation (1). Much of the issues associated with spatial scaling of soil hydrological processes were presented in Hopmans *et al.* (2002a). It is also the focus of this treatise to review the current state-of-the-art of solving the unsaturated water flow equation (1) across spatial scales.

SCALE-DEPENDENCY OF SOIL PROPERTIES AND PROCESSES

Upscaling requires integration and aggregation of spatial information into larger spatial units, for example, as in the estimation of an effective field soil water retention or conductivity curves from small-scale laboratory core measurements. As pointed out by Baveye and Boast (1999), Darcy's experiment can in effect be interpreted as yielding an upscaled, effective saturated hydraulic conductivity. In contrast, downscaling is the disaggregation of scale into smaller scales, for example, as in distributed hydrological modeling. Baveye and Boast (1999) discuss the confusion on concepts of scales in vadose zone hydrology. In contrast to the "perceived" clear hierarchy of spatial and temporal scales, they point out that the differentiation between scales is partly arbitrary, and depends, for example, on the scale of measurement and system scale. Moreover, whatever the spatial scale considered, it has its own characteristic dynamics, and should be treated that way, so that focus should be placed on experimentation and measurement methods that are representative for the different scales. Loosely, one may define the microscopic pore scale, the local scale, and the regional scale such as agricultural fields and watersheds. The macroscopic Darcy equation is considered to be valid for the local scale, with a typical size in the range of centimeters to meters. It is the local scale for which equation (1) is considered to be generally valid. It is also this scale, for which the Darcy equation can be derived from the volume averaging of the Stokes equations at the microscopic scale level. Increasingly, innovative measurements and modeling techniques are becoming available to measure and model pore size scale properties and processes. The regional scale typically applies to agricultural fields and watersheds for which the relevant soil hydrological properties become increasingly nonstationary. Yet, it is at these larger spatial scales that solutions are increasingly sought, putting the validity of equation (1) into question.

When increasing the spatial scale, soil properties typically become nonstationary, as evidenced by the delineation of soil map units by a soil survey. As one moves through a sequence of increasing sampling scales, nonstationarities at smaller spatial scales may be eliminated, and soil properties may change from deterministic to random, with the smaller-scale variations filtered out by the larger scale process or aliasing (Kavvas, 1999). The spatial organization and its evolvement across spatial scales can be viewed as continuous with deterministic patterns evolving as the field-of-view changes. At each field-of-view, the large-scale variation can be regarded as deterministic, whereas the smaller scale variations within each main unit can be treated stochastically. As explained earlier, this hierarchy of spatial scales (Cushman, 1990) can be described by structural and textural elements, as defined by the scaleway approach of Roth *et al.* (1999), with the structural elements describing the dominating soil patterns that affect the hydrological mechanisms operating at the *a priori* defined field-of-view. For the purpose of using soil information towards hydrological modeling, one must be careful on focusing on soil properties only, since spatial patterns of soil properties may be different from the functional organization of soil hydrological processes that may also be determined by landscape position and land use. It may be argued that as different flow processes may be dominant at each scale, different mathematical relationships may be required to describe the underpinning physical process at each spatial scale.

According to the scaleway approach, 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. For example, if the scale of interest is an agricultural field, one defines the structural elements based on the dominant soil hydrological mechanism that causes the major differences in soil water regime between structural units. Most recently, Becker and Braun (1999) defined these units as hydrotopes or hydrological response units (HRU's) based on differences between vegetation types, shallow groundwater presence, soil type or hillslope. 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.

SPATIAL SCALING APPROACHES

In soil hydrological studies, soil map units may define the structural units across the landscape (Ferguson and Hergert, 1999), or soil types may need to be regrouped, classifying soils by their hydrologic functioning (Dunn and Lilly, 2001). By combining GIS with fuzzy logic techniques, Zhu and Scott Mackay (2001) generated spatial continuous soil information as input to a distributed watershed model. This provided a gradual transition between HRU's, depending on soil type, position in the landscape, and land use, instead of the discrete and generally coarse resolution of soil maps. This distribution or disaggregation of a watershed in structural units is deterministic (distributed modeling) and their aggregation to the scale of interest may be possible by simple mass conservation principles. The selection of the main HRU's or hydrotopes with their corresponding effective hydrological parameters is determined by calibration, such as was presented by Eckhardt and Arnold (2001) using parameter optimization. Rather than expecting a unique solution for the distributed hydrologic parameters, nonlinearity and measurement uncertainty, Beven (2001) introduced the equifinality concept, indicating that many solutions may be acceptable. Recent optimization algorithms now allow for multiple objective functions for multiparameter distributed watershed modeling, with effective hydrologic parameter values determined by the choice of the most relevant hydrological variables. Increasingly, efficient global optimization algorithm's are developed such as the shuffled complex evolution (SCE) algorithm (Duan *et al.*, 1993) to calibrate for a large number of parameters for distributed watershed models. Madsen (2003) demonstrated the successful application of SCE using multiple objective functions for calibration of a multiparameter distributed watershed model. He showed that if multiple measurement types of different importance are available, a so-called Pareto set of solutions provides trade offs between the different objectives. The current state-of-the-art in calibration of watershed models is presented in Duan *et al.* (2003), and appears ready to be applied to unsaturated water flow modeling (*see* **Chapter 84, Inverse Modelling of Soil Hydraulic Properties, Volume 1**).

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 (*see* **Chapter 86, Assessing Uncertainty Propagation Through Physically-based Models of Soil Water Flow and Solute Transport, Volume 1**). The exact nature of the functional dependence of both soil water retention and unsaturated hydraulic conductivity 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 procedure consists of using scaling factors to relate the hydraulic properties at a given location to the mean properties at an arbitrary reference point. This physically based scaling concept provides for the simultaneous scaling of the soil water retention (Kosugi and Hopmans, 1998) and unsaturated hydraulic conductivity functions (Tuli *et al.*, 2001), leading to scaled mean soil hydraulic functions for each structural unit, to serve as effective soil hydraulic functions (e.g. Mohanty *et al.*, 1997).

Stochastic approaches to upscale soil hydrological processes from the local to the regional scale include Monte-Carlo (MC) analysis and solution of a stochastic form of equation (1). A common assumption in using the stochastic approach is that of ergodicity, that is, the ensemble average is equivalent to the spatial average. Typically, in MC analysis, numerical solutions of equation (1) are repeated using different realizations of spatially variable soil hydrological properties. Realizations are generated using a random number generator from *a priori* knowledge of the statistical distribution of the parameter(s) in questions, including their spatial correlation. Repeated solutions will yield the stochastic information needed for the relevant output variables. An example of this approach was used by Hopmans and Stricker (1989). In this study, scaling factors and soil hydraulic functions were generated for different soil map units and soil horizons to study the soil water regime in a 650-ha watershed, specifically the influence of soil heterogeneity on plant transpiration.

Although MC analysis is conceptually straightforward, it can become computationally very intensive. Another approach is to use a perturbation approximation of equation (1), by representing local soil hydraulic properties as the sum of a deterministic and a stochastic component (Zhang, 2002). The result is that the local Richards equation (1) with deterministic parameter values is replaced by an upscaled equation with stochastic parameters, that is, the means, variances, and covariances of hydrological parameter values. A disadvantage of this method is that it is mostly restricted to relatively small fluctuations of the stochastic parameters. A third approach assumes that local-scale flow can be simplified so that analytical expressions may be derived that describe the flow statistics at a larger scale. As an example, Chen *et al.* (1994) present a solution for the area-averaged Green and Ampt infiltration model that is applicable for large parameter uncertainties.

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 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.* (2002b). Although the inverse method may suffer from nonuniqueness (e.g. Beven, 2001), the application of inverse methods in general to estimate soil hydraulic functions across spatial scales is very promising, yielding effective hydraulic properties that pertain to the scale of interest.

EXAMPLES OF SOIL WATER FLOW AT DIFFERENT SPATIAL SCALES

The application of the various modeling techniques for unsaturated water flow is presented. First, at the microscale, the measurement of porosity at the pore scale is demonstrated using X-ray computed tomography. Examples are presented for local-scale unsaturated water flow models, whereas the application of using effective soil hydraulic functions is presented at the regional scale for an irrigation water district in California, USA.

Pore Scale

Although equation (1) is not applicable at the pore scale, this example is presented to demonstrate the existence of a Representative Elementary Volume (REV) for porosity, for the first time as it is known (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 μm, resulting in $(18.4\,\mu\text{m})^3$ voxel volumes (see Figure 1a). 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 $8 \times 8 \times 8$ 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 $8 \times 8 \times 8$ averaging volume centered in the air phase, and subsequently with the averaging volume centered in the glass phase. The resulting curves are presented in Figure 1(b), suggesting a REV of about three to five times the bead diameter. Using lattice-Boltzmann modeling, Zhang *et al.* (2000) showed that the REV may depend on the specific soil property measured. In a subsequent study, Clausnitzer and Hopmans (2000) showed that X-ray CT can be used to measure the spatial and temporal distribution of a tracer through this glass-bead medium with a spatial resolution of about 85 microns. Although we have a general good understanding of macroscopic flow and transport, much additional work is needed to describe processes at the scale of pores, thereby improving our understanding of the effects of variations in pore-water velocity and air–water interfaces on flow and transport in unsaturated porous media. Numerical modeling techniques are now becoming available to solve for streamlines and velocities at the pore scale by lattice gas automata (LGA) and the lattice–Boltzmann method.

Local Scale

Most unsaturated water flow and transport models have been developed for applications at the local scale, that is, the laboratory column and field plot scale. Whereas the initial applications were dominantly agricultural, many recent applications are mostly environmental. Also, whereas the earlier models focused on unsaturated water flow only, recent applications require coupling of water flow with models that simulate chemical and biological processes. Although many excellent models are available, we present only a few here as these appear to be applied more often than others. RZWQM (Ahuja *et al.*, 1999) is an integrated physical, biological, and chemical one-dimensional process model, simulating crop growth and movement of water, nutrients, and pesticides over and through the root zone. The model includes a generic crop-growth simulator, estimates soil evaporation and plant transpiration, and links total root water and nutrient extraction to atmospheric demand. The (*see* **Chapter 85, Models of Water Flow in the**

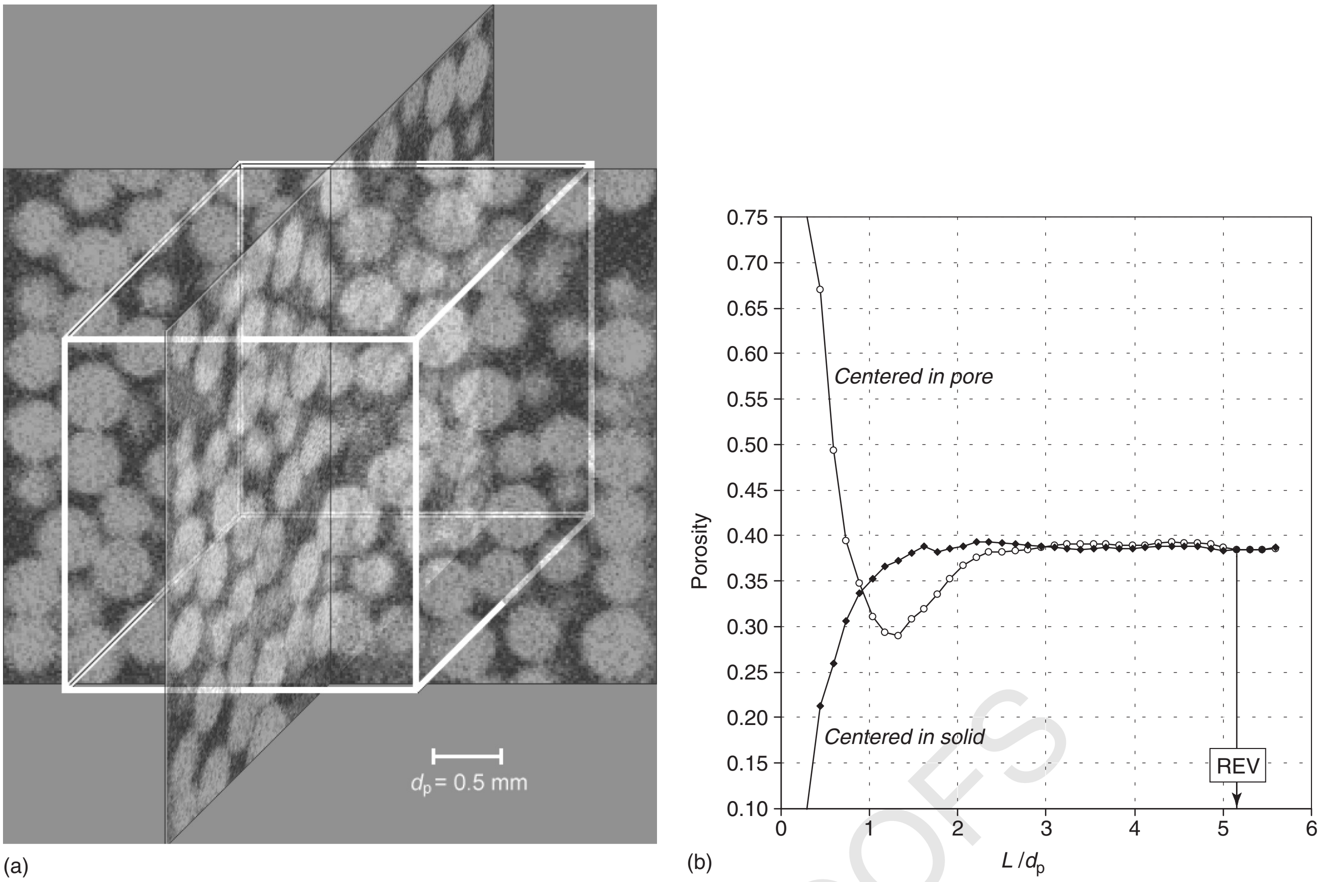

Figure 1 (a) Three-dimensional image of dry glass beads (light gray) and pore space occupied by air (dark grey) (after Clausnitzer and Hopmans, 1999). Two vertical cross-sections of a glass-bead pack with 2.576 mm side length. (b) Estimated porosity for a cubic domain of increasing size within a glass-bead pack, centered either within the air or the glass phase. Cube side length is expressed as multiple of the bead diameter d_p (0.5 mm) (after Clausnitzer and Hopmans, 1999) (Reprinted from Advances in Water Resources, **22**(6), Clausnitzer *et al.*)

Unsaturated Zone, Volume 1) SWAP model (Van Dam *et al.*, 1997) combines a one-dimensional water flow and nutrient transport model with a universal crop-growth simulator. Since SWAP has been designed for interactions with surface water and regional drainage, applications are primarily at the field scale. Increased computer capability and development of more efficient computer algorithms has increased the spatial dimension of solutions of equation (1) from one-dimensional to two and three-dimensional. An example of a three-dimensional water flow, coupled with nutrient transport, root water and nutrient uptake, and root growth models was presented by Somma *et al.* (1998).

The application of the aforementioned calibration techniques to a field-scale level was presented in de Vos *et al.* (2002). In this study, four major hydrologic zones with different soil hydraulic functions were identified in a tile-drained field. Soil water matric potential, groundwater level, and piezometric heads, at various locations within the experimental field, field discharge rate and nitrate concentrations were measured during a four-month leaching period. Soil water retention, saturated and unsaturated hydraulic conductivity data for four distinct hydrological soil units were measured from laboratory soil cores. The HYDRUS-2D model (**`http://www.ussl.ars.usda.gov/models/hydrus2d.HTM`**), as presented by Šimunek *et al.* (1999) was used to simulate two-dimensional flow regime and nitrate transport for a 2 by 6 m field plot, matching drainage rates and nitrate concentrations 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. The study concluded that 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. Mohanty *et al.* (1997) demonstrated the application of a two-dimensional local-scale model to describe preferential flow of a tile-drained field using field-averaged piecewise-continuous hydraulic functions for different soil horizons.

Successful applications such as these and the SWAP model demonstrate that local-scale models can be used to spatial scales as large as agricultural fields.

Regional Scale

Soil hydrological information can be fairly easily assigned to local-scale unsaturated water flow models, using small-scale soil properties measurements in the laboratory or field scale. However, in applications at the field to watershed scale, a prohibitively large number of sampling sites are needed to characterize the vadose zone. An alternative approach is to estimate effective values for the hydraulic parameters by inverse modeling. In the presented example study, the inverse approach is applied to the 9700-acres Broadview irrigation district that is located in the San Joaquin Valley, California. The area consists of about 60 tile-drained 160-acre fields. Drains are located at a depth of approximately 2 m with horizontal spacings of 100–200 m. Subsurface drainage flow is measured weekly at 25 sumps, hence each sump collects subsurface drainage from one or more fields. The main crops in the area are cotton, tomatoes, alfalfa, melons, and wheat. Fields are either furrow or sprinkler irrigated. The amount of irrigation water applied to each field is measured every two days from water meters at irrigation turnouts. Rainfall data were obtained from a nearby weather station. A total of 48 shallow groundwater wells are distributed throughout the district from which monthly water table depth readings were available. Topography is nearly flat. The majority of the soils are mapped as vertisols with an average clay content of 50%. The numerical model used in this study was MODHMS (**http://www.modhms.com/modhms.cfm**), which is a MODFLOW-based distributed watershed model. It simulates in an integrated manner evapotranspiration, overland flow, channel flow, and subsurface flow and transport. Three-dimensional variably saturated subsurface flow was simulated with the three-dimensional Richards equation. Input data include spatially distributed crop types, and weekly irrigation and rainfall amounts for each field in the district. Subsurface drains are simulated using a head-dependent function, with drain discharge proportional to head above the drain and the drain conductance, C_d. Separation of crop transpiration and soil evaporation was based on a method developed by Allen *et al.* (1998). Field-specific actual crop transpiration values were determined by a depth-dependent root water uptake distribution, a time-varying crop coefficient, and a water-stress response function. Actual field evaporation was estimated from a wetness function that defines the reduction of soil evaporation with soil surface water content. The Broadview water district was divided into 1 536 200 × 200 m square cells, using approximately 16 grid cells per field. Vertically, the flow system was divided into four layers with layer thicknesses of 0.9 m, 0.9 m, 1.8 m, and 2.4 m, with a total model thickness of 6 m, resulting in a total of 6144 cells. Adaptive time-stepping was used to solve the variably saturated flow equation. Simulations were done for the 1998-crop year, which started on October 1, 1997, and ended on September 30, 1998. The water flux between the bottom of the model domain at the 6-m depth and the regional aquifer was simulated assuming a linear relation between the head difference of the bottom grid cell and a 10-m deep measured total head in the district, with a proportionality constant defined by the regional conductance, C_b. It was assumed that no lateral flow occurred across the other district boundaries.

Reference soil hydraulic functions $K_{ref}(\theta)$ and $h_{ref}(\theta)$ for clay were estimated based on the neural network analysis (**http://www.ussl.ars.usda.gov/models/rosetta/rosetta.HTM**) of Schaap *et al.* (1998). As part of the calibration, these functions were scaled using a single district-wide scaling factor, α, relating the effective water district hydraulic properties to the reference functions. Calibration parameters included α, C_d, C_b, and the initial head in the unsaturated zone h_{ini}. The latter calibration parameter was added, since it was very sensitive to the initiation of subsurface drainage. These parameters were estimated from weekly district-scale drainage discharge measurements and monthly district-average water table levels using an inverse modeling approach based on the Levenberg–Marquardt algorithm of PEST (**http://www.parameter-estimation.com/html/pest_overview.html**), while minimizing the residuals between simulated and measured drainage discharge and water table levels. Average evapotranspiration (ET), infiltration, drainage rate, and groundwater table levels are presented in Figure 2(a). Optimized district-wide parameter values were: $\alpha = 10.0$, $C_d = 0.08\ \mathrm{m\ yr^{-1}}$, $C_b = 3.6 \times 10^{-4}\ \mathrm{m\ yr^{-1}}$, and $h_{ini} = -380\ \mathrm{cm}$. A comparison of measured with optimized drainage rates and groundwater tables is presented in Figure 2(b).

As can be seen in Figure 2(b), the approach of treating the entire district as a homogeneous system in terms of hydraulic properties works surprisingly well, if the interest is only in predicting district-average hydrological conditions. Calibration results were disappointing when comparing drainage data from individual sumps within the district, even though field-specific boundary conditions were used. The optimized district-representative scaling factor was much larger than one, indicating that the district-wide response to irrigation is much faster than that initially estimated from pedotransfer functions on laboratory-scale measurements. This result indicates preferential water flow at this larger scale. However, physical interpretation of the optimized hydraulic functions is difficult since they represent effective properties that are likely not a function of the porous system only, but also depend on the boundary conditions (Blöschl *et al.*,

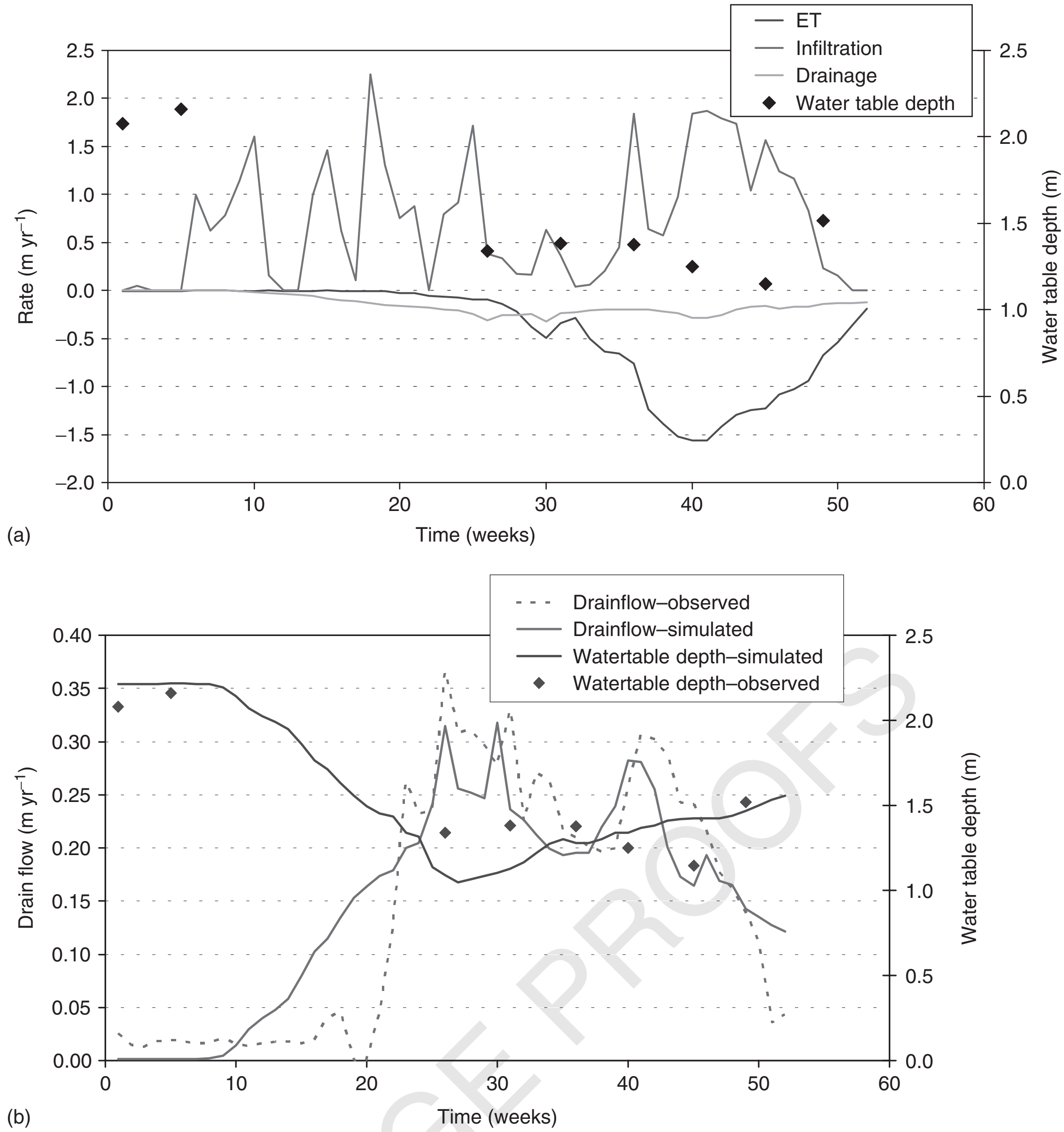

Figure 2 (a) Annual water balance for Broadview Water District, crop year 1998. (b) Comparison of observed and simulated values of district-scale drainage discharge and water table depth after optimization

1995). Therefore, it may be argued that application of the Richards equation at this scale is conceptual rather than physically based. (Beven, 2001). It is expected that the presented calibration approach may be improved by including spatially distributed scaling factors based on the soil map. The selection of using a single scaling factor for the calibration of the entire water district was based on parameter identifiability limitations of the optimization algorithm. Optimization algorithms that can efficiently optimize larger number of parameters, such as SCE, are likely much more appropriate when calibrating distributed scaling factors.

CONCLUDING REMARKS

It is becoming increasingly obvious that there is a pressing need for unsaturated water flow modeling, monitoring and characterization at the regional scale, such as for an agricultural field or watershed. To date, soil hydrologists are quite comfortable in measuring and modeling flow processes at local scales, since physical characterization methods are applicable at the laboratory or at a small field plot scale. However, the need for hydrological and associated environmental and ecological solutions is becoming increasingly needed at the regional scale. In response, hydrological scientists mostly apply soil hydrological concepts that are considered valid at the local scale and extend those to the regional scale. Whereas this type of approach requires an enormous amount of experimental observations, one may also question whether this is valid.

The scale problem is extremely complex because of the general presence of large spatial and temporal variability of soil hydrological properties and their highly nonlinear nature. Hence, much more developmental work is needed regarding fundamental concepts and measurement technologies to establish appropriate soil hydrological parameters for the description of unsaturated water flow at the larger spatial scales. Simultaneously, the need arises to develop appropriate scale-dependent measurement techniques that allow for model calibration and the estimation of effective soil hydrological properties. Present theory and applications of remote sensing may potentially improve the understanding of large-scale hydrological processes such as runoff, infiltration, and evapotranspiration, including their spatial distribution and scale-dependency. For example, the monitoring of transient soil moisture changes by remote sensing may provide the essential information to estimate upscaled soil hydrological parameters such as needed for the unsaturated hydraulic functions.

Although it is evident that large-scale measurements and modeling is needed, there is also increasing awareness within the scientific community that vadose zone processes are controlled by mechanisms operating at the pore size scale. Improved understanding of these processes will likely be a function of the development and application of innovative noninvasive measurement techniques that operate at the microscopic level. Examples of such techniques are NMR, CT, and laser technologies. Finally, we note that the required improved integration of vadose science in hydrologic models requires interdisciplinary partnerships with surface and groundwater hydrologists, experts in remote sensing, numerical modeling and parameter optimization, water management and policy, experimentalists, and others.

SOFTWARE LINKS

HYDRUS

Software description: Finite element model for simulating the one-dimensional movement of water, heat, and multiple solutes in variably saturated media.

Typical applications: Analysis of water flow and solute transport in soils.

URL: **`http://www.ussl.ars.usda.gov/models/hydrus2d.HTM`**

Reference: Šimunek J., Šejna M., and van Genuchten M.Th. (1999). *The HYDRUS-2D software package for simulating two-dimensional movement of water, heat, and multiple solutes in variable saturated media.* Version 2.0, IGWMC-TPS-53, International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado.

MOD-HMS

Software description: MODFLOW-based, fully integrated and comprehensive hydrologic flow and transport modeling system, including 3-D variably saturated subsurface flow, 2-D aerial overland flow, and 1-D channel flow

Typical applications: Integrated analysis of regional-scale flow and transport

URL: **`http://www.modhms.com/modhms.cfm`**

Reference: HydroGeoLogic Inc. (2001). *MOD-HMS: A Comprehensive MODFLOW-based Hydrologic Modeling System.* Herndon, VA.

ROSETTA

Software description: Neural network pedotransfer functions to estimate unsaturated hydraulic properties from surrogate soil data such as soil texture data and bulk density.

Typical applications: Parameterization of regional-scale vadose zone flow and transport models.

URL: **`http://www.ussl.ars.usda.gov/models/rosetta/rosetta.HTM`**

Reference: Schaap M.G., Leij F.J., and van Genuchten M.Th. (1998). Neural network analysis for hierarchical prediction of soil–water retention and saturated hydraulic conductivity. *Soil Sci. Soc. Am. J.*, **62**, 847–855.

PEST

Software description: Nonlinear parameter estimation package based on the Levenberg-Marquardt algorithm

Typical applications: Inverse estimation of soil hydraulic parameters using a hydrologic model and observed data

URL: **`http://www.parameter-estimation.com/html/pest_overview.html`**

Reference: PEST Software (1998). *PEST: Model-Independent Parameter Estimation*. Watermark Computing.

NEURAL MULTISTEP

Software description: Algorithm for prediction of soil–water retention and hydraulic conductivity data.

Typical applications: Soil hydraulic data are required for unsaturated water flow modeling purposes.

URL: **`http://www.usyd.edu.au/su/agric/acpa/software/multistep.htm`**

Reference: Minasny, B., J.W. Hopmans, T.H. Harter. A.M. Tuli. S.O. Eching and D.A. Denton. 2004. Neural network prediction of soil hydraulic functions for alluvial soils using multistep outflow data. *Soil Science Soc. Amer. J.* 68:417–429.

REFERENCES

Ahuja L.R., Rojas K.W., Hanson J.D., Shaffer M.J. and Ma L. (1999) *Root Zone Water Quality Model: Modeling Management Effects on Water Quality and Crop Production*, Water Resources Publication LLC: Highlands Ranch.

Allen R.G., Pereirea L.S., Raes D. and Smith M. (1998) *Crop Evapotranspiration. Guidelines for Computing Crop Water Requirements*, FAO Irrigation and Drainage Paper 56, FAO: Rome.

Baveye P. and Boast C.W. (1999) Physical scales and spatial predictability of transport processes in the environment. In *Assessment of Non-Point Source Pollution in the Vadose Zone*, Geological Monograph Series 108, Corwin D.L., Loague K. and Ellsworth T.R. (Eds.), American Geophysical Union: Washington, pp. 261–280.

Becker A. and Braun P. (1999) Disaggregation, aggregation and spatial scaling in hydrological modeling. *Journal of Hydrology*, **217**, 239–252.

Beven K. (1995) Linking parameters across scales: subgrid parameterizations and scale dependent hydrological models. *Hydrological Processes*, **9**, 507–525.

Beven K. (2001) How far can we go in distributed hydrological modeling. *Hydrology and Earth System Sciences*, **5**, 1–12.

Blöschl G., Grayson R.B. and Sivapalan M. (1995) On the representative elementary area (REA) concept and its utility for distributed rainfall-runoff modeling. *Hydrological Processes*, **9**, 313–330.

Chen Z.Q., Govindaraju R.S., and Kavvas M.L., (1994) Spatial averaging of unsaturated flow equations under infiltration conditions over areally heterogeneous fields: 1. Development of models. *Water Resources Research*, **30**, 523–533.

Clausnitzer V. and Hopmans J.W. (1999) Estimation of phase-volume fractions from tomographic measurements in two-phase systems. *Advances in Water Resources*, **22**, 577–584.

Clausnitzer C. and Hopmans J.W. (2000) Pore-scale measurements of solute breakthrough using microfocus computed tomography. *Water Resources Research*, **36**, 2067–2079.

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

Dane J.H. and Hopmans J.W. (2002) Soil water retention and storage – introduction. In *Methods of Soil Analysis. Part 4. Physical Methods*, Dane J.H. and Topp G.C. (Eds.), Soil Science Society of America Book Series: No. 5, pp. 671–674.

De Vos J.A., Raats P.A.C. and Feddes R.A. (2002) Chloride transport in a recently reclaimed Dutch polder. *Journal of Hydrology*, **257**, 59–77.

Duan Q.Y., Gupta H.V. and Sorooshian S. (1993) Shuffled complex evolution approach for effective and efficient global optimization. *Journal of Optimization Theory and Applications*, **76**, 501–521.

Duan Q.Y., Gupta H.V., Sorooshian S., Rousseau A.N. and Turcotte R. (2003) *Calibration of Watershed Models*, Water Science and Application 6, AGU: Washington.

Dunn S.M. and Lilly A. (2001) Investigating the relationship between a soils classification and the spatial parameters of a conceptual catchment-scale hydrological model. *Journal of Hydrology*, **252**, 157–173.

Eching S.O., Hopmans J.W. and Wallender W.W., (1994) Estimation of in situ unsaturated soil hydraulic functions from scaled cumulative drainage data. *Water Resources Research*, **30**, 2387–2394.

Eckhardt K. and Arnold J.G. (2001) Automatic calibration of a distributed catchment model. *Journal of Hydrology*, **251**, 103–109.

Ferguson R.B. and Hergert G.W. (1999) Sampling and spatial analysis techniques for quantifying soil map unit composition. In *Assessment of Non-Point Source Pollution in the Vadose Zone*, Geological Monograph Series 108, Corwin D.L., Loague K. and Ellsworth T.R., (Eds.), American Geophysical Union: Washington, pp. 79–94.

Hopmans J.W., Nielsen D.R. and Bristow K.L. (2002a) How useful are small-scale soil hydraulic property measurements for large-scale vadose zone modeling. In *Heat and Mass Transfer in the Natural Environment, The Philip Volume*, Geophysical Monograph Series No 129, Smiles D, Raats P.A.C. and Warrick A. (Eds.), AGU: pp. 247–258.

Hopmans J.W., Simunek J., Romano N. and Durner W. (2002b) Simultaneous determination of water transmission and retention properties. Inverse methods. In *Methods of Soil Analysis. Part 4. Physical Methods*, Soil Science Society of America Book Series No. 5, Dane J.H. and Topp G.C. (Eds.), AGU: pp. 963–1008.

Hopmans J.W. and Stricker J.N.M. (1989) Stochastic analysis of soil water regime in a watershed. *Journal of Hydrology*,**105**, 57–84.

Kavvas M.L. (1999) On the coarse-graining of hydrological processes with increasing scales. *Journal of Hydrology*, **217**, 191–202.

Klute A. and Dirksen C. (1986) Hydraulic conductivity and diffusivity: laboratory methods. *Methods of Soil Analysis. Part 1. Physical and Mineralogical Methods*, Agronomy Monograph Number 9, *Second Edition*, ASA: Madison, pp. 687–734.

Kosugi K. and Hopmans J.W. (1998) Scaling water retention curves for soils with lognormal pore size distribution. *Soil Science Society Of America Journal*, **62**, 1496–1505.

Mohanty B.P., Bowman R.S., Hendrikx J.M.H. and van Genuchten M.Th. (1997) New piece-wise continuous hydraulic functions for modeling preferential flow in an intermittent flood irrigated field. *Water Resources Research*, **33**, 2049–2063.

Madsen H. (2003) Parameter estimation in distributed hydrological catchment modeling using automatic calibration with multiple objectives. *Advances in Water Resources*, **26**, 205–216.

National Research Council (1991) *Opportunities in the Hydrologic Sciences*, National Academy Press: Washington.

Roth K., Vogel H.-J. and Kasteel R. (1999) The scaleway: a conceptual framework for upscaling soil properties. In *Modelling of Transport Processes in Soils at Various Scales in Time and Space*, Feyen J. and Wiyo K. (Eds.), International Workshop of EurAgEng's Field of Interest on Soil and Water:

24–26 November, Leuven, Wageningen Pers, Wageningen, pp. 477–490.

Schaap M.G., Leij F.J. and van Genuchten M.Th. (1998) Neural network analysis for hierarchical prediction of soil water retention and saturated hydraulic conductivity. *Soil Science Society Of America Journal*, **62**, 847–855.

Šimunek J., Šejna M. and van Genuchten M.Th. (1999) *The HYDRUS-2D Software Package for Simulating Two-Dimensional Movement of Water, Heat and Multiple Solutes in Variable Saturated Media*, Version 2.0, IGWMC-TPS-53, International Ground Water Modeling Center, Colorado School of Mines: Golden, Colorado.

Somma F., Clausnitzer V. and Hopmans J.W. (1998) Modeling of transient three-dimensional soil water and solute transport with root growth and water and nutrient uptake. *Plant and Soil*, **202**, 281–293.

Tuli A., Kosugi K. and Hopmans J.W. (2001) Simultaneous scaling of soil water retention and unsaturated hydraulic conductivity functions assuming lognormal pore size distribution. *Advances in Water Resources*, **24**, 677–688.

Van Dam J.C., Huygen J., Wesseling J.G., Feddes R.A., Kabat P., van Walsum R.E.V., Groenendijk P. and van Diepen C.A. (1997) *Theory of SWAP Version 2.0*, SC-DLO, Wageningen Agricultural University: Report 71, Department of Water Resources, The Netherlands.

Zhang D. (2002) *Stochastic Methods for Flow in Porous Media. Coping with Uncertainties*, Academic Press: San Diego.

Zhang D., Zhang R., Chen S. and Soll W.E. (2000) Pore scale study of flow in porous media: scale dependency, REV and statistical REV. *Geophysical Review Letters*, **27**, 1195–1198.

Zhu A.-X. and Scott Mackay D. (2001) Effects of spatial detail of soil information on watershed modeling. *Journal of Hydrology*, **248**, 64–77.

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Keywords: vadose zone; unsaturated water flow; flow modeling; scaling; calibration

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