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Role of vadose-zone flow processes in regional-scale hydrology: review, opportunities and challenges

Thomas Harter and Jan W. Hopmans[#]

Abstract

At the regional scale, vadose-zone processes are recognized for controlling both short-term dynamics in watershed hydrology and long-term water balances of hydrologic basins. In this paper we explore the various conceptual and mathematical models that have been proposed or could be considered to represent water fluxes in the vadose zone at the catchment, watershed or regional scale. Such models have been in existence in two largely disconnected disciplines: on the one hand, watershed hydrologists and, more recently, climate modelers frequently conceptualize the vadose zone as a zero-dimensional black box represented by lumped parameter models. On the other hand, soil physicists, equipped with tools to measure system and system-state properties directly in the vadose zone at scales of 10^{-2} – 10^{0} m, have relied on Richards' equation, a physically based, fully parameterized four-dimensional space–time model to represent unsaturated flow at the laboratory or field-plot scale. Over the past thirty years, the modeling efforts of the two disciplines have increasingly converged: hydrologists downscale their models by employing distributed (rather than lumped) models of varying complexity, while soil physicists have employed stochastic methods to upscale from their local-scale measurements and their local-scale physical understanding of flow processes to the field and regional scale. The lead question in this work is how the typical small-scale vadose-zone measurements relate to the large-scale representative or 'effective' parameter values of variously complex regional vadose-zone models. Recent advances in both, downscaling (from the regional scale) and upscaling (from the laboratory scale) and the use of inverse models have led to promising tools. As a result, at the regional scale, the Richards' equation and some of its simplifications, but also mass-balance and storage-based bucket models have been employed to represent spatially distributed unsaturated flow. All of these approaches have been employed with some success and under typically rather restrictive assumptions, whereby the least complex models seem to apply exclusively to the largest (and smallest) spatial and temporal scales. Various stochastic analyses have shown that simple averaging of local-scale measurements across the regions is associated with significant errors. Inverse modeling has relied on *a priori* assumptions about the physical framework that can be tested *a posteriori*. Both, downscaling and upscaling, regardless of the approach, yield increasingly complex models as they move from their opposing and well-understood starting points towards a unified mathematical representation that appropriately spans the hierarchy of significant process scales. To date, a physically and geostatistically

[#] Department of Land, Air, and Water Resources/Hydrology, University of California, Davis, CA 95616-8628, USA. E-mail: ThHarter@ucdavis.edu and JWHopmans@ucdavis.edu

consistent solution to describe regional vadose-zone flow in terms of local-scale measurements still eludes researchers.

Keywords: vadose zone; water balance; stochastic analysis; upscaling; infiltration; recharge; basin yield; watershed hydrology; SVAT

Introduction

The vadose zone is an intrinsic part of the hydrologic cycle, essentially controlling interrelationships between precipitation, infiltration, surface runoff, evapotranspiration and groundwater recharge. The vadose zone regulates the transfer of water from the land surface to groundwater and vice versa, while providing protection, screening, filtering, transfer and attenuation of potential groundwater contaminants that are delivered via the land surface. Yet, unlike the groundwaters below and surface water resources above, the dynamics of the vadose zone have not been subjected to regular monitoring at regional scales. For that reason, and because the vadose zone itself is not considered a resource reservoir, the vadose zone is generally not an explicit part of regulatory or planning guidelines that control or protect its waters.

Dichotomy of scales: horizontal versus vertical scale

When considering the vadose zone and its linkages to groundwater and surface water at the regional scale, it is helpful to remind ourselves of the vast differences between its horizontal and vertical extent: the vadose zone is but a thin film stretched across the continents, confined to a roughly 10^1 m thick zone, give or take one order of magnitude, separating the groundwater below from the sky above while stretching at length scales of 10^7 m over six continents. Even at the watershed or catchment scale (10^3 m-10^5 m), the ratio between horizontal extent and vertical thickness of the vadose zone is several orders of magnitude. In this paper, we focus on regional-scale representations of the vadose zone at scales much larger than 10^2 m. There, the dichotomy of scales between the horizontal and vertical extent of the vadose zone is a key consideration in building a framework for regional-scale vadose-zone hydrology.

Watershed hydrologists and water-resources engineers often consider the vadose zone as a thin skin, separating surface water resources from groundwater resources, with a horizontal-to-vertical scale ratio much larger than one, perhaps viewing it mostly as a black box that merely serves to connect – and separate – surface water and groundwater. Soil physicists, on the other hand, are mostly concerned with the pore, plot scale or field scale. In that case, horizontal length scales are on the same order as the vertical extent of the vadose zone. At these local scales, the vadose zone is therefore often considered as a fully three-dimensional system with interacting lateral and vertical fluxes of water, solutes, contaminants and air. It is also at this local or plot scale, at which soil physicists take measurements, including those used by hydrologists at the regional scale.

In watershed hydrology, perhaps the least contrast in horizontal extent to thickness is observed in small catchments with hillslope lengths on the order of 10^1-10^2 m. There, lateral flow processes in the vadose zone (interflow), rather than vertical transfer towards the saturated zone can be the dominant hydrologic process. In fact, one may contemplate that the hillslope scale is intermediate between the local and regional scale, thereby providing an ideal flow domain to investigate both small-scale and large-scale hydrological processes. In this treatise, hillslope vadose-zone processes will not be considered. We do so, not because of a belief that these are not important within a regional context. Rather it reflects our lack of experience in this particular area of vadose-zone hydrology.

In recent years, we have observed a convergence of the work by regional-scale hydrologists and that of local-scale soil physicists: as available computational resources and tools become more sophisticated, the conceptual understanding of the pore and plot scale has become more powerful. At the same time, regional-scale hydrology has moved from lumped to distributed hydrologic modeling of hydrologic systems coupled with global climate modeling. As a result, among the key challenges before us is to address the hierarchy of scales in the vadose zone appropriately in light of the dichotomy presented by the horizontal-to-vertical scale ratio, to explore the proper dimensionality of vadose zone processes, and to find their appropriate regional-scale representation without losing the link to local-scale soil physics.

The big picture: role of the vadose zone in regional-scale hydrology

The vadose zone serves many functions that are relevant at the regional scale. They can be summarized as follows (Figure 1):

1. To separate precipitation and applied irrigation water into infiltration, runoff, evapotranspiration, interflow and groundwater recharge;
2. To store and transfer water in the root zone between the atmosphere above and the deeper vadose zone or groundwater below, including interflow;
3. To store and transfer water in the 'deep vadose zone', that is, between the root zone above and groundwater below;
4. To store, transfer, filter, adsorb, retard and attenuate solutes and contaminants before these reach the ground water.

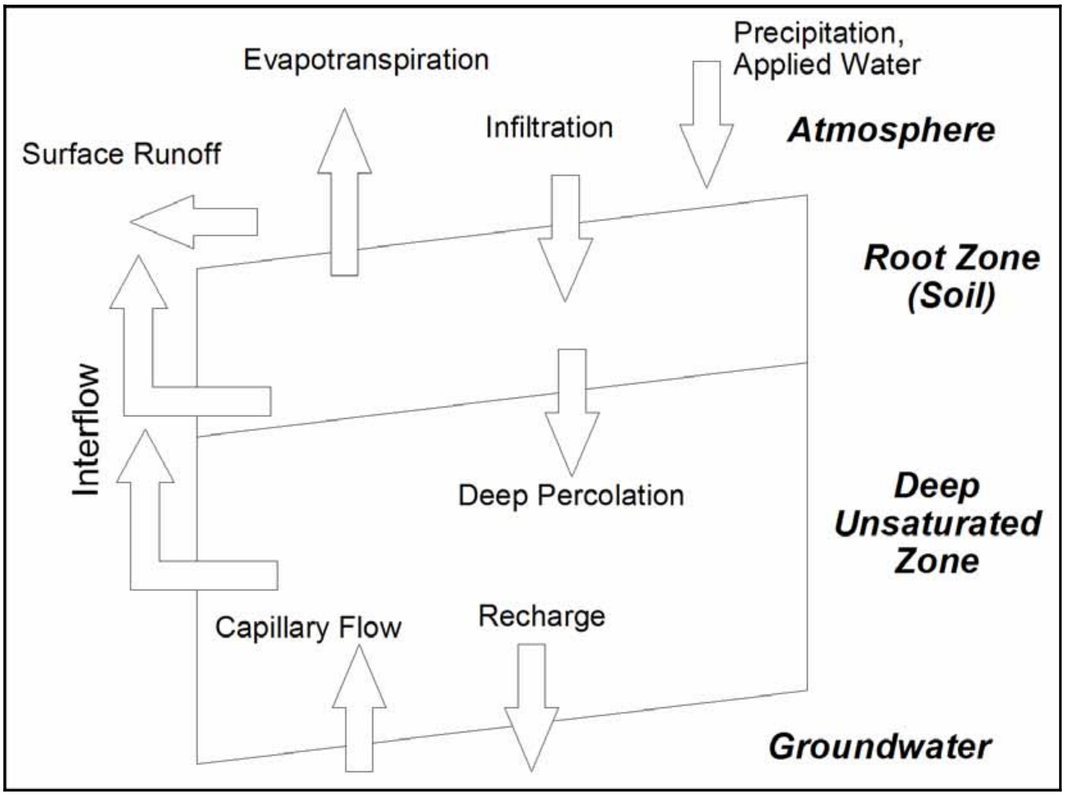

Figure 1. Water fluxes associated or controlled by the vadose zone

As a result, regional-scale vadose-zone hydrology is closely linked to watershed/basin hydrology, atmospheric/climate processes, agrohydrology, irrigation science, ecohydrology, groundwater-basin hydrology and contaminant hydrology.

Outline

In this review, we summarize and discuss the role of the vadose zone in regional-scale hydrology. By regional scale, we mean the catchment, watershed or basin scale (10^3-10^6 m). We use the terms regional, watershed and basin interchangeably, without explicit distinction.

While developing this paper, we pose two overarching questions: (1) What is known about the appropriate representation of the vadose zone (models, parameters, measurements) at the regional scale? (2) Is there a link between the regional and smaller scale representations of the vadose zone at the local scale?

Our goal is not to provide a rigorous physical or mathematical framework. Rather, our objective is to order and summarize the various concepts that have been applied to understand regional-scale vadose-zone flow and its linkages to vadose-zone processes at the local scale. We provide our own biased view, shaped by our mentors and colleagues as much as through our wide portfolio of projects, primarily in subsurface hydrology.

We begin with the following five principal statements summarizing the state of regional-scale vadose-zone hydrology:

1. Currently, there is no unified, universally accepted mathematical representation of regional-scale flow or transport in the vadose zone.
2. Regional-scale vadose-zone hydrology has been approached by either upscaling or downscaling, depending on the scientist's primary field of interest. For example, soil physics is a field of study that has historically been confined to small spatial and temporal scales, and is applied to larger scales from an upscaling point of view. Alternatively, groundwater recharge or basin runoff, traditionally treated by hydrologists in a lumped 'black box' fashion, is increasingly downscaled in a distributed modeling approach, to understand mechanisms better;
3. Richards' equation is the universally accepted local-scale mathematical model of vadose-zone flow, and the reactive advection–dispersion equation (RADE) is the universally accepted local-scale mathematical model of transport. However, both equations are physically meaningless when applied to the regional scale.
4. The role of the deep vadose zone at the regional scale has mostly been overlooked. This may be well justified in the context of long-term regional hydrology, as the deep vadose presents but an intermediary storage component. It does not affect long-term net fluxes in regional-scale hydrologic systems. However, the deep vadose zone plays a critical role in regional-scale transport processes;
5. The relevance of regional-scale vadose-zone flow to watershed hydrology and the hydrologic cycle is different from its relevance to regional-scale solute and contaminant transport. To address the latter (regional-scale contaminant transport) properly would overextend the scope of this paper.

Regional-scale vadose-zone flow

Control of ET and basin yield

The importance of the vadose zone in controlling regional-scale runoff dynamics has long been recognized and has been a central theme of soil hydrology for more than 50 years. More recently, dynamic modeling of basin yield and basin water balances (e.g., Eagleson 1978a; 1978b; Milly 1994) has further highlighted the key role of the shallow vadose zone. In the following, we will refer to the shallow vadose zone interchangeably as 'soil' or as the 'root zone', to highlight root-zone processes.

Soil hydrology controls, to a large degree, the separation of precipitation and applied water by irrigation into runoff and infiltration, and the partitioning of infiltration into evapotranspiration and groundwater recharge. At the regional scale, groundwater and the deep vadose zone serve as intermediate water storage pools, whereas the 'basin yield' quantifies the amount of runoff generated within the watershed. In basins with significant groundwater development, 'basin yield' also includes groundwater recharge used for groundwater production (Ruud, Harter and Naugle in press).

The estimation of evapotranspiration and groundwater recharge from precipitation has been a basic part of hydrology (Milly 1994), whether one is considering short-term or long-term flow dynamics in watersheds. Short-term processes include both rainfall-runoff dynamics and flood routing, while long-term issues of hydrologic research deal with the understanding of inter-annual and intra-annual (seasonal) variations in basin water balances.

Figure 2 illustrates the fundamental issues of the long-term water-balance dynamics. In humid climates, evapotranspiration, E, is not limited by available water from precipitation, P, and approaches potential evapotranspiration, $E_{p,}$ as indicated by the 1:1 asymptote *B*. Precipitation in excess of E_p generates basin yield by runoff and groundwater recharge. On the other hand, in arid climates, the available atmospheric energy supply exceeds available precipitation. There, all precipitation is subject to evapotranspiration (asymptote *A*), leaving no basin yield. In most basins around the globe, especially those with E_p values approximately equal to P, the asymptotic behavior of curve *A-B* may not be attained, and instead curve *C* is a typical hydrological response. This is so because of the 'inefficiency' of the short-term water flux dynamics in the vadose zone, which cannot deliver precipitated water to plant roots without losses to runoff, interflow and deep percolation (and, subsequently, groundwater recharge).

Understanding the controlling dynamics of shallow vadose-zone processes (i.e., the root zone) is critical in understanding the short-term dynamics of rainfall runoff, infiltration, evapotranspiration and recharge, which in turn determine the long-term water balance (Figure 3). Under most climate conditions, the ability of the root zone to match E with P (line *A*-B) depends on the soil's infiltration capacity, root zone storage and water-holding capacity, as well as on the temporal dynamics of the precipitation process relative to that of evapotranspiration. In the short term, evapotranspiration will usually lag precipitation, as P is larger during the rainfall event (usually) than E_p. Hence, the root zone acts as a temporary finite-volume storage reservoir. Under water-limited conditions, the departure of *C* from *A-B* is determined by many factors, including rainfall distribution and intensities, soil heterogeneity, root-zone depth, vegetation type and coverage, and its potential to overcome soil water stress. The closer the vadose zone can match E with P in the

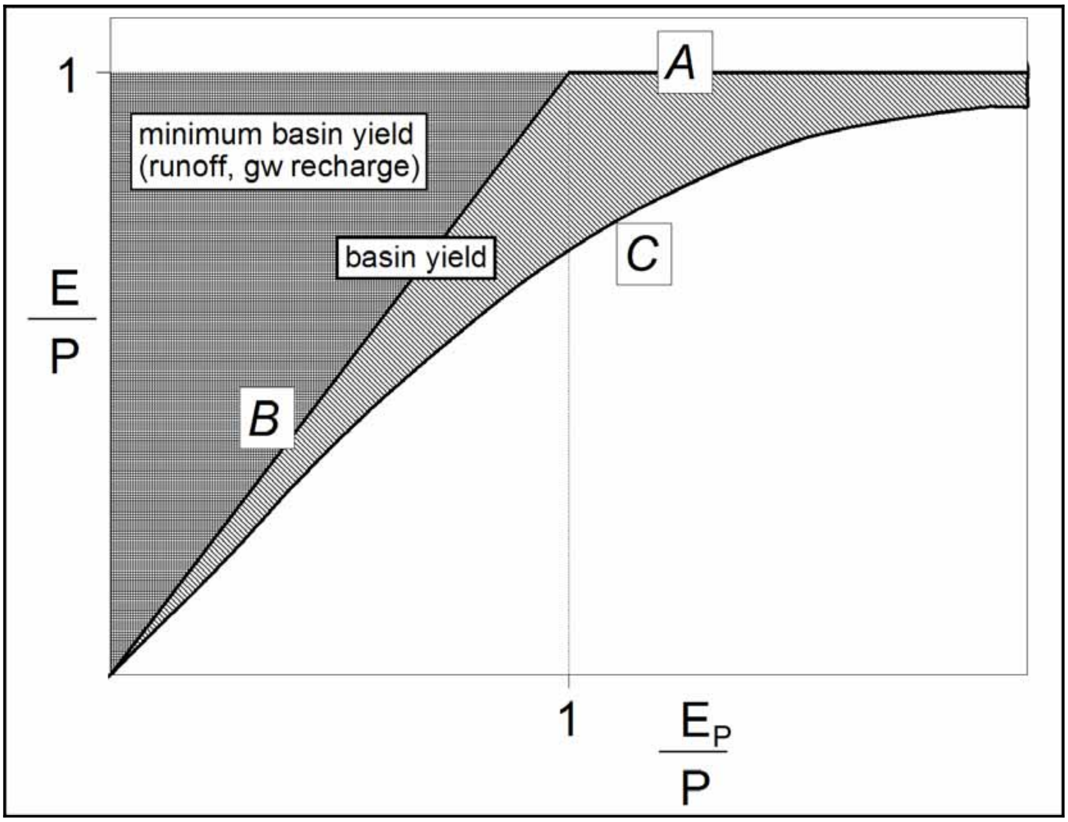

Figure 2. Schematic basin-yield diagram showing the relationship between evapotranspiration, E, potential evapotranspiraction, E_P, precipitation, P, and actual basin yield, Q (shaded area above curve C). Relative basin yield Q/P is the vertical distance between the curves *A*-*B* or *C* and E/P=1. Hence, the dark shaded area (above curve B) indicates the theoretical minimum basin yield (precipitation in excess of potential evapotranspiration)

short term, the more curve *C* will approach the asymptotic behavior of curves *A* and *B* in the long term, generating only the minimum basin yield. Hence, at the regional scale, local-scale vadose-zone flow processes and their dynamics provide the key for our understanding and prediction of curve *C* and its functional description relative to the asymptotic behaviors of curves *A* and *B,* and are therefore critical in estimating long-term basin yield. Furthermore, from a practical point of view, the vadose zone most critically controls and regulates the short-term runoff, the long-term base flow, and the availability of groundwater for production.

In summary, regional-scale vadose-zone hydrology is about predicting the functional relationships in Figure 3, thereby providing a signature of the watershed in question from which to understand long-term hydrologic and climate dynamics (Figure 2). An understanding of regional-scale hydrology and its dynamics, as defined in Figures 2 and 3, is therefore intrinsically linked to the dynamics of the soil–vegetation–atmosphere energy and water transfer (SVAT) processes.

Vadose-zone parameterization

At the watershed scale, the traditional hydrologic approach consists of the empirical fitting of observations (precipitation, runoff, potential evapotranspiration) to the lumped, basin-scale hydrologic fluxes that characterize basin-scale behavior ('lumped parameter approach'). Although not explicitly considered, the role of the vadose zone in the integrated hydrologic system is intrinsically reflected by the hydrologic response function or unit hydrograph inasmuch as the hydrograph reflects the separation of runoff, interflow and baseflow (Figure 3). Similarly, the measured regional-scale water balance as estimated from available land-surface energy (E_P) and water input (P) merely characterizes the partial control by the vadose zone, but does not assume the critical role of the root zone.

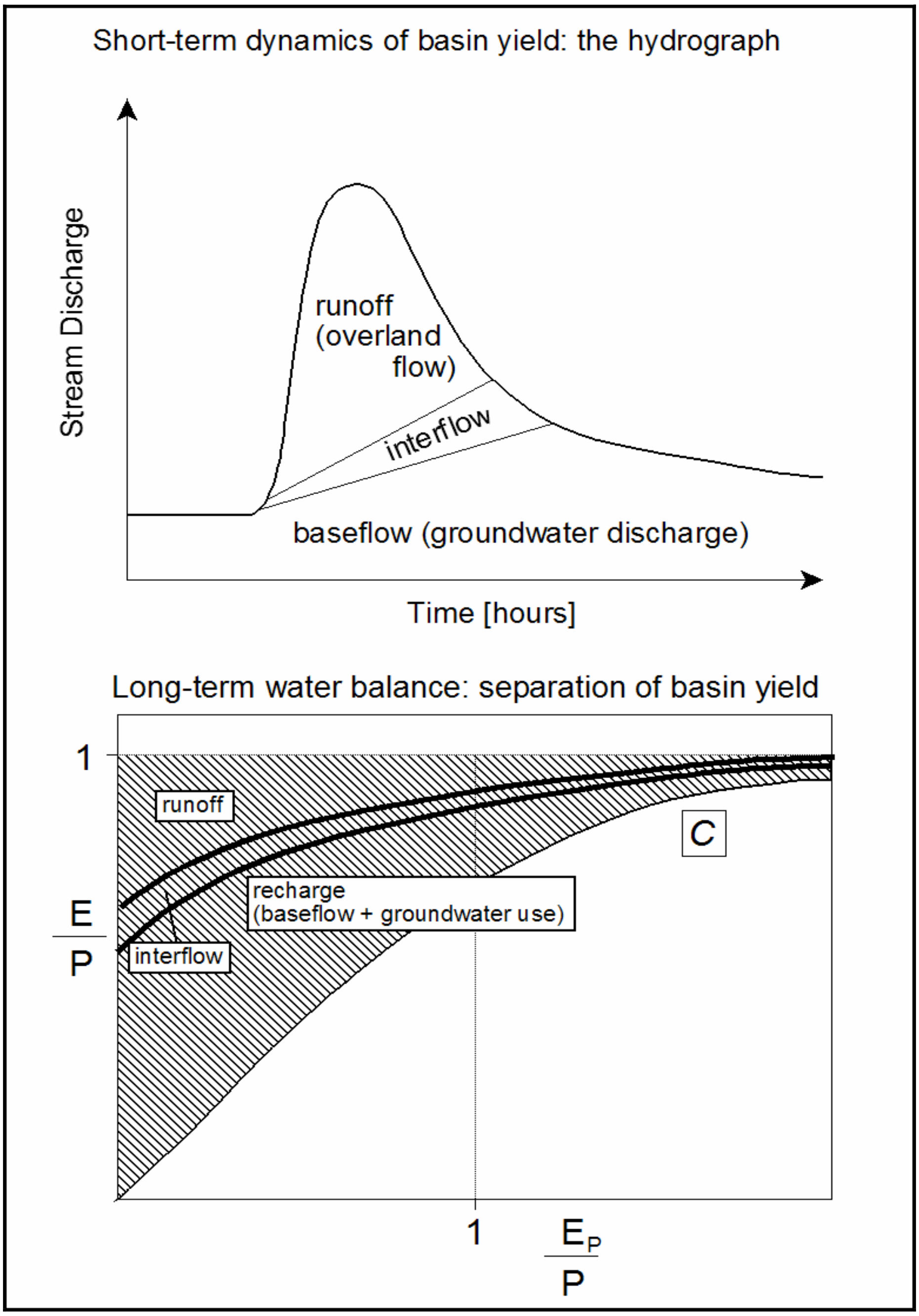

Figure 3. Separation of both short-term (top) and long-term (bottom) basin yield into overland flow (runoff), interflow and baseflow

In contrast, the current need to predict hydrologic behavior in watersheds is driven by questions on hydrologic responses for changing climatic conditions, and our scientific interest in understanding hydrological controls on ecosystem behavior.

Solutions require process-based models that predict the hydrograph (short-term dynamics) and water balance (long-term dynamics) from spatially distributed and spatially variable climatic, geomorphological, geological and soil-physical property measurements using the so-called distributed parameter approach. Because of the potential control exerted by short-term dynamics on long-term water balances and ecosystem behavior, these distributed watershed models depend on a physically based, regional-scale vadose-zone flow-process representation (cf. Beven and Feyen 2002).

Given the relatively large-scale focus, these regional-scale vadose-zone models mostly ignore internal lateral water fluxes and predict vertical fluxes such as infiltration, ET, runoff and deep percolation, with the vadose zone simply lumped into a single root zone that is explicitly treated as a black box. Sometimes a higher vertical resolution is considered to capture the dynamics of the vadose-zone flux and the separation of infiltration into evapotranspiration and deep percolation. In either case, the vadose-zone flow model is reduced from a complex three-dimensional to a simplified one-dimensional flow system that is representing horizontal scales that are much larger than the plot or field scale. In the simple lumped (spatially zero-dimensional) form, the water balance is typically written as (Rodriguez-Iturbe et al. 2001):

$$d_{rz}\frac{\partial\hat{\theta}(t)}{\partial t} = +P(t) - Int(t) - EV(\hat{\theta}(t),t) - TR(\hat{\theta}(t),t) - Q(\hat{\theta}(t),t) \qquad (1)$$

where $\hat{\theta}$ denotes average water content of the root zone with thickness d_{rz} (L), *Int* denotes plant-canopy interception, *EV* is bare-soil evaporation, *TR* denotes plant transpiration by root water uptake, and *Q* denotes the net water yield, computed from the sum of surface runoff, Q_r, groundwater recharge (drainage/percoloation), Q_d, and interflow, Q_i, all expressed as a flux rate. The functional relationships between these fluxes and water content are determined by flux-specific parameters, $\mathbf{p}_i$, ($i = EV, TR, Q_j$, $j=r, d, i$). In defining the regional-scale processes, a key issue is the natural variability of soil properties or system variables, measured at the local scale, and how they affect the regional-scale components of the water balance.

At the local scale, Richards' equation is universally considered the appropriate mathematical model for vadose-zone water flow. The Richards' equation in its most general form, which includes a root water-uptake function, *WU(h),* is defined as:

$$\frac{\partial\theta}{\partial t} = -\frac{\partial\mathbf{q}(h)}{\partial\mathbf{x}} + WU(h,\mathbf{p}_{WU}) \qquad (2)$$

subject to the appropriate initial and boundary conditions. θ is the volumetric water content, *h* is the soil water pressure head, **q** is the Darcian flux vector, and $\mathbf{p}_{WU}$ denotes a parameter vector that defines the control of soil water pressure head and spatial root distribution on root water uptake. When integrated over the whole root-zone domain, this sink term is equal to *TR*. Dependence on space, ***x***, and time, *t*, is implied. Water content and pressure head are related through the water retention function $\theta(h, \mathbf{p}_\theta)$, where $\mathbf{p}_\theta$ denotes the parameter set that defines the shape of the soil water retention curve. The Darcian flux vector, **q**, is defined as:

$$\mathbf{q}(h) = -K(h, \mathbf{p}_K)\frac{\partial(h + x_3)}{\partial \mathbf{x}} \tag{3}$$

where the function, $K(h,\mathbf{p}_K)$, defines the unsaturated hydraulic conductivity as a function of h through the parameter vector $\mathbf{p}_K$. The vertical dimension is expressed through x_3. Various models are used for the constitutive relationships $\theta(h, \mathbf{p}_\theta)$ and $K(h,\mathbf{p}_K)$. Many different types of hydraulic functions have been proposed, including the Brooks and Corey, Gardner-Russo, and Van Genuchten functions (Kosugi, Hopmans and Dane 2002).

For application at the regional scale (e.g., Feddes et al. 1993; Kabat, Hutjes and Feddes 1997), regional-scale surface boundary conditions are imposed to solve Eq. (2). Boundary conditions implicitly are a function of the internal state of the vadose-zone domain. That is, the partitioning of rainfall into infiltration and runoff, evaporation and transpiration rates are controlled by soil water content and/or pressure head. Therefore, as for the hydraulic functions, constitutive parametric models are defined to determine these external fluxes. However, one must question whether the Richards' equation or other derived simplified models, all of which are based on the concept of Darcy-Buckingham flow and mass conservation, are appropriate physical models to simulate vertical flow and the partitioning of fluxes between infiltration, evapotranspiration and deep percolation at regional spatial scales (Beven 1995; 1989) and how effective, scale-dependent hydrologic parameters relate to measurements.

Finding appropriate regional-scale solutions to (2) is the focus of regional-scale vadose-zone hydrology. A key condition for the validity of this model is the existence of a local scale, the representative elementary volume (REV), at which Darcy's law (3) is valid and for which the constitutive parametric process models for $\theta(h,\mathbf{p}_\theta)$ and $K(h,\mathbf{p}_K)$ can be measured. The scale of the REV or Darcy scale is about 10^{-2} m, and Richards' equation with the associated hydraulic functions is most commonly used to represent vadose-zone properties at a measurement scale of $10^{-2} - 10^{0}$ m. Thus, one would conclude that Eq. (2) applies only to flow models with a grid-scale resolution of that order of magnitude. Yet, distributed-parameter hydrologic models that explicitly account for vadose-zone processes, such as MIKE SHE (Refsgaard and Storm 1995) are applied with discretized horizontal spatial units much larger than 10^{0} m (Figure 4). Global climate models that include SVAT processes, are discretized to even larger horizontal scales of $10^{4} - 10^{5}$ m. This scale problem does not explicitly present itself in the lumped approach where hydrologic parameters are representative of the spatial scale at which the model is applied.

To satisfy the Darcy-scale requirement, one may be tempted to cast the regional-scale flow problem (2) into a fully three-dimensional numerical implementation with local-scale discretization of soil properties across the regional-scale domain. Assuming that proper local-scale discretization is on the order of 10^{-2} m vertically and 10^{0} m horizontally, this explicit modeling approach for a watershed with an area of 10^{2} km^{2} and a 10^{0} m thick root zone requires 10^{10} nodes. As a reference, the current maximum number of nodes to solve a transient, three-dimensional Richards' model within a reasonable amount of time is approaching 10^{6}. Further assuming that the historic growth of the maximum unsaturated-zone model size (total number of grid cells) will continue at approximately one order of magnitude per decade, we are half a century away from implementing such highly resolved climate grid-scale or watershed-scale regional models.

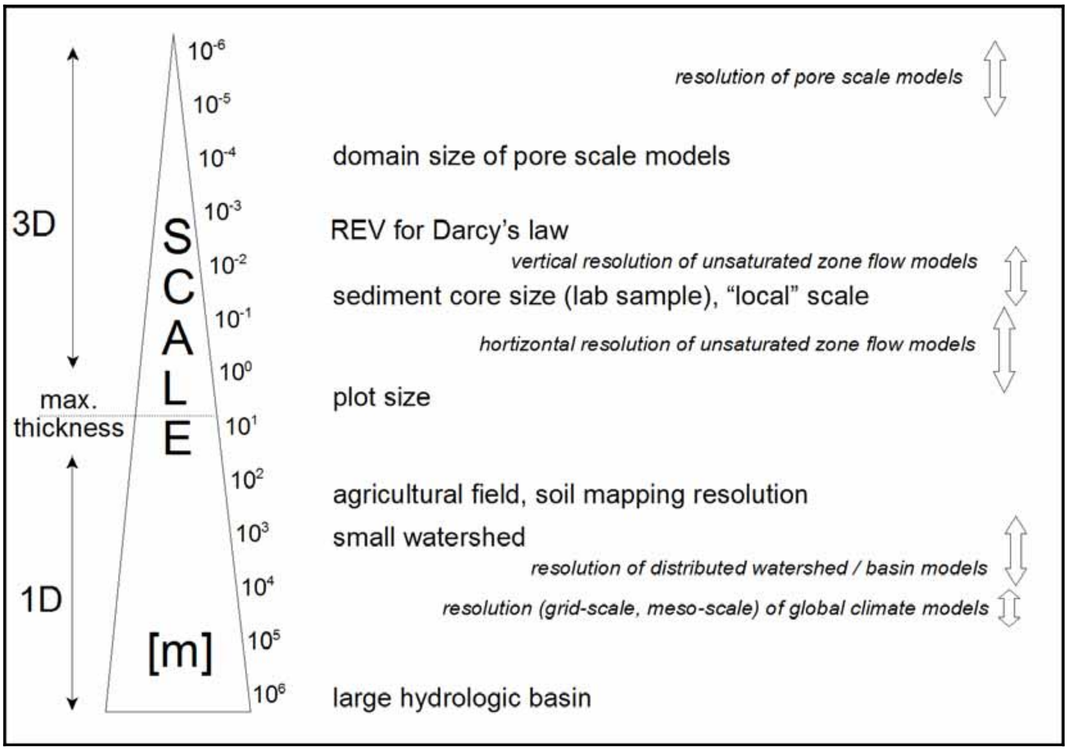

Figure 4. Illustration of the various scales of the vadose zone and associated modeling and measurement. Indicated on the left are the maximum space dimensions typically used for modeling the associated scale processes

Consequently, current process-based regional-scale models apply the Richards' equation and approximations thereof using grid-size scales of 10^3 m or larger, thereby making the implicit assumption that vadose-zone flow processes are scale-invariant. That assumption, however, is challenged. We will further discuss the potential implications hereafter.

When considering vadose-zone processes at the regional scale, inevitably we need to consider the hierarchy of scales, as introduced by Cushman (1990) and Roth, Vogel and Kasteel (1999) who conceptualize the soil as a hierarchical heterogeneous medium with discrete spatial scales that each may require different effective process models. Natural patterns of soil variability may show embedded, organizational structures that lead to non-stationary soil properties or processes. 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 level, different mathematical relationships may be required to describe the underpinning physical process at each scale. The vadose zone can be similarly characterized by this approach (Figure 4). In this regard, the recent applications in regional-scale vadose-zone hydrology can be viewed as a two-pronged approach. First, there is the need for downscaling of lumped hydrologic models to conceptual models with distributed parameter modeling. Second, starting from fundamental properties and processes at the pore, laboratory or field-plot scale, the hydrologic conceptualization must be upscaled to make regional-scale predictions. In the following we attempt to summarize the current state-of-the-art for both as a basis for outlining current strengths, weaknesses and challenges in regional-scale vadose-zone hydrology (*highlighted in italics*).

The upscaling approach

Starting with the analysis of field data by Biggar and Nielsen (1976), much quantitative evidence has been presented that demonstrates the tremendous variability of vadose-zone hydraulic properties. Field variability of the saturated hydraulic conductivity and of pore size distribution-related parameters can be extremely large (Zhang 2002, p. 223; Rubin 2003, p. 290). Field data consistently show that vadose-zone properties, measured at scales of 10^{-2}-10^{-1} m vary significantly over vertical scales of 10^{-1}-10^{0} m and horizontal scales of 10^{-1}-10^{1} m.

Within the context of regional-scale modeling of the vadose zone and especially of the root zone, this tremendous variability raises three related fundamental questions:

1. Is there a correct physical model that accurately predicts the dynamics of vadose-zone water fluxes at the regional scale?
2. If so, what is the relationship of these model parameters to the spatially-distributed measurement data collected with small-scale measurement devices?
3. Can the accuracy of the upscaled regional model in light of both the model and parameter uncertainties be quantified?

A review of the upscaling research in vadose-zone hydrology shows various distinct approaches. Whereas some work has been analytical, others used a numerical or strictly field-based approach. Some of the reviewed analyses must assume steady-state flow while others focus primarily on the effects of a transient moisture regime. Most of the analytical stochastic upscaling research assumed simple and homogeneous boundary conditions, with some considering spatially-variable or temporally-varying boundary conditions. Most studies ignore the three-dimensional variability of the vadose-zone system and instead focus solely on the horizontal variability using a parallel column model with vertically-homogeneous soils. Some modeling approaches consider a fully three-dimensional, heterogeneous system. Quite surprisingly, only a handful of stochastic upscaling studies consider heterogeneous flow within the SVAT framework to drive the upper boundary condition of the vadose zone. Table 1 makes an attempt to classify the various different upscaling studies that apply to regional-scale vadose-zone processes, although not all of them have been developed with that scale in mind.

Table 1. Literature review of models that upscale local-scale vadose-zone processes to the field-/meso-/regional scale. Non-highlighted articles are theoretical models. Lightly highlighted articles focus on numerical applications, darkly highlighted articles focus on modeling of field applications. References with an asterisk (*) indicate watershed or basin models that assume an effective soil water model at a resolution equivalent to or larger than the field scale. All other models are founded on the validity of Richards' equation at the local scale. The inclusion of any article in this table does not imply particular importance or significance. Rather this is an arbitrary, random selection of some of the significant papers. Model complexity, in general, increases from upper left to lower right.

Dynamics:	(Quasi-) Steady-state conditions			Transient conditions			
Upper Boundary Condition	Explicit (lumped)	Water balance (SVAT)-coupled		Explicit (lumped)		Water balance (SVAT)-coupled	
Lateral variability of BC (at scales smaller than the regional/watershed scale: / Vertical variability of soil properties:	homogeneous	homogeneous	heterogeneous	homogeneous	heterogeneous	homogeneous	heterogeneous
Vertically homogeneous or lumped		Milly (1994)*, Atkinson, Woods and Sivapalan (2002)*; Farmer, Sivapalan and Jothityangkoon (2003)*		Bresler and Dagan (1983), Dagan and Bresler (1983)	Chen, Govindaraju and Kavvas (1994a), Chen, Govindaraju and Kavvas (1994b)	Kim, Stricker and Torfs (1996)	Albertson and Montaldo (2003)*, Montaldo and Albertson (2003)*
Vertically distributed – stationary soil properties	Yeh, Gelhar and Gutjahr (1985a; 1985b; 1985c), Yeh (1989), Rubin and Or (1993), Harter and Yeh (1998), Harter and Zhang (1999)			Mantoglou and Gelhar (1987c; 1987a; 1987b), Ünlü, Nielsen and Biggar (1990), Polmann et al. (1991), McCord, Stephens and Wilson (1991), Chen, Govindaraju and Kavvas (1994a, b), Smith and Diekkrüger (1996)	Foussereau, Graham and Rao (2000)		Hopmans and Stricker (1989), Kim and Stricker (1996), Kim, Stricker and Feddes (1997)
Vertically distributed – non-stationary properties				Mantoglou (1992), Zhang (1999; 2002)		Jensen and Mantoglou(1992)	

Stochastic upscaling methods have been developed for the Richards' equation to provide physically-consistent models for important spatially-averaged vadose-zone variables, such as hydraulic conductivity, pressure head, water content, and flux. The upscaled dimension typically considered is the field scale, not the regional scale. Hence, most studies have considered a fully two- or three-dimensional domain. The upscaled models are mostly driven by spatially homogeneous and constant boundary conditions, and include spatially-variable soil properties to define the spatially-variable unsaturated hydraulic functions. Spatial variability is characterized using geostatistical techniques including variogram modeling. In the stochastic upscaling approach, one solves for the geostatistial moments of the dependent state variables (K, h, θ, q), using the geostatistical moments (mean, variance, correlation scale) of the independent system parameters (K_s, and other hydraulic function parameters).

Beginning with the seminal studies of Russo and Bresler (1981), Bresler and Dagan (1983), Yeh, Gelhar and Gutjahr (1985a; 1985b; 1985c) and Mantoglou and Gelhar (1987c; 1987a; 1987b), a suite of increasingly complex upscaling relationships were developed to determine 'effective' field-scale hydraulic properties from local-scale measurements. These include models for steady-state and transient flow conditions, stationary and non-stationary random fields, one-dimensional and multi-dimensional analyses. Recent reviews have been presented by Govindaraju (2002), Zhang (2002) and Rubin (2003). In the context of this paper, the critical question is: what have we learnt from these models with respect to a regional-scale representation of the vadose zone?

Yeh, Gelhar and Gutjahr (1985a; 1985b; 1985c) provided a three-dimensional stochastic analysis of steady-state vadose-zone flow for heterogeneous soils. Their analysis suggested that the effective hydraulic properties are primarily a function of the geometric mean of the local-scale saturated hydraulic conductivity and the arithmetic mean of the local pressure head (or water content). Since their analysis assumed steady-state gravity flow, *the effective hydraulic conductivity* K_{eff} *was equal to the field-scale, average downward flux,* q_z*, which in turn was shown to be approximately a function of the hydraulic conductivity obtained from the average of the local parameter values,* $<\mathbf{p}_K>$. Hence:

$$\log K_{eff} = <\log q_z> \cong \log K(<\mathbf{p}_K>) \tag{4}$$

This same result was later confirmed by Ünlü, Nielsen and Biggar (1990) and Harter and Yeh (1998) using Monte Carlo simulations.

However, as illustrated by both Yeh, Gelhar and Gutjahr (1985c) and McCord, Stephens and Wilson (1991) this effective hydraulic conductivity is also a function of the variance of the pore size distribution parameter and the degree of layering or anisotropy in the vadose zone. Accounting for the resulting higher order moments of a heterogeneous soil system, a more exact form of (4) yields:

$$<\log q_z> = \log K(<\mathbf{p}_K>) + \Delta \tag{5}$$

where Δ stands for additional terms obtained from the stochastic analysis. These, in part, account for the high nonlinearity of the water flow equation (2), and in part they account for the higher-order joint moments of the spatially varying system and state parameters. Values of Δ can be as low as -40% for horizontal anisotropic flow conditions and as high as +50% for isotropic soils leading, among other things, to *potentially significant lateral flow, even under gravity flow conditions*.

Direct application of these results to the regional scale is limited because steady-state flow was assumed for an equivalent infinite porous medium, with uniform spatial moments of both the system parameters and the state variables ('stationarity'). However, analytical solutions for the more common transient flow conditions in heterogeneous soils can only be obtained for special cases.

An example of transient stochastic analyses is the work by Dagan and Bresler (1983) and Bresler and Dagan (1983), who derived general approximate semi-analytical solutions for the effective field-scale hydraulic conductivity under transient conditions. Two major assumptions were implied in the solution. First, the vadose zone was conceptualized as a bundle of independent parallel columns, each with different but internally homogeneous hydraulic properties, to mimic soil heterogeneity in the horizontal direction only. Second, rather than solving Richards' equation explicitly, a simplified Green-Ampt type approximation with a rectangular water-content profile was used to represent one-dimensional infiltration and redistribution for each individual homogeneous soil column. Their analysis illustrated that 'effective' soil hydraulic parameters and their variability are highly nonlinear functions of depth and time, and only in the special case of steady gravity-drainage flow did the simple averaging of equation (4) apply.

The first stochastic upscale models that considered the complexity of non-stationarity and transient flow in three-dimensions were presented by Mantoglou (1992), expanding on the stationary model of Mantoglou and Gelhar (1987c; 1987a; 1987b), which in turn followed the steady-state, stationary model of Yeh, Gelhar and Gutjahr (1985a; 1985b; 1985c). The Mantoglou (1992) study provides the most general result for large-scale vadose-zone flow under non-stationary, transient flow conditions. Zhang (1999; 2002) explicitly solved the same problem but used an alternative linearization technique to reduce the truncation error in the perturbation analysis. Both studies point out the *tremendous theoretical and mathematical complexity of solving the fully-coupled non-stationary, transient 3-D flow system for effective parameters.*

Mantoglou (1992) and Zhang (1999) presented general upscaled equations that solve for the spatially-averaged water content and pressure head, using a spatio-temporally varying effective hydraulic-conductivity function (similar to Liedl (1994) and Li and Yeh (1998)). To close the physico-mathematical statement of the problem, truncations and linearizations were introduced. The resulting closed form of the field-scale equation is indeed identical to the local-scale Richards' equation, with the field-scale 'effective' hydraulic conductivity being dependent on the spatio-temporally varying covariances between system properties and pressure potential or water content (state variables). Figure 5 captures the principal components of the iterative numerical algorithm that must be used to solve these transient upscaling problems. *With respect to regional-scale flow processes, the solutions showed that at sufficiently large scales and in the absence of interflow, the average lateral flow component is negligible, so that the large-scale Richards' equation becomes one-dimensional.* Most importantly*, these studies suggest that there is a physical basis for applying Equations (2) and (3) at the field or possibly regional scale, at least under conditions of mild (as opposed to strong) heterogeneity.*

As an alternative to the highly restrictive analytical stochastic models, numerical stochastic methods using Monte Carlo (MC) simulation have been used to understand better the field and small watershed-scale behavior based on small-scale discretizations of the heterogeneous hydraulic-parameter fields (e.g., Hopmans, Schukking and Torfs 1988; Ünlü, Nielsen and Biggar 1990; Polmann et al. 1991;

Harter and Yeh 1998; Russo, Zaidel and Laufer 1998). These MC simulations have confirmed the general validity of the stochastic results, but also demonstrated the limitations of the perturbation approach. Specifically, under highly variable soil moisture conditions, such as occur during a drainage process, first-order perturbation methods and the linear upscaling approximation of Equation (4) fail to predict spatially averaged water fluxes accurately. At given mean head, the flux rate obtained from fully non-linear MCs is as much as half of that predicted by first-order perturbations. As a corollary, at given flux rates, the mean head (and, consequently, the mean water content and mean unsaturated hydraulic conductivity) are higher (wetter) than predicted by first order perturbation models (e.g., Harter and Yeh 1998; Harter and Zhang 1999).

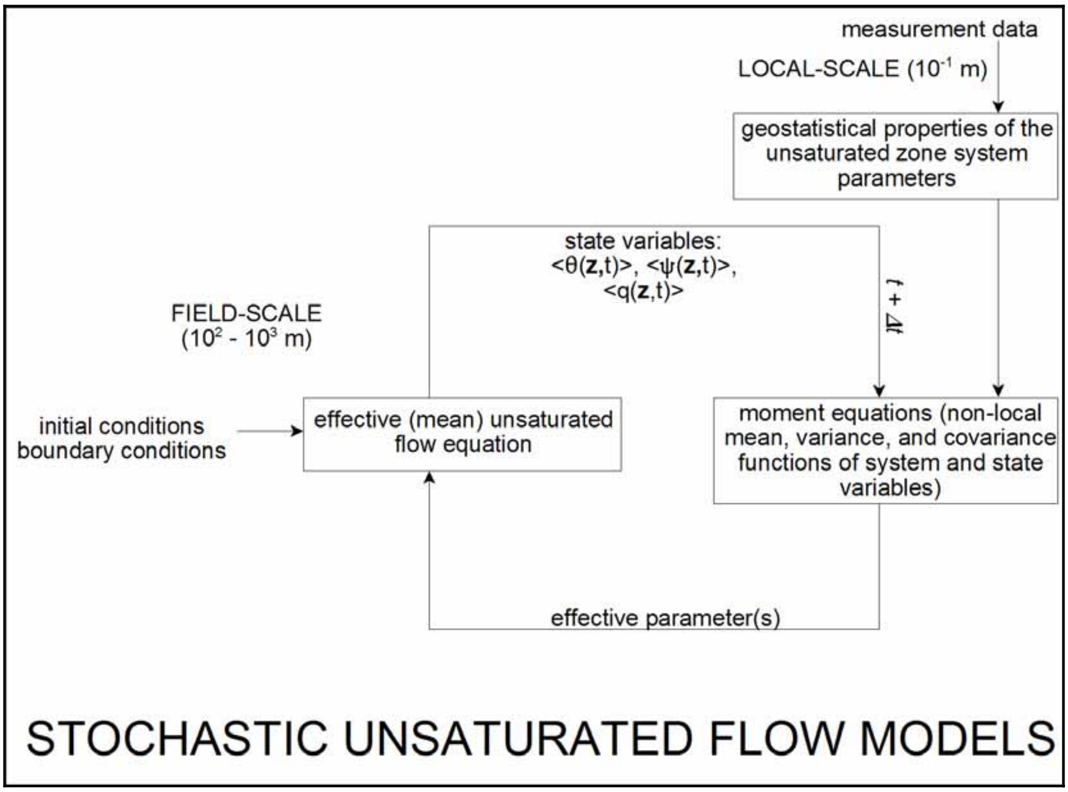

Figure 5. Flow diagram of the modeling process for stochastic transient unsaturated flow models

Testing these developed concepts for actual field conditions has been and will continue to be critical to understand the general applicability of the stochastic upscaling method. Jensen and Mantoglou (1992) have presented perhaps the most comprehensive field application of a fully three-dimensional stochastic upscaling model for transient, non-stationary flow conditions. It was a unique attempt to validate the rationale of stochastic upscaling theory. Their work demonstrates that *the application of stochastic methods to field sites may be excessively complex.*

Despite an extensive sampling campaign, the lack of data to estimate appropriate geostatistical models of local-scale hydraulic properties forced the modelers to make significant simplifications. As a result, Jensen and Mantoglou (1992) also compared their field data to models that use more simple upscaling relationships, such as (4). While the stochastic framework (Figure 5) clearly provides improved predictions of the field conditions, the improvement gained by solving a highly nonlinear, complex stochastic model appears to be small or even irrelevant in light of the data uncertainty. Clearly, *more studies of this type are needed to test the relevance of the non-local, non-linear terms of the large-scale equations for a variety of field conditions.*

Modeling approaches discussed to this point have not addressed critical aspects of regional-scale hydrological modeling with spatially-variable boundary conditions at the soil surface, such as infiltration and root water uptake. However, the experimental evidence and the analytical work provided in these studies clearly suggest that the variability of the local-scale flux in the root zone is potentially very large and is persistent in time. They also suggest that these may have complex interactions with spatio-temporally varying boundary conditions or spatio-temporally varying internal sink conditions (root water uptake). It is thought that the integration of imposed boundary fluxes with root-zone dynamics at the local scale and the nonlinearity of the upscaling process largely control the large-scale hydrologic behavior.

For simplified conditions, this issue was investigated by Rubin and Or (1993), who solved a steady-state non-stationary stochastic flow problem that included root water uptake. Their approach was based on the parallel-column model. The analysis focused on the effect of root water uptake on the spatially-averaged moisture profile. Surprisingly, they concluded that the spatially-averaged soil water pressure and water content were functions solely of the mean soil parameters, thereby confirming the simplified stochastic solution of Equation (4). However, their solution would not apply in arid climates, where transient flow conditions prevail.

Fousserau, Graham and Rao (2000) considered a more realistic random three-dimensional heterogeneous soil system with spatio-temporally variable infiltration rates. Their derivations confirm the fundamental proposition of the work by Mantoglou (1992) and Zhang (1999) and suggest that the effective large-scale equations are non-local, non-homogeneous partial differential equations. However, under conditions of spatio-temporally varying infiltration, the large-scale effective equations resemble the advection–dispersion equation (not the Richards' equation) with non-constant boundary conditions. The 'effective parameters' in the large-scale equation are spatio-temporally varying covariance and cross-covariance terms. These include covariances and cross-covariances of the spatially varying conductivity, recharge, and water content, which effectively represent physical forces capable of generating or destroying variability in soil water fluxes.

The advective-dispersive form of the large-scale equation with spatio-temporally variable large-scale production and decay terms suggests that large-scale flux through the unsaturated zone under conditions of spatially variable precipitation, infiltration and root water uptake is not unlike a reactive solute transport system. Unfortunately, Fousserau, Graham and Rao (2000) solve and illustrate the governing large-scale system of equations only for some extremely simplified and highly restrictive examples, which then reduce the solution to a form equivalent to (4) (Foussereau, Graham and Rao 2000, eq. 90). Also, like the study of Rubin and Or (1993), their results do not present quantitative insights regarding the effects of root-zone heterogeneity on the large-scale fluxes (as opposed to large-scale mean head).

It appears that the reluctance to take more often advantage of the stochastic models offered by, e.g., Mantoglou (1992), Zhang (1999) or Fousserau, Graham and Rao (2000) in regional scale models is also due to the fact that neither soil physicists nor watershed or climate modelers are familiar with the stochastic methods employed, or have the institutional and educational capacity to employ these. *We propose that – despite their limitations – the use of stochastic models would be beneficial in the analysis of regional-scale vadose-zone processes; and that 'packaged', well-*

documented stochastic software is needed to make these models more accessible to practitioners.

As a final note at this juncture, we offer an additional consideration that appears relevant for root-zone processes although it has not been studied in the context of stochastic models. The inherent large soil heterogeneity induces the potential for locally heterogeneous flow. The root system grows in direct response to the local heterogeneity of soil water fluxes. Since plant root growth and uptake are largely controlled by soil water status and its variability, root–soil interactions tend to equalize soil water content in all directions. Specifically, roots tend to explore soil regions that have large water and nutrient availability, and grow in the direction where water and nutrients are most plentiful (Clausnitzer and Hopmans 1994; Hopmans and Bristow 2002). Hence, the heterogeneity of the root-zone water-uptake system may effectively result in significant homogenization of soil water content, pressure head and vertical water fluxes. *The tendency of homogenizing soil water content reduces soil water flux variability, thereby providing a justification for one-dimensional or simple bucket-type flow models to simulate regional-scale soil water flow.* However, this large-scale approach was not considered by Rodriguez-Iturbe et al. (2001), who advocated a spatial scale of not more than a few meters, characteristic of the scale of a single plant root, extrapolating these root-zone-scale results to the regional scale.

Downscaling: from lumped to distributed parameter models

Historically, watershed and climate modeling has been applied using large-scale water-balance equations such as (1), with a focus on the interaction between the various boundary fluxes of the root-zone domain (Figure 6). Work in this direction was recently initiated by, e.g., Eagleson (2002), Rodriguez-Iturbe (2000) and Rodriguez-Iturbe et al. (2001) as part of an effort to define eco-hydrology as a subdiscipline that considers spatially-variable precipitation and dynamic rooting-zone processes as critical input to ecosystem models, especially for water-limited systems. Downscaling has also become important to meet a particular challenge of large-scale climate models: The lack of correspondence between model grid boundaries and basin or watershed boundaries does not afford climate models the use of water balances as a validation tool.

In the most simple case (and at the largest scale), the root zone is treated as a zero-dimensional black box with input (precipitation, infiltration), output (surface runoff, interflow, evapotranspiration, drainage), and with a variable finite soil water storage capacity. Thus, in the dynamic regional-scale water-balance model (1), the root zone and its dynamics play a prominent role. Yet, as discussed earlier, the vertical extent of the root zone is orders of magnitude smaller than the lateral extent of the vadose-zone domain. Correspondingly, the typical discretization at the horizontal scale is much larger than the field scale and may be as large as the 'grid scale' of a climatological model with daily, monthly or annual time steps. The hydrologic dynamics of (1) are driven by the surface boundary conditions, i.e., precipitation and available energy (ET_p) and their spatial and temporal variations. Vertically and horizontally distributed root-zone processes control the partitioning of total water input into *EV, TR*, runoff, interflow and drainage at all spatial scales.

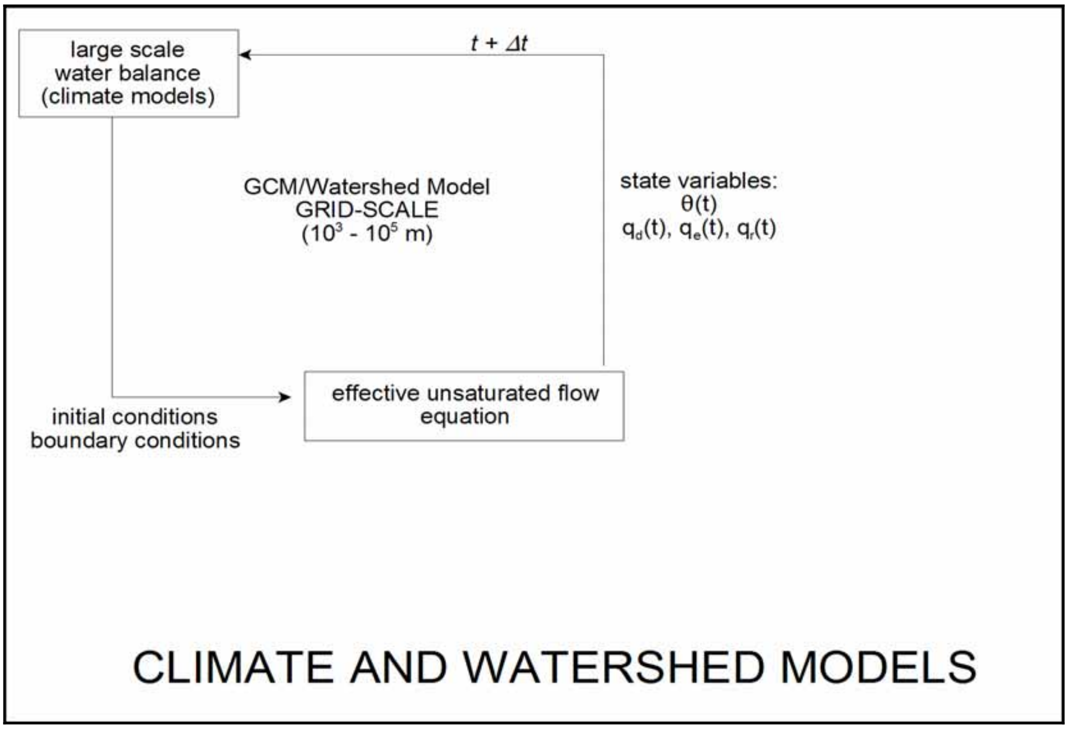

Figure 6. Flow diagram of the modeling process in climate and watershed models

Despite the complex dependence of the regional-scale flow dynamics on the spatial and temporal variability of the local-scale processes and vice versa, regional hydrologic modeling typically considers the root zone as a single thin homogeneous soil layer that uniformly extends across the watershed, of which $<\hat{\theta}>$ and $<\mathbf{p}>$ represent spatial averages of their local equivalents.

Two key questions can be raised in applying this simple upscaled concept of the dynamic water balance to regional-scale vadose-zone hydrology. These are:

1. Which process model and what vertical discretization is required to simulate the dynamics of all possible fluxes in (1) satisfactorily?
2. What degree of horizontal spatial resolution is needed to delineate appropriately the individual mapping units, representative elementary areas (REA) or hydrological response units (HRU), as determined by geographical, geomorphological, land-use, or other hydrologically-relevant watershed characteristics?

Milly (1994) used a simple storage bucket model, representing the root zone as a lumped storage reservoir with root-zone thickness and effective water-holding capacity as the selected reservoir parameters. This study used spatially-distributed precipitation and potential evapotranspiration data for the eastern United States, resolved at a grid scale of 0.5 degrees, as the basis for their analysis. Their approach successfully reproduced the continental-scale spatial distribution of the average long-term basin yield $\{<Q>\}$ and evaporation $\{<E>\}$, where {} indicates time-averaged values.

Alternatively, one-dimensional regional models consider the transient, vertically distributed soil moisture, hydraulic conductivity and root water uptake (e.g., Hopmans and Stricker 1989). Salvucci and Enthekabi (1994) compared the performance of the simple storage bucket-type model with the one-dimensional approach, and concluded that *long-term spatially and temporally averaged fluxes computed from the bucket-*

type approach (e.g., Eagleson 1978a; 1978b) are sufficiently accurate. In other words, long-term soil water dynamics can be modeled using a simple storage bucket model. Guswa, Celia and Rodriguez-Iturbe (2002) expanded this approach to include root water uptake and evapotranspiration. They also concluded that the bucket-type approach is adequate, even in water-limited systems, provided that the soil moisture dependency of root water uptake is considered through introduction of a macroscopic root compensation factor.

Model results have demonstrated that the water balance (1) is highly sensitive to the root-zone storage capacity (Figure 6). Atkinson, Woods and Sivapalan (2002) and Jothityangkoon, Sivapalan and Farmer (2001) concluded that such sensitivity is especially high for arid and semi-arid water-limited watersheds, where $ET_P/P > 1$ (Figure 2). Ruud, Harter and Naugle (in press) confirmed this result for a semi-arid, irrigated basin, showing that groundwater recharge is highly sensitive to root-zone storage. On the other hand, as $ET_P/P \rightarrow 0$ (humid climates), the role of root-zone storage capacity in determining the water balance diminishes.

Clearly, a relationship must exist between the temporal resolution defined *a priori* (long-term, inter-annual or intra-annual variations of basin yield), the required spatial resolution (horizontal and vertical), and associated model complexity, that defines the conditions needed for accurate basin yield predictions using (1). Using a comparative downscaling approach, Atkinson, Woods and Sivapalan (2002) and Farmer, Sivapalan and Jothityangkoon (2003) investigated this relationship for a series of watersheds, ranging in size from a few square kilometers to several tens of square kilometers. These watersheds were located in Australia and New Zealand across a variety of climatic conditions. Their work demonstrated that *horizontal across-the-watershed and vertical across-the-root zone spatial resolutions must increase to predict the water balance dynamics accurately at increasingly shorter time scales* (Figure 7). If one is interested in a single-valued long-term basin yield, a simple bucket-type modeling approach with water balances computed across REAs was adequate. This confirms results by Ruud, Harter and Naugle (in press), who concluded that a zero-dimensional, bucket-type root-zone storage model, with spatially variable soil parameters and boundary conditions resolved at the field scale (10^1-10^3 m), was sufficiently accurate to predict both spatial variability and temporal variations (at the inter-annual and seasonal time scales) in basin yield for a 2,300 km^2 semi-arid, irrigated watershed.

Consistent with Figure 2 and reported regional-scale studies, we conclude that *model complexity increases as climates become increasingly water-limited (drier climates), requiring increasing spatial resolutions in both horizontal and vertical directions, regardless of the temporal scale of interest.*

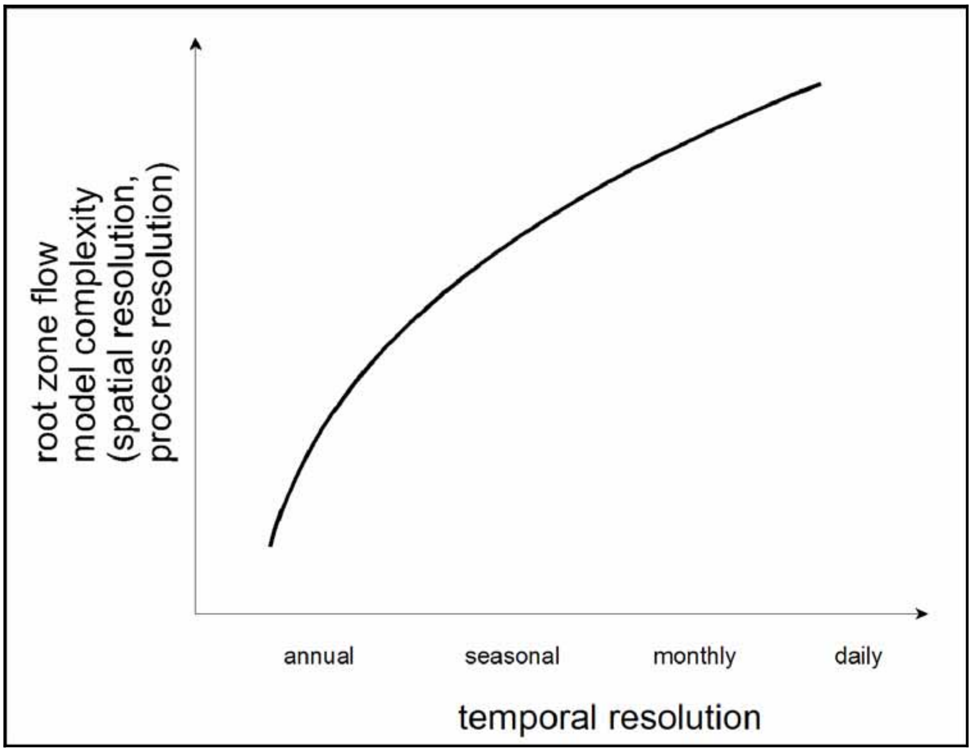

Figure 7. Dependence of spatial model complexity on temporal resolution

Bridging upscaling and downscaling efforts: effect of soil-moisture spatial variability on the regional-scale water balance

To understand better the issues related to spatial discretization and parameterization in regional water-balance models, one must recognize that hydrological models which are based on (1) make the following key assumption, one that is equivalent to (4):

$$< Q_j(\mathbf{p}_Q, \hat{\theta}) > \; = \; Q_j(< \mathbf{p}_Q >, < \hat{\theta} >) \tag{6a}$$

$$< E(\mathbf{p}_E, \hat{\theta}) > \; = \; E(< \mathbf{p}_E >, < \hat{\theta} >) \tag{6b}$$

where $j = [r,i,d]$ represents runoff, infiltration and drainage, respectively. Stochastic analyses by Russo and Bresler (1981) and Bresler and Dagan (1983) questioned the validity of (6), and they concluded that this simplification only applies for restrictive conditions. Moreover, as concluded by Smith and Diekkrüger (1996), the effective soil dynamic characteristics cannot be directly measured for hydrologic systems with significant heterogeneity. Herein lies the key challenge in the modeling of regional-scale vadose-zone hydrologic processes.

Over the past 25 years, various studies have explicitly demonstrated the limitations of (6) when solving (1) within the context of SVAT, and have sought alternative relationships that are valid at the watershed scale. The study by Sharma and Luxmoore (1979) was perhaps the first of this kind, followed later by similar studies by Milly (1987), Entekhabi and Eagleson (1989), Hopmans and Stricker (1989), Chen, Govindaraju and Kavvas (1994a; 1994b), Kim and Stricker (1996), Kim, Stricker and Feddes (1997), Kabat, Hutjes and Feddes (1997) and, most recently, Albertson and Montaldo (2003) and Montaldo and Albertson (2003).

Kim, Stricker and Torfs (1996) derived a one-dimensional analytical set of solutions to compute the transient water budget for the vadose zone coupled with SVAT processes. While based on the Richards' equation principles, their scheme used some critical assumptions not uncommon in similar models. Specifically they assumed instantaneous redistribution of infiltrating water in the root-zone reservoir, no evaporation and deep percolation during precipitation, a linear relationship between root-zone saturation and evapotranspiration, and gravity drainage describing deep percolation. The simplified solution was chosen to compare explicitly the regional long-term average $\{<E(\mathbf{p_E})/P>\}$ with the lumped approach $\{E(<\mathbf{p_E}>)/P\}$, where $\mathbf{p_E}$ included two surrogate parameters α and m representing the soil's saturated hydraulic conductivity and pore size distribution. The parameters varied horizontally (distributed, parallel-column model). Spatial variations were generated from independent random log-normal distributions using soil- and climate-dependent mean and variance values for **p** (stationary distribution). This approach is an extension of Bresler and Dagan's (1983) parallel-column model for use within a regional water-balance model. For a number of different climate–soil-texture combinations, their results indicated that the long-term spatially-averaged evaporative flux $\{< E(\mathbf{p_E})/P>\}$ was larger than the regional evaporative flux computed from averaged parameters, $\{E(<\mathbf{p}_E>/P\}$ (1). The reverse result applied only to fine-textured soils under arid climate conditions. Unfortunately, their work did not discuss equivalent implications of the model with respect to effective, regional scale Q_d (deep percolation).

'Equivalent parameters' $\mathbf{p}_{eq,}$ such that $\{<E(\mathbf{p}_E)/P)>\} = \{E(\mathbf{p}_{E,eq})/P\}$ were shown to depend on the mean and variance of $\mathbf{p}_E$ and on climate parameters. Equally important, their work demonstrated that the use of equivalent parameters in the local-scale equations cannot explain short-term regional-scale variability. This conclusion confirms results from using Monte Carlo simulations of the nonlinear Richards'-type model (Kim and Stricker 1996), where differences between $\{<E(\mathbf{p},\theta)/P>\}$ and $\{E(<\mathbf{p}>,<\theta>)/P\}$ were the largest for low-permeable soil conditions with surface runoff dominating.

Chen, Govindaraju and Kavvas (1994a; 1994b) took a step further in model complexity and developed two stochastic models to solve for a horizontally-averaged, but depth-dependent transient water content. The 'averaged Green-Ampt' method was based on an analytical statistical integration across the horizontal spatial dimension, with local infiltration simulated as a Green-Ampt process. For comparison, they also derived a stochastic perturbation-approach model using a stochastic representation of the fully three-dimensional Richards' equation. In both models, the saturated hydraulic conductivity was the single spatially-variable soil parameter. Furthermore, soil variability was considered in the horizontal direction only, as in the parallel-column model by Bresler and Dagan (1983). Clearly, the upscaling based on the Green-Ampt approach is much simpler than the perturbation method and, therefore, has the potential to be widely used in water-balance modeling using appropriate boundary conditions. Results from both models were compared to numerical Monte Carlo simulations for a fully three-dimensional parameterization of Richards' equation, which was considered the 'real world' standard. Their study concluded that the perturbation method gave better results than the simplified Green-Ampt model if vadose-zone heterogeneity was limited. However, with increasing soil variability, the errors due to simplifications of the Green-Ampt approximation were not nearly as large as the truncation errors of the analytical perturbation approach. Hence, a simplified soil physical representation of the vadose zone (such as the Green-Ampt approach) appears to be justified in the context of analytical stochastic models. Even though the stochastic analysis itself is physically and conceptually more consistent with reality than the Green-Ampt approach, the closure of the governing system of stochastic equations requires simplifications that introduce errors of similar order of magnitude to those introduced by the conceptual simplification of the flow system represented in the Green-Ampt model.

The work by Chen, Govindaraju and Kavvas (1994a; 1994b) comes closest to bridging the upscaling efforts of local stochastic modeling with the downscaling approach of regional dynamic water-balance modeling (Figure 8). Moreover, their results provided insight into why simplified root-zone models are appropriate choices for regional-scale water-balance purposes. Also, from a practical point of view, the work by Chen, Govindaraju and Kavvas (1994a; 1994b) has important implications that warrant further study. Their work *explicitly confirms that upscaling by simple parameterization using a simple statistical integration is a valid approach that yields much better results than simply assuming that (4) or (6) holds true*. Neither the fully three-dimensional numerical models based on local-scale parameterization of Richards' equation nor the upscaled stochastic equations are currently of practical significance, because of their complexities and computational needs. *This again points to the need for packaging these methods into user-friendly software*. Without these tools, application of (1) at the regional scale, using simplified process-based models that operate at a sub-regional scale and that use a relatively simple parametric upscaling method to circumvent the limitations of (6) is a sound alternative. This approach is also consistent with other studies, such as Rubin and Or (1993).

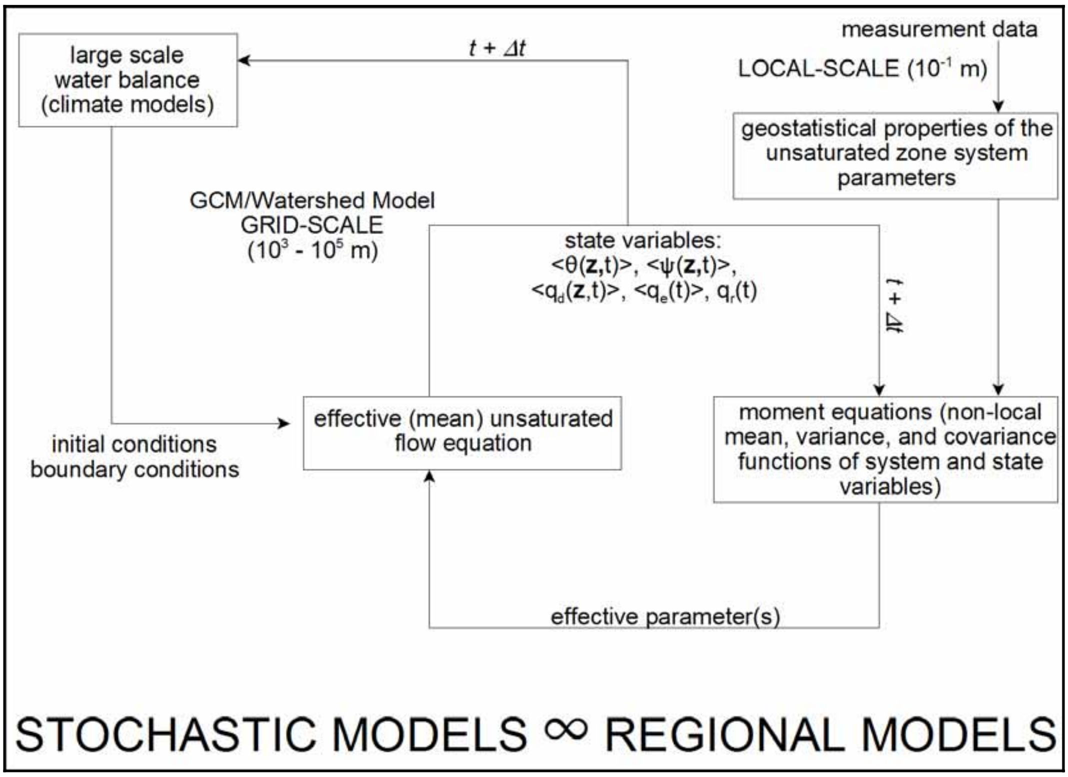

Figure 8. Flow diagram of the modeling process needed to integrate local-scale and large-scale data into a unified stochastic modeling framework at the regional scale

More recent studies are considering the spatial variability in climate forcing, in addition to soil spatial variability for transient conditions. For example, Albertson and Montaldo (2003) investigated relationships between spatio-temporally varying parameters of the water balance (initial conditions in water content, hydraulic parameters, precipitation, evapotranspiration, deep percolation), using a water-balance perturbation approach to hypothetical examples. In their investigations, flux boundary conditions were prescribed through a separate precipitation model. They showed that the mean water content of a spatially-variable vadose zone, $<\hat{\theta}(\mathbf{p})>$, was generally different from the water content of the homogeneous (mean state variable) soil, $\hat{\theta}(<\mathbf{p}>)$. Their study demonstrated how these differences were the result of the covariances and cross-covariances between water content and soil–climate system parameters. The important role of these covariances was also highlighted in studies by Mantaglou (1992), Mantoglou and Gelhar (1987c; 1987a; 1987b), Harter and Zhang (1999) and Foussereau, Graham and Rao (2000), but for field-scale applications and outside the SVAT framework.

Despite these most recent advances, much less information is currently available on the formulation and solution of an appropriate stochastic framework of regional-scale vadose-zone flow processes within the SVAT-type context given by (1) and illustrated in Figure 8. Clearly, from a practical point of view, simplification works well as shown in the applications of Milly (1994), Jothityangkoon, Sivapalan and Farmer (2001), Atkinson, Woods and Sivapalan (2002), Farmer, Sivapalan and Jothityangkoon (2003) and Ruud, Harter and Naugle (in press).

But from a theoretical point of view, we have yet to come to a rigorous understanding of why the simple bucket-type models really work or how their parameters can be computed from local-scale measurements. Moreover, we note that when requiring dynamics of water and nutrient limitations on root activity, models become even more complex than those considered thus far (Hopmans and Bristow 2002). Some have argued that such an increase in system complexity inevitably leads to vadose-zone fluxes being dominated by spatially-variable boundary conditions such as T and P (Laio et al. 2001; Porporato et al. 2001) rather than spatially variable soil properties.

Inverse modeling of regional-scale vadose-zone flow

Not having a physically-based forward model that relates locally measured system parameters to the effective system parameters driving simplified regional models leads to the use of inverse modeling approaches directly at the larger scales. The inverse method (also referred to as 'calibration' or 'parameter optimization') offers a powerful procedure to estimate effective flow system properties across spatial and temporal scales given any arbitrary model structures. As numerical models have become increasingly sophisticated and powerful, inverse methods are found to be applicable to laboratory, field and watershed data, no longer limited by the physical dimensions of the soil domain or type of imposed boundary conditions. The application of inverse modeling to estimate soil hydraulic functions for laboratory soil cores has been extensively reviewed by Hopmans et al. (2002). Inverse methods might be especially appropriate for estimating field- and regional-scale effective soil hydraulic parameters given measurements of boundary fluxes (Feddes et al. 1993; Hopmans, Nielsen and Bristow 2002). Regional-scale inverse models determine effective regional-scale model parameters through fitting to measurements of state variables that represent the regional-scale system. The principal regional-scale state variables measured in watersheds are surface water flows and water-table depths. Although application of inverse methodology may suffer from non-uniqueness (e.g., Beven 2001), the application of parameter optimization methods for the estimation of soil hydraulic functions across spatial scales is generally very promising, yielding effective hydraulic properties that pertain to the scale of interest.

In soil hydrological studies at the regional scale, hydrological response units may define the relevant structural units that partition the watershed domain into units by their hydrologic functioning. The distribution or dis-aggregation of a watershed into structural units is deterministic (distributed modeling) and their subsequent aggregation to the scale of interest may be possible by simple mass-conservation principles. The selection of the main HRUs or hydrotopes with their corresponding effective hydrological parameters is determined by inverse modeling (e.g., Eckhardt and Arnold 2001). Recent optimization algorithms allow for multiple objective functions in distributed watershed modeling, with effective hydrological-parameter values determined by the choice of the most relevant hydrological variables. Increasingly efficient global optimization algorithms include the shuffled complex evolution (SCE) algorithm (Duan et al. 2003), which has been applied to calibrate a large number of parameters for distributed watershed models. More importantly, the method allows for a direct estimation of the associated parameter uncertainty without making an *a priori* assumption about their probability distribution. Madsen (2003) demonstrates the successful application of SCE using multiple objective functions for calibration of a multi-parameter distributed watershed model. We believe that these sophisticated calibration techniques, which have proven to be successful in surface-water hydrology, are ripe for application to regional-scale vadose-zone flow models.

In Vrugt et al. (2004), we explored the usefulness and applicability of the inverse method to estimate effective vadose-zone parameters at the small watershed scale based on measurements of spatially-distributed tile-drainage data (calibration targets). The study area was the 3880-ha tile-drained Broadview Water District (BWD), which is an intensively irrigated agricultural region on the west side of the San Joaquin Valley of California. In this study, we compared different hydrologic models, representing different levels of model complexity, at various spatial resolution scales. The models were compared for their ability to minimize uncertainty in the calibration parameters while also minimizing model prediction errors. Inverse modeling was conducted with a recently developed global optimization SCEM-UA algorithm (Vrugt et al. 2003) that provides an efficient estimate of the most likely parameter set with its underlying posterior probability distribution. Results demonstrated that measured spatially distributed patterns of drainage flux data were particularly inadequate for estimation of the soil hydraulic properties at those scales. The study showed that the only parameters estimated with reasonably narrow confidence intervals were related to drain conductance and bypass flow, indicating that these were the critical parameters controlling drainage flow processes at the relevant space (field/drainage system) and time scales (weeks). Clearly, for any model calibration to be successful, the parameters to be optimized must be sensitive to the model solution. In practice, this means that the calibration parameters must characterize the most relevant hydrologic processes. Additional complications arise if multiple measurement types need to be fitted to corresponding model predictions. For example, the recent study by Schoups et al. (submitted) showed the presence of non-uniqueness and resulting large parameter uncertainties for these multiple-objective conditions. However, this same study also demonstrated that the forceful combination of model simulations with experimental data, as is done in the inverse-modeling approach, can provide much information on model deficiency and/or experimental error.

This perspective on inverse modeling is not incidentally consistent with the findings of forward-modeling studies that have investigated to which degree model structure (as opposed to model parameters) must be adapted to explain basin scale flux (i.e., basin yield, recharge) satisfactorily at seasonal or inter-annual time scales, including the work by Ruud, Harter and Naugle (in press), Farmer, Sivapalan and Jothityangkoon (2003), Atkinson, Woods and Sivapalan (2002), Jothiyangkoon, Sivapalan and Farmer (2001) or Milly (1994), to name a few.

Status quo versus opportunities and challenges

A solid understanding of regional-scale flow and transport processes provides the key to the sustainable management of soil and water resources at the watershed scale, offering practical solutions to wide-spread environmental problems and a better understanding of regional-scale hydrology. However, most vadose-zone research efforts to date have focused on explaining local-scale physical processes, without paying much attention to their extrapolation at the regional scale. On the other hand, conventional hydrologic models only implicitly consider the vadose zone, treating the soil as a thin, passive skin, merely to separate surface water from the groundwater. Increasingly though, recent hydrologic applications seek to couple hydrologic modeling with chemical transport and climate-forecasting models. For that purpose, it is now widely recognized that a better understanding of the dynamical flow and transport processes in soils and the vadose zone is needed. Hence, the incentive of the presented review on regional-scale vadose-zone hydrology.

First and foremost, we conclude that vadose-zone processes provide a signature of watershed function, as they control the partitioning of all hydrologic fluxes. Historically, vadose-zone modeling is carried out either through complex multi-dimensional flow models that can be applied to the local scale only, or by simplistic lumped water-balance models that strictly apply to the regional scale. Neither approach is very satisfying. There is still a great need for the development of new concepts and models that simulate and predict the intricate flow dynamics at regional scales in a physically consistent manner considering that most measurements of the vadose-zone system are taken at the local scale.

In hydrology, an attractive approach was offered through the concept of hierarchy of scales, whereby the soil is conceptualized as a hierarchical heterogeneous medium with discrete spatial scales that each may require different effective process-based models. Spatial patterns of soil properties, geomorphology and other landscape properties within and between scales (structural hierarchy) might be different from the organization of the relevant soil hydrological processes (functional hierarchy) across spatial scales. As different flow processes may be dominating at each spatial-scale level, different mathematical relationships may be required to describe the underpinning physical hydrologic process at each scale.

We believe that the vadose zone can also be characterized by this approach. We suggest that combined developments in downscaling of lumped hydrologic models with the upscaling of complex mechanistic flow models are needed to achieve a satisfactory middle ground. Whatever model solution is selected, it must include the key hydrological process(es) that control(s) the flow in the watershed. Inverse-modeling approaches can present solutions where hydrologic parameters become increasingly empirical, with the model calibration providing parameter uncertainty, determined by model structure and measurement errors and uncertainty of boundary conditions. If that recommendation is followed, studies have shown that simple one-dimensional or even zero-dimensional flow models provide adequate solutions to regional-scale problems. The need of model complexity will further depend on the requirements regarding temporal resolution and variability of boundary conditions.

Regional-scale modeling approaches tend to oversimplify the role of the plant with associated root water uptake. Simplicity may be justified, considering the 'homogenizing' power of roots, with root growth and uptake directed towards areas of the root-zone domain where water and nutrients are most plentiful. However, we also conclude that model complexity must increase where climates are more water-limited, requiring higher spatial resolutions in both horizontal and vertical directions at all temporal scales.

As a side-note, we point out that the seemingly limited amount of information on regional-scale vadose-zone processes that is available from twenty years of stochastic modeling is somewhat misleading. Generally, stochastic models have not been developed to address regional-scale flow problems. Their primary purpose has been to explain the spatial variability of water content, soil water tension, and fluxes at the field and sub-field scale. The main application of the stochastic theories has in fact been the prediction of solute transport at the local to field scale, and the prediction of measurable variability of soil water content and suction head at the field scale.

Many opportunities exist in this field. Specifically, there is the challenge to infuse the climate and watershed hydrologic sciences with improved soil physical representation, including that of soil–vegetation–atmosphere transfer processes. But perhaps the most critical challenge is to build more capacity within the vadose-zone hydrology community – soil physicist, climate modeler, watershed modeler and soil scientists alike – to deal with the highly complex physico-mathematical concepts behind the work presented here.

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