Reality and fiction of models and data in soil hydrology

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Abstract

The objective of this paper is to contribute to the ongoing discussion on strengths, weaknesses, opportunities and trends of existing modeling approaches in soil hydrology. In modern hydrology, complexity of models and detail of data grow at increasing pace. The prevailing attitude has been that if a model is comprehensive enough, it should be possible to represent the site uniqueness with a specific set of model parameters. Recent advances in instrumentation have revealed complexity of flow pathways that may be easily perceived but difficult to represent in mathematical terms without making strong simplifying assumptions. This implies that many different model structures could be consistent with available observations. The same appears to be true for parameter sets obtained by calibration for a specific model. The multiplicity of models and the parameter deficit are the emerging issues that present both obstacles and opportunities for hydrologic modeling. We present a comprehensive case study of using integrated data to build a model of groundwater pollution for a watershed, and use this case study to illustrate current opportunities and problems related to quantifying soil variability with remote sensing, geophysical methods and topographic information. The value of pedotransfer functions and publicly available databases is discussed. Mismatch between measurement and modeling scales creates the need to incorporate scale effects in the hydrologic models. Techniques for comprehensive comparative evaluation of models need to be developed and tested. In the absence of unique model selection criteria, it can therefore be best to consider a variety of alternative models based on reasonable alternative hypotheses.

Introduction

In the historical course of studies on the soil-vegetation-atmosphere system, many models and measurement methods have been developed. Having said that truism, one actually opens a Pandora's box of questions. Is there a better or the best model for a specific site or watershed? Should measurement methods correspond to the model selected? How complex does a model have to be? Being far from having answers to these questions, we still see a value in reflecting on them.

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Over the past 40 years there has been (and continues to be) an exponential increase in computing power and the consequent ability to provide numerical solutions to highly non-linear equations for a wide variety of changing initial and boundary conditions. Prior to this development, hydrologists were limited to analytical solutions for very special cases, i.e. Burgers solution and the Dirac delta solution for linearizing the soil hydraulic properties in order to provide analytic solutions to Richards' equation (Smith, Smettem and Broadbridge 2002). Although these solutions still provide insights into checks for numerical models, it appears that numerical modeling has become the 'tool of choice' in hydrological studies. Another important development in setting the direction of hydrological modeling has been the increasing availability and resolution of digital elevation models. This development coincided with the emerging concepts of 'variable source area' hydrology that broke away from the earlier Hortonian notions of runoff dominated entirely by the infiltration-excess process. The advent of geographical information systems and the consequent ability to store, retrieve and rapidly manipulate spatial data gave further impetus to the development and application of spatially distributed deterministic hydrologic models.

Overall, complexity of models and data detail grow at increasing pace. Many researchers are now beginning to question openly whether the reductionist or 'bottomup' approach to model development that pursues ever-greater detail in the understanding of processes and their interactions is the only approach. Instead, can general limits and controls be elucidated that provide an overarching framework for understanding and interpreting system behavior? Can such a framework lead to model structures that are consistent with the available data and inform us about the key processes that need to be incorporated into our models?

We commence this paper be exploring some of these emerging issues in more detail.

Overview

A comprehensive contemplation on the non-uniqueness of modeling in environmental sciences was recently presented by Beven (2000; 2002a). Referring to hydrology, Beven (2000) poses an interesting question: why are predictions so uncertain if all hydrological principles are known? The primary reason is that in practice one deals with specific instances of real sites that are unique in their characteristics, including atmospheric and human impact (Neuman and Wierenga 2003). In the past, the attitude was that if a model is comprehensive enough, it would be possible to represent the site-uniqueness with a specific set of model parameters.

In addition to burgeoning growth in computer models, there has been a major increase in detailed studies which, generally, have revealed a complexity in flow pathways due to heterogeneity at different scales and interactions between geometry of the flow domain and prevailing hydraulic gradients including both 'preferential flow' and 'stagnant zones'. Indeed, some hydrologists now accept that preferential flow is ubiquitous – a situation that soil physicists would have found hard to accept even 40 years ago. Similarly, much of our hydrological modeling effort has been built around the 'variable source area' (VSA) concepts of runoff (Dunne 1978). McDonnell (2003) points out that new field evidence of water source, flowpath and age provides a different picture of runoff generation. There is now recognition that pre-event water can dominate storm runoff (Kirchner 2003), whereby catchments store water for considerable periods of time and then release it promptly during storm events. This

paradox of prompt release of old water within a flashy hydrograph is one example of a process not captured by existing VSA-structured models (McDonnell 2003).

Complexity of flow pathways may be easily perceived but difficult to represent in mathematical terms without making strong simplifying assumptions. This implies that many different model structures could be consistent with available observations. Likewise, it may well be impossible to identify a single correct set of model parameters, especially if one seeks a rational physical basis to the parameters. For example, at the Representative Elementary Volume scale, where macroscopic average parameters are typically used in flow equations (typically, over scales of 1 to 10 m² for macroporous soils), preferential flow is a non-equilibrium process, so the (often unstated) assumption of equilibrium between water content and soil water potential at any given position in the soil does not apply. Ross and Smettem (2000) addressed this problem by introducing a time constant to describe the non-equilibrium between the soil water matric head, and the soil water content during preferential wetting. Other modelers have empirically separated the soil into two (or more) 'domains' that may be independent or interconnected (e.g. Jarvis et al. 1991; Šimůnek et al. 2003) and need to be extensively parameterized.

Even if a reasonable description of the representative elementary volume (REV) scale macrostructure is possible, upscaling remains a major problem. Difficulties include meaningful representation of soil macrostructure in soil mapping and the inherent temporal variability of structure in agricultural soils. Identification of threshold conditions for preferential flow is also problematic. For example, runoff can occur in structured soils when the rainfall intensity is less than the saturated hydraulic conductivity. The reason for this is that runoff can occur between structural features and this may also be compounded by macropore sealing during rainfall (Somaratne and Smettem 1993).

In terms of model choice, Beven (2000) argues that no matter how intensively a site is studied, there is a wide range of models and parameter sets for each model that will yield acceptable simulations. Such multiplicity of models is simply a summed expression of the limitations to current models in representation of flow systems, limitations of measurement techniques with respect to scales of public interest, and limitations in defining initial and boundary conditions. One cannot also exclude the possibility that there still exists a lack of fundamental understanding in fluid and chemical transport processes in the environment, and this precludes building of widely applicable models.

If there is a wide range of models and parameter sets for each model that will yield acceptable simulations, then what can be an approach to model selection? One approach is, in essence, based on scale(s) of interest. Recently, in recognition of (or in response to) the limitations of detailed models, there has been considerable interest in what has been referred to as the 'downward approach' in hydrological modeling. The motivation comes from work such as Klemes (1983), who suggests that calibration-based models suffer from structural arbitrariness and over-parameterization. This theme is echoed by Perrin, Michel and Andreassian (2001), who show that complex models outperform simple ones in calibration mode but fail to do so in verification mode.

The philosophy of the downward approach is that laws at higher levels of scale may express integration of laws at lower scales (Klemes 1983). This has motivated a search for parsimony in model parameterization and structure and a systematic method of model selection that makes trade-offs between model complexity, accuracy and predictive uncertainty (Atkinson, Woods and Sivapalan 2002). Characteristically, the approach starts by postulating very simple models with physically meaningful parameters in order to capture the signature of, say, the annual runoff response of a catchment (Milly 1994). Progressive complexity is added as space and/or temporal scales diminish (Jothityangkoon, Sivapalan and Farmer 2001). In this way, spatial and temporal scales are associated with the complexity scale.

In the related field of plant physiology, a similar dilemma concerning the complexity of models has arisen. Calder (1998) has proposed a limits-on-evaporation concept to guide the development of models of varying complexity for estimating water use of forests in different regions and for predicting differences in water use between forests and shorter crops. Calder (1998) makes the important point that in dry climates, where evaporative systems are limited by supply and where demand greatly exceeds supply, detailed modeling of the meteorological demand in the evaporative equations becomes largely irrelevant. This implies that there will be a shift in model sensitivity between temperate wet and dry climates, with advection dominating in the wet environment and soil-water and physiological processes dominating in the dry climate.

Other approaches to the model selection are based on the availability of input data, on previous experience or on physically meaningful model performance with reasonable scenarios using, i.e., the Generalized Likelihood Uncertainty Estimation (GLUE) methodology (Beven 2002b). However, an impeccable way to select 'the model' is unknown. A variety of formulations exists for any component of soil-vegetation-atmosphere models, and in any specific project a choice is made on the model type and the source and availability of the parameter values. Either the choice has to be justified or outcomes of several models have to be used simultaneously.

To examine general issues of model parameterization and testing, we commence with a short introduction to modeling soil–vegetation–atmosphere processes using Richards' equation and present an example from a study in which subsurface water fluxes and pesticide transport are modeled using integrated datasets in a 20 km² area in order to predict the groundwater quality.

Spatial modeling using integrated datasets: a case study

Model development

To describe water movement in the subsurface, Richards' equation may be written

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \mathbf{K} \nabla (\psi + z) - S \tag{1}$$

where θ (L³ L⁻³) is the volumetric water content, **K** (L T⁻¹) the hydraulic-conductivity tensor, ψ (L) the pressure head, z (L) the elevation head, and S (T⁻¹) a sink term that accounts for water uptake, among other things water uptake by plant roots. The functions $\theta(\psi)$ and **K**(ψ) are highly non-linear, and an approximate solution of Eq. (1) can only be obtained using numerical methods. The TRACE code (Vereecken et al. 1994), which was developed at the Forschungszentrum Jülich, has been used in this work to solve the 3-D Richards' equation numerically.

The soil hydraulic properties are related to other soil properties like soil texture, bulk soil density and organic carbon content. By pedotransfer functions, parameters of the $\theta(\psi)$ and $\mathbf{K}(\psi)$ functions can be estimated from other soil properties (e.g.

Vereecken et al. 1989; 1990). For larger-scale modeling, information is extracted from soil maps to obtain the spatial distribution of hydraulic soil properties.

The root water-uptake sink term, S(z,t), is a function of depth which is defined by the root density and the potential transpiration. When plants are not subjected to stress, the root uptake is at its potential maximum: $S(z,t) = S_p(z,t)$, where $S_p(z,t)$ is the potential root water uptake. The integral of S(z,t) with depth corresponds with the potential transpiration T_p (L T-1) by the plant cover :

$$T_p(t) = \int_0^{L_r} S(z,t) dz$$
⁽²⁾

where L_r (L) is the rooting depth. The potential transpiration is a boundary condition that is estimated from meteorological and plant-cover parameters (see below). When the soil is too wet or too dry, plants are under stress and roots cannot take up sufficient water. The reduction of root water uptake due to stress is modeled using a stress factor $\alpha(\psi)$ (-) that reduces the sink term with respect to the potential sink term:

$$S(z,t) = \alpha(\psi) S_p(z,t) \tag{3}$$

The stress factor α depends on the matric head and the plant (Feddes, Kowalik and Zaradny 1978).

In order to solve flow equation, the boundary conditions must be defined. We focus on the boundary conditions at the soil surface, which are relevant for remote sensing: the water that infiltrates in the soil I (L T-1), that evaporates from the soil surface, E_a (L T-1), and that is taken up by the plant roots and transpired by the crop, T_a (L T⁻¹).

Based on an energy balance at the soil surface, the reference evapotranspiration, ET_0 (L), can be calculated from meteorological parameters using the Penman/Monteith equation (Monteith 1975; Allen et al. 1998). ET0 corresponds to the evapotranspiration of a well-watered grass surface. The potential evapotranspiration, ETp (L) of a cropped or bare soil surface is calculated from ET0 using the dimensionless Kc factor (Doorenbos and Pruitt 1977), which depends on the plant, plant-cover development stage and climatic region:

$$ET_{p}(t) = K_{c}(t) ET_{0}(t)$$
(4)

The potential evapotranspiration is split up into the potential evaporation from the soil surface, E_p , and transpiration from the crop using an empirical model that is controlled by the leaf-area index LAI (-):

$$E_p(t) = ET_p(t)e^{(-0.6 \text{ LAI})}$$
 (5)

Then the potential transpiration can be obtained from the difference between potential evapotranspiration and potential evaporation.

The evaporation and transpiration rates obtained until now are potential evaporation rates when both the soil and the plant can supply the atmospheric demand. Under water-stress conditions, plant roots cannot take up enough water and the transpiration is reduced according to Eq. (3). When plants suffer from water stress,

hydraulic soil properties influence plant transpiration rates through the stress factor $\alpha(\psi)$. Changes of the stress factor with water loss from the soil profile are controlled by soil hydraulic properties.

Due to evaporation from the soil surface, the upper soil layer dries out and the hydraulic conductivity of the surface layer drops. To guarantee upward water flow to an evaporating soil surface, the matric potential at the soil surface must drop. It is assumed that the potential at the soil surface cannot drop below a critical threshold value. When this threshold is reached, the potential at the surface remains constant so that the evaporation rate decreases with time. The reduction of the potential evaporation rate when the soil dries out is determined by the hydraulic soil properties and can be predicted using the Richards' equation when hydraulic soil properties are known (Figure 1).



Figure 1. Evaporation from a bare loamy soil surface predicted by the Richards equation for a potential evaporation of 0.3 cm d^{-1}

Since surface boundary conditions and internal sinks in a water flow model are to a major extent controlled by plants, a water flow model should be coupled to a crop growth model. Therefore, for cropping systems, the simple crop growth model SUCROS (Spitters, Van Keulen and Van Kraalingen 1989), which calculates drymatter accumulation of a crop as a function of irradiation, temperature and crop characteristics, was coupled to the soil/groundwater flow model TRACE. In Figure 2, the effect of the crop type on the matric head in the soil profile as simulated by the coupled TRACE/SUCROS model is shown (see Color pages elsewhere in this book).

Model application

The TRACE/SUCROS model is applied in the PEGASE project to predict groundwater quality in a 20-km² area around the Forschungszentrum Jülich (Figure 3, see Color pages elsewhere in this book). In a first step, a 3-D hydrogeological model is built using the soil map and geological data (Figure 4, see Color pages elsewhere in this book). From the soil map, four characteristic soil profiles with typical soil layers were identified. Using a pedotransfer function, the hydraulic functions were determined for the different soil layers. Geological information was used to determine the base of the unconfined aquifer. Since the modeled area was not hydrologically confined at the lateral boundaries, groundwater-table depths at the boundaries were interpolated from piezometers and were used as Dirichlet boundary conditions. Land

use was derived from statistical information. Because the parcel size was smaller than the size of the used computation grid (200 x 200 m) and since no data were available on the land use in the different parcels for the considered simulation period, the land use of the non-forested and unsealed surfaces was attributed randomly to the grid cells and conforms to the land-use statistics (Figure 5, see Color pages elsewhere in this book). The soil surface boundary conditions: precipitation and potential evapotranspiration are derived from meteorological data that were recorded in the meteorological station of the Forschungszentrum Jülich. ET_0 was calculated using the Penman/Monteith approach according to the revised FAO methodology (Allen et al. 1998).

The matric potential at the soil surface, the actual evaporation and transpiration predicted by the TRACE model are shown in Figure 6 for two exemplary days (see Color pages elsewhere in this book). Since the model considers three-dimensional flow, spatially variable soil properties and land use, the spatial structure and heterogeneity of the flow processes at the soil–atmosphere surface are represented by the model. Furthermore, the model also represents the dynamics of water flow in the soil in response to the dynamics of the boundary conditions. However, the predicted fluxes and state variables are not validated against measurements. The example of this case study illustrates the typical choices that have to be made in any concerted effort to integrate existing data and existing models to address practical questions of public interest. We now turn our attention to the question of the uncertainty behind some of those choices and the potential to mitigate this uncertainty.

Quantifying spatial variability of soil parameters using geophysical, remote-sensing and topographic data

The example case study raises the question of whether the input datasets adequately capture the inherent spatial variability in both the horizontal and vertical co-ordinates. This question arises in almost every application where map information is utilized to define the spatial pattern of input parameters but formal recognition of this source of error is comparatively recent (Heuvelink and Goodchild 1998).

Over the last few decades, the heterogeneity of soil properties has been subject of extensive research. The spatial variability of hydraulic properties has received especially large interest since the pioneering work of Nielsen, Biggar and Erh (1973). Extensive field experiments have been conducted both in the vadose zone and aquifer systems (Butters and Jury 1989; Ellsworth et al. 1991; Gelhar, Welty and Rehfeldt 1992). The theoretical framework developed to understand the relationship between soil properties and flow and transport is based on a stochastic description assuming that soil properties are space random variables. In order to obtain analytical expressions and to interpret field data, simplifying assumptions such as second-order stationarity have been introduced (Russo, Dagan and Bresler 1993; Dagan 1989; Russo and Dagan 1991; Neuman 1997). For simplified linearized cases, approximate closed-form expressions for effective parameters have been derived (e.g. renormalization methods for hydraulic conductivity K, effective dispersivity). In soil hydrology, due to the strong non-linearity and the limited spatial extent of the system, these approximate expressions may be unreliable and only numerical analyses can be made at present.

Traditional soil and landscape mapping defines 'units' and performs a taxonomic partition with distinct boundaries. The resulting classification usually only provides a rudimentary guide to the soil hydraulic properties and gives little insight into the

spatial structure within the units. To overcome this problem, geostatistical methods such as variogram analysis and kriging techniques are now routinely used to identify the spatial structure and to derive continuous fields from point measurements. However, field measurement costs can be high because large numbers of samples are required to characterize adequately the semi-variogram which is the main source of geostatistical inference.

Despite our improved capability to provide continuous surface mapping of relevant soil attributes, the major limitation is still our inability to verify experimentally the validity of our estimates of effective parameters at scales larger than a soil column. Non-invasive methods including tomographic geophysical techniques and remote sensing offer an enormous potential to tackle some of the above issues (Vereecken, Yaramanci and Kemna 2002).

Recent advances in mapping the distribution of relevant soil properties include the direct generation of continuous surfaces from a variety of remote-sensing and geophysical techniques.

Kemna et al. (2002) used electrical-resistivity tomography (ERT) to monitor bromide concentration changes in an ERT plane during a tracer test in an unconfined aquifer. The concentration images were interpreted using equivalent transport models. They used a 3-D equivalent convection-dispersion model to quantify the longitudinal and lateral spreading of the solute plume. The spreading process and the observed heterogeneity were characterized using a 1-dimensional stochastic stream-tube model. Zhou, Shimada and Sato (2001) proposed a 3-D ERT method for monitoring spatial and temporal variations of soil water content in the field. Moisture contents were derived from 3-D distributions of soil resistivity and Archie's law which was calibrated on field data. They compared the obtained water contents with measured values obtained from heat-probe-type soil moisture sensors. Although considerable differences were found between calculated and measured moisture contents, a linear relation between both existed, which enabled the investigation of temporal variations. Ground-penetrating radar (GPR) is being used to monitor changes in soil moisture content. Huisman (2002) used GPR to map the soil water content at the field scale in which a spatial structure in soil water content was created by irrigation. He found that GPR is well suited to capture the spatial water-content variation as expressed by the variogram. Lambot (2003) used a contact-free GPR system to predict the moisture retention characteristic of a disturbed sandy soil in a laboratory experiment. This method shows considerable potential for mapping soil water content under real field conditions.

Remote-sensing techniques show large potential in evaluating spatial variability of SVAT components. Taylor et al. (2002) used airborne gamma-radiometric sensing to estimate the clay content of surface soils across a catchment. Active microwaveradar methods are presently used to map continuously spatial and temporal changes of moisture content (Burke et al. 1997; Mancini, Hoeben and Troch 1999; Ulaby, Dubois and Van Zyl 1996). The passive microwave remote sensing can also be used to determine the water content of the soil surface (reviews by Engman and Chauhan 1995; Njoku and Entekhabi 1996; Schmugge 1998; Wigneron et al. 2003). Overviews of the use of remotely sensed data for hydrological modeling are given by, e.g., Droogers and Kite (2002) and Schmugge et al. (2002). Reflectance spectra of sunlight can be used to characterize land cover/land use (Hall, Townshend and Engman 1995), which is an important input parameter for hydrological models. Furthermore, the LAI can be derived from reflectance spectra using the NDVI index. The LAI can be predicted by a crop growth model and plays a crucial role by splitting up the evapotranspiration in crop transpiration and soil evaporation. Therefore, the remotely sensed LAI can be used to validate or even calibrate crop growth models or to define the upper boundary fluxes better, which improves the model performance of soil–plant–atmosphere models (e.g. Andersen et al. 2002).

The thermal microwave emission or brightness temperature, T_B, in the 1-5 GHz frequency range is considered to be the most useful for determining surface soil moisture. Besides soil moisture, the emitted radiation depends as well on the surface roughness, the depth profiles of the soil water content and soil temperature (e.g. Schneeberger, Stamm and Flühler in press), and the vegetation (e.g. Ferrazzoli, Guerriero and Wigneron 2002). Therefore, microwave remote-sensing data must be 'assimilated' in radiation transfer models that model the effect of soil roughness, water-content profiles and vegetation on the emitted radiation, and soil-vegetationatmosphere models (SVAT), which model water and energy fluxes (e.g. Wigneron et al. 1999; 2002). If multi-angular and dual-polarization passive microwave measurements are acquired, effects of soil and vegetation on the microwave signature can be discriminated and the outcomes of this assimilation process are root-zone water contents and parameters that describe the crop development (Wigneron et al. 2002). Besides microwave emission data, IR surface brightness temperatures and short-wave reflection spectra can also be assimilated in SVATs to calculate sensible and latent heat fluxes (e.g. Bastiaanssen et al. 1998; 2002; Olioso et al. 1999a; 1999b; Mauser and Schädlich 1998; Boulet et al. 2000; Van der Keur et al. 2001). Assimilation schemes were in most cases developed and tested based on measurements in agricultural field plots, cropped or bare. How the microwave emission from a forest can be related to the forest soil water content is the subject of current research projects. The SVATs that are commonly used in assimilation schemes are based on a capacity model to describe water and energy fluxes in the soil. These models currently have limited capability to describe the spatial dependence of water flow and root water uptake in soils.

Based on monitored soil moisture data, hydraulic soil parameters and parameters of a root water-uptake model can be estimated using inverse modeling. Musters and Bouten (1999) and Hupet and Vanclooster (2002) derived root water-uptake parameters (root depth and root density) using a 1-D flow model and found that the root uptake parameters vary considerably in space. Two-dimensional soil moisture patterns were considered by Vrugt, Hopmans and Šimůnek (2001) in the calibration of a two-dimensional root water-uptake model. However, Hupet and Vanclooster (2002) remarked that root water-uptake parameters are difficult to estimate when hydraulic soil parameters are uncertain. Musters and Bouten (2000) also found that root water uptake was difficult to estimate based on soil water dynamics alone. Additional measurements of root densities, sap flow and actual plant transpiration would help to confine root parameters within physically reasonable bounds. Alternatively, a comparison of the behavior of the system with and without root activity may be used to discriminate root activity and its spatial heterogeneity from the heterogeneity of soil hydraulic properties. However, in winter, when roots are not active and the evaporation is low, soils remain relatively wet and the dynamics of the soil water content is small. Tracer experiments can be used to identify zones of high and low leaching velocity, which are related to zones of differing hydraulic conductivity.

The potential of remotely-sensed parameters, soil moisture and actual evapotranspiration in combination with inverse modeling of unsaturated flow has first been discussed by Feddes et al. (1993). Soil hydraulic properties were estimated from remotely-sensed surface soil moisture content (Burke et al. 1997; Mattikalli et al.

1998; Chang and Islam 2000). Given the control of hydraulic soil properties on the reduction of both potential evaporation and transpiration, soil hydraulic properties may be derived from actual evapotranspiration data obtained from remotely-sensed thermal infrared signals (e.g. Jhorar et al. 2002). Chanzy, Bruckler and Perrier (1995) suggested combining both thermal infrared and microwave remote sensing to confine the estimation of soil parameters. A combination of multispectral remote-sensing data, including areal subsurface information has a great potential to improve the parameterization of subsurface water flow models. Especially the effect of heterogeneity on flow and transport processes can be considered when the spatial information of subsurface soil water contents is included. For instance, Schneeberger, Stamm and Flühler (in press) illustrated that the dynamics of the soil surface moisture content, which can be derived from microwave radiometers, was equally well described by a unimodal model, which does not account for preferential flow, and by a preferential-flow model. This implies that surface water-content dynamics does not contain sufficient information for discrimination between these two models. It is therefore assumed that inclusion of subsurface information about the soil watercontent dynamics may better constrain the model identification.

Our case-study model does not directly include remotely-sensed parameters. However, remotely-sensed parameters like IR surface-brightness temperature, LAI derived from NDVI, short-wave reflection or albedo, can be used as direct input in an expanded Soil–Vegetation– Atmosphere–Transfer models (SVAT) to calculate latent and sensible heat fluxes (e.g. Olioso et al. 1999a; 1999b; Mauser and Schädlich 1998; Boulet et al. 2000; van der Keur et al. 2001). Additional input parameters are the resistances for heat and vapor transfer in the atmospheric surface boundary layer and meteorological parameters. Sensible heat-transfer resistances are only determined by meteorological parameters whereas resistances for vapor transport are linked to the soil water content. Therefore the coupling between soil moisture status and actual evapotranspiration requires the use of SVAT models to interpret remotely-sensed variables. A further advantage of a SVAT is that fluxes can be predicted at times for which no remote-sensing data are available. Since remotely-sensed data are instantaneous data of variables with a high temporal dynamic, a physically based model may be useful to predict the systems behavior between observation times.

However, a disadvantage of SVATs is the larger number of parameters that is needed to run the model. Especially the spatial variability of meteorological parameters like air temperature, air humidity and wind-speed profiles make a parameterization of SVAT cumbersome. This may be overcome using the SEBAL procedure proposed by Bastiaanssen et al. (1998). In this procedure, area effective resistances for sensible heat transfer are derived from the relation between surface brightness temperature and albedo for regions where the latent heat flux can be neglected. Surface-air temperature differences are derived from surface temperatures. Latent heat fluxes are obtained by closing the surface energy balance. In order to extrapolate the estimated evaporation rates in time, it is assumed that the evaporative fraction, i.e. the ratio of the energy used for evapotranspiration to the total net radiation, remains constant in time (e.g. Bastiaanssen, Ahmad and Chemin 2002). This assumption is only valid for moderate temporal variations in soil moisture content. When the soil dries out, actual evapotranspiration will be less than the potential evapotranspiration so that the fraction of the sensible heat flux will increase. Since the change in actual evapotranspiration with time is controlled by soil hydraulic properties, a soil-vegetation-atmosphere model can be combined with remotelysensed surface parameters to evaluate evapotranspiration rates in time.

Finally, topographic spatially dense data can be related to soil properties. Separating hill slopes into distinct sections, showed that soil properties within a section vary much less than between sections, so that distinct values of soil properties can be assigned to each section (Lark 1999). Regression equations could be developed to correlate soil properties in the sections (Brubaker et al. 1994). Geomorphometry was proposed as a data source to predict soil properties (Moore et al. 1993; McKenzie and Austin 1993). Terrain attributes, i.e. mathematical characteristics of the land surface shape, such as slope, profile, plan and tangential curvatures, and aspect, could be used for statistical correlation with soil properties (Odeh, Chittleborough and McBratney 1991). Such relationships have a general validity (Rawls and Pachepsky 2002); they become more accurate when site-specific soil-survey information is available (Pachepsky, Timlin and Rawls 2001).

Using pedotransfer functions

Because of the difficulties and high labor costs associated with measuring soil hydraulic properties, there is often a need to resort to estimating modeling-related soil parameters from other readily available data. Modeling in a wide range of scales, from general circulation models to the fine-scale precision-agriculture decision support, experiences the need for such estimations. Statistical regression equations expressing relationships between soil properties were proposed to be called '*transfer functions*' (Bouma and Van Lanen 1986) and later '*pedotransfer functions*' (PTFs) (Bouma 1989). Estimating soil hydraulic properties dominates the research field, although soil chemical and biological parameters are also being estimated. Several reviews on PTF development and use have been published (e.g. Rawls, Gish and Brakensiek 1991; Van Genuchten and Leij 1992; Pachepsky, Rawls and Timlin 1999; Wösten, Pachepsky and Rawls 2001). Large databases, such as UNSODA (Leij et al. 1996), HYPRES (Lilly 1997; Wösten et al. 1999), WISE (Batjes 1996) and NRCS pedon database (USDA Natural Resources Conservation Service 1997) are suitable for PTF development. Our case study heavily relies on the use of PTFs.

Evaluation of PTFs is an essential element of their development and use. Pachepsky, Rawls and Timlin (1999) have broadly defined the accuracy of a PTF as a correspondence between measured and estimated data for the data set *from which a PTF has been developed*. The reliability of PTF was assessed in terms of the correspondence between measured and estimated data for the data set(s) *other than the one used to develop a PTF*. Finally, the utility of PTF in modeling was viewed as a correspondence between *measured and simulated environmental variables*. The concept of the PTF uncertainty (Schaap and Leij 1998) encompasses the ambiguity in PTF predictions and parameters caused by the input data variability and uneven representation of soils with different properties in the database.

The apparent ease of developing PTFs by applying statistical regressions should not overshadow several basic questions about PTFs that need to be answered by hydrologists and soil scientists. Why do PTFs exist? How do we assess the accuracy and reliability of PTFs? Will a grouping of soils by some criterion enhance both the accuracy and the reliability of PTFs? Is there a limit of accuracy and reliability of PTFs and on what does this limit depend? What are the most appropriate techniques to evaluate a PTF? What input variables are more preferable or necessary to be included in a PTF? An inventory of existing PTFs (Pachepsky and Rawls in press) has been assembled to begin answering these questions in a systematic fashion. Estimating solute transport parameters remains a weak point of the PTF development. Although a progress has been made in estimating solute dispersivity for small soil cores (Griffioen, Barry and Parlange 1998; Oliver and Smettem 2003), no methodology exists for such estimates at the pedon scale and at coarser scales. A notable attempt was recently made by Nimmo (2002), who collected published results of field experiments on conservative tracer transport in soils and unsuccessfully tried to relate the solute travel time to soil properties. Results of this work in Figure 7 show that the only parameter suitable to predict the presence or absence of fast preferential flow is the type of water supply at the soil surface. Ponded infiltration inevitably causes a fast breakthrough whereas an intermittent water supply does not. A likely reason for this failure is the fact that soil transport properties are largely dependent on soil structure. Quantitative information on soil structural parameters that could be used in PTFs is not available.



Figure 7. Maximum tracer velocity in 34 documented field experiments (from Nimmo 2002)

The PTF research is a fast-developing field driven by the high demand in hydraulic and related parameters existing in environmental modeling. Recently the volume of PTF applications increased due to development of GIS-based regional modeling. Relying on PTFs presumes a level of the PTF accuracy and reliability sufficient to obtain acceptable uncertainty in results of modeling. As many PTFs have been developed and are under development, the users face the problem of selection of PTF. Discussions of reasoning and consequences of such selection are currently underrepresented in literature. One criterion of PTF selection is its reliability. Although no general conclusion could be derived from the review of the PTF reliability studies, some general observations can be made. PTFs developed from regional databases give good results in regions with similar soil and landscape history. Water-retention PTFs developed in Belgium (Vereecken et al. 1989) were the most accurate as compared with 13 others for the data base of Northern Germany (Tietje and Tapkenhinrichs 1993). Water-retention PTFs developed for the Hungarian Plain (Pachepsky et al. 1982) were applicable for the Caucasian Piedmont Plain. PTFs developed in Australia were more accurate for the Mississippi Delta as compared with other regional PTFs (Timlin et al. 1996). It remains to be seen whether this

observation holds for other cases, and which soil and landscape features have to be similar in two regions to assure the mutual reliability of the PTFs developed.

The database size and measurement methods are among important factors affecting PTF accuracy and reliability. The number of samples has to be large enough to develop both accurate and reliable PTF (Pachepsky, Rawls and Timlin 1999). PTFs developed from the USA database by Rawls and Brakensiek (1985) are more robust than PTFs developed from regional databases. When the reliability of the all-USA PTFs has been compared with the accuracy of several other regional databases, and the PTFs were ranked by their reliability, the all-USA PTFs usually had one of the highest rankings (Tietje and Tapkenhinrichs 1993; Kern 1995; Timlin et al. 1996). Collection and analysis of data suitable for the PTF development is an important step in providing essential parameters for the environmental and agricultural modeling.

There may exist a limit in accuracy and reliability of PTFs caused by temporal variation of soil properties related to the changes in vegetation and soil management. Incorporation of organic-matter content (Felton and Ali 1992), soil erosion (Fahnestock, Lal and Hall 1995), tillage practice (Azooz, Arshad and Franzluebbers 1996) can cause variations in hydraulic properties that are comparable with variations within regional data bases. Pachepsky, Mironenko and Scherbakov (1992) have reported 20% changes in water retention at -1 kPa and 5% changes in water retention at -30 kPa in soils under wheat during the growing season in three different climatic zones. The amount of published data on temporal variations of soil hydraulic properties remains small. A temporal component may be required in PTFs to improve their reliability.

A relatively new promising direction in PTF development is the use of spatially dense physical information related to the soil cover. Smettem et al. (in press) presented an example of using airborne gamma-radiometric sensing to estimate the clay content of surface soils and using a simple PTF (Smettem et al. 1999) to convert this information into a spatial representation of the slope of the Brooks and Corey water-retention function. Another idea is to use geophysical and/or topographic information as a direct input in PTFs. Ground-penetrating radar, penetrometers, electric-conductivity meters, etc., all provide spatial coverage that shows a potential to be included in PTFs (an example for the penetration resistance as a PTF input can be found in Pachepsky et al. (1998)). Romano and Palladino (2002) used terrain attributes to recalibrate a PTF, and soil water retention exhibited strong dependence on terrain attributes in the study of Pachepsky, Timlin and Rawls (2001).

The reliability of a PTF is not directly related to its utility. The latter is affected by the sensitivity of the model to PTF predictions, and also by the uncertainty in other model inputs (Leenhardt 1995). When the PTF uncertainty is factored in a modeling effort, the variation in predictions of different PTFs has to be considered along with uncertainty of individual PTF predictions. The procedures to do that have yet to be developed. Using weighted-average predictions of several different PTFs instead of predictions of a single PTF may be a viable option for obtaining an estimate of the hydraulic property and to guess-estimate the uncertainty of this estimate. As the hydrological model calibration technology develops, more opportunities appear to compare calibrated and PTF-estimated hydraulic properties (Wang et al. 2003) and also to use PTF predictions as initial estimates for model calibration (Jacques et al. 2002).

An emerging challenge is the upscaling of PTF estimates, i.e. determination of equivalent hydraulic parameters for large spatial units using PTF estimates and information on their variations in space. Scale dependencies in soil hydraulic properties have become recognized (Bork and Diekkrüger 1990; Feddes et al. 1993). Currently these dependencies are ignored and may limit PTF reliability. Scale dependencies of hydraulic properties need to be included in PTFs. As the scale becomes coarser, hydrologic models change and so do the hydrologic parameters. Soil field capacity presents an example of such parameter that cannot be predicted as water retention at some fixed value of soil matric potential. PTF predictions of waterretention curves have to be supplemented with a scale correction to become utilizable at coarser scales.

Quantifying scale effects

It seems that all parameters of the models in hydrology are scale-dependent, and yet very little is known about those dependencies. An example of the scale effect on the solute dispersivity in soils is shown in Figure 8. One plausible explanation of the increase in dispersivity with distance or with travel time is the lateral mixing developing in time (Flühler, Durner and Flury 1996).

When the transport time is shorter than the mixing time, the dispersivity increases with time or travel distance. A constant dispersivity is reached when the travel time is much longer than the mixing time. The mixing time is defined by soil structural features that either enhance lateral mixing, such as soil layering, or prevent mixing and induce preferential flow such as large interconnected interaggregate pores, water repellent layers etc. (Vanderborght et al. 2001). The occurrence of these morphological features is not related to soil texture so that soils with similar soil texture may have completely different dispersivity and scale dependence of dispersivity. However, quantitative information of soil morphology is used in soil classification. As a consequence, inclusion of categorical soil-type information in PTFs may improve the estimation of transport parameters. Some data on dependencies of hydraulic conductivity with the core size is well pronounced.



Figure 8. Observed dependencies of the solute dispersivity on distance in soils (after Pachepsky, Benson and Rawls 2000). Different symbols show data of different



Figure 9. Examples of scale dependence in soil saturated hydraulic conductivity; \circ -loamy sand, Ap horizon, \Box - loamy sand, A₂ horizon, Δ - sandy clay loam, B₁t horizon, Λ - clay loam, B₁t horizon (after Pachepsky and Rawls 2003)



Figure 10. Relationship between field and laboratory water contents at the same soil-water matric potential; \bigcirc - samples with sand content more than 50%, \bigcirc - samples with sand content less than 50%; lines show the quadratic regression (____) with 95% prediction interval (____). Data from the UNSODA database (Leij et al. 1996)

Scale dependence of parameters affects the performance of methods of parameter determination. Comparison of field and laboratory water-retention data is shown in Figure 10. At the same matric potentials, field water contents of fine-textured soils are markedly less than the laboratory values. Comparison of unsaturated hydraulic conductivity obtained with the tensiometer-influx method and with profile drainage method is shown in Figure 11. The difference in hydraulic conductivity is more than one order of magnitude.

Scale dependencies in hydrologic parameters have led to a general rule of selecting the size of grid cells corresponding to the scale at which the measurements were made (Neuman and Wierenga 2003). However, this becomes impractical as the grid size increases in large-scale modeling. No scale dependence of hydraulic parameters has been introduced in our case study.

In soil physics, the description of water flow in soils is based on the gradients in soil water potential, which in soils is predominantly determined by capillary and gravitational forces. This concept has been applied and thoroughly tested at the scale of a soil column. The upper scale limit is determined by the measurement scales of water fluxes and water contents in soils. Predictions of water fluxes in soils at larger scales are, therefore, an extrapolation based on the reductionist assumption that the hydraulic properties of the soil, which are experimentally determined on a local scale, may represent the properties of the system at a larger scale. However, many studies have revealed that soil properties vary considerably in space. Therefore, upscaling procedures need to derive effective parameters that describe the system's behavior at a scale that is relevant for the watershed management. Therefore, if effective parameters cannot be adequately specified, a change of scale may dictate changing models and parameters. For example, capacity-based rather than Darcy's-law-based models are often used at coarse spatial and temporal scales. Difficulties arise when parameters of coarser scales and finer scales have to be related. Several attempts were



Figure 11. Unsaturated hydraulic conductivity of soil measured at two different scales; • - drainage in soil profile, O - in proximity of the tensiometer cup (after Timlin and Pachepsky 1998); (a) and (b) show data in two field locations

made to relate soil water-retention curves measured on small cores to field capacity measured as water content measured after two days of drainage following a ponded infiltration event. Some results of relating field capacity to water contents measured at specific soil water matric potential are shown in Figure 12. No single value of the matric potential appears to be suited to estimate field capacity from soil water-retention curves.



Figure 12. Soil field capacity and soil water retention at fixed matric potentials; CS - coarse sand, MS - medium sand, FS - fine sand, LFS - loamy fine sand at -5 and -10 kPa sol matric potentials (data from Rivers and Shipp 1978); \circ and \Box - topsoil and subsoil of varying texture at -33kPa (data from Haise, Haas and Jensen 1955)

Soil physicists have approached the upscaling problem in two ways as shown in Figure 13. In the first (Vogel and Roth 2003) approach, the smaller-scale structure and heterogeneity of the properties at a smaller scale are explicitly considered in a small-scale model that predicts processes considering small-scale spatial variability and its spatial structure. Essentially, it is proposed to generate parameters of a coarser scale by the Monte Carlo simulation of a coarse-scale representative elementary volume (REV) as composed of many small representative elementary volumes at a finer scale (Faybishenko et al. 2003). The predicted processes and variables at the smaller scale



Figure 13. Schematic representation of the upscaling of processes in heterogeneous media, effective parameters and inverse parameter estimation

finer scale (i.e., macropores), are represented in the 'composite' coarse-scale REV. Deriving soil profile parameters from the parameters of soil horizons (Jhorar et al. 2004; Zhu and Mohanty 2003) presents another example of work along those lines. In the second approach, the behavior of the system is observed at the larger scale and effective parameters are derived using inverse modeling. Effective parameters are parameters that lump the system's subscale heterogeneity and describe its behavior at a larger scale (e.g. Grayson and Blöschl 2001). Here, remote sensing has a potential to determine area-wide states of the system (e.g. surface soil-moisture content, leaf-area index) and surface fluxes (Feddes et al. 1993).

Using publicly available data

Large databases have recently become available containing data that can either serve directly as model inputs, as climatic data, or be used in pedotransfer functions to estimate soil hydraulic properties. Several publicly available datasets have been used in our case study. There is not enough experience with such databases to compare the relative value of such data with site-specific information. The first examples of such comparisons have brought mixed results. The HYPRES database served as input in a study by Nemes, Schaap and Wösten (2003), in which the authors used national-, continental- and intercontinental-scale data collections to derive PTFs for the estimation of soil water retention, using artificial neural networks. The goal of the study was to identify the relevance of PTF from international data collections for individual countries that contributed to the database or for countries located in areas with comparable climatic conditions. The same methodology and the same sets of predictors were used while the source database was changed. Soil-moisture time series of seven soils were simulated, using water-retention characteristics estimated by the different PTFs. Small differences were found between simulations based on different-scale data collections. Moreover, PTF estimates resulted in simulations that were only marginally worse than simulations with estimates using laboratorymeasured water retention. Wang et al. (2003) simulated water flow and bromide transport in soils and sediments of a desert research site for a 100-day period. They found that publicly available information could not be satisfactorily translated in model transport parameters. In situ measured hydraulic properties also did not provide good parameters for the transport simulations. A calibration of the models to the monitoring data was needed for successful simulations. The authors concluded that the value of publicly available data consists in providing estimates of the stratigraphy, *a priori* estimates of input-parameter distributions, and initial estimates of parameters for inverse modeling. Similar conclusions were reached by Jacques et al. (2002), who simulated a full year of water and chloride transport in loamy soil in Belgium. We note that the two latter research groups used large international or all-USA databases, and did not make an attempt to use smaller regional subsets to estimate hydraulic properties like Nemes, Schaap and Wösten (2003) did.

Evaluating performance, predictive ability and prediction uncertainty

The root-mean-square model error or the determination coefficients are often used as measures of model performance. These measures may suffice for investigating the performance of a single model against a single data set, yet fail to recognize that a model should not be more accurate than the data. The χ^2 test, the goodness-of-fit test (Whitmore 1991) or the normalized root-mean square (Loague and Green 1991) value would account for that, but things become more complex if a choice of model is presented and/or datasets on different variables are available to evaluate model performance.

Apart from conceptual differences, a major difference between models is in the number of parameters that are free to be adjusted. This leads to a recognition of the need for information-based measures of model performance in which the root-mean-square error is corrected to reflect the number of adjustable parameters (Akaike 1977). These criteria leave aside the issue of data quality and availability. Kashyap (1982) has suggested the criterion that combines measures of complexity, data quality and goodness-of-fit.

Soil-vegetation-atmosphere models serve as both explanatory and predictive tools. Suitable forecasts can hardly be expected from a model that fits observations well but produces a wide range of predictions given reasonable variations of parameters and forcing variables. The Monte Carlo simulations present a viable way of predicting uncertainty estimations, but Latin Hypercube (LH) sampling is more efficient. In contrast to the Monte Carlo method, which is a random-sampling simulation, LH sampling is a numerical simulation of a distributed parameter. The probability-density function is divided into M equal areas and the centroid of each area is used to determine a sample value. The major advantage is that a similar level of accuracy to the Monte Carlo method can be achieved with an order of magnitude fewer samples. With both methods, a measure of uncertainty is generated after multiple model runs. The LHS method was used by Vachaud and Chen (2002) to investigate the sensitivity of computed water and nitrate leaching to within-textureclass variability of transport parameters using the ANSWERS model. For their simulations, within-class variability had no effect in long-term simulations for soils with saturated hydraulic conductivity greater than 100 mm/d. Corresponding soil classes could be identified by a single set of parameters (the barycentre (centroid) of the class) with a small loss of information compared to a very important gain in terms of input-data requirements and simulation time. This has profound consequences for large-scale distributed models, since it reduces considerably the number of measurements necessary to describe the soil; in particular there may be no need, in this range, to account for spatial variability of textural parameters within a class. With saturated hydraulic conductivity of 100 mm/d, however, within-class variability of transport parameters was a much more important source of uncertainty.

Providing probability distributions for simulations is not a trivial matter. In ecological modeling, input values and their ranges are often taken from personal beliefs or from literature. Neuman and Wierenga (2003) indicate that such estimates are rarely realistic. Adjustable, or calibrated, model parameters also have to be reported and used as random values. One way to obtain their probability distributions is to do multiple calibrations of the model within the Monte Carlo framework by using random input parameters with known or estimated distributions. Correlations between parameters, both input and adjustable, are of utmost importance in Monte Carlo assessment of the predicted uncertainty. Rechov (1994) gives examples of the decrease in uncertainty from 300% to 30% after such correlations have been accounted for. Clearly, there is much work to be done in this area, with the goal of achieving parsimony in the model input parameters and data requirements.

Quo vadis?

The multiplicity of models, the parameter deficit, and the uncertainty of predictions are not new problems in hydrologic modeling. The need to address these problems directly is a relatively new issue.

Soil hydrology gives a representative example of model multiplicity. Onedimensional flow and transport in soils can be modeled using Richards' equation or by simpler mass-balance approximations. For two- and three-dimensional flow problems, Richards' equation still applies but is often forsaken in favor of more approximate models that require less computing time and input data. Preferential flow is accounted for with separate submodels or ignored. Parameters of models exist in many functional forms, more than ten equations for water content being but one example. A similar multiplicity can be found in watershed hydrology.

In absence of unique selection criteria, it can therefore be best to consider a variety of models (National Research Council 2001) based on reasonable alternative hypotheses. More examples of working with multiple models can be expected, and comparison of models will undoubtedly enhance the understanding of the validity of hypotheses behind them. The need to balance complexity and robustness of models begins to materialize in developments of the model abstraction technology that seeks to reduce the complexity of a simulation model while maintaining the validity of the simulation results with respect to the question that the simulation is being used to address.

In the absence of reliable methods to measure directly fluxes in the vadose zone, parameter deficit will remain a substantial difficulty. Pedotransfer functions present a viable way to obtain first-guess estimates that may be sufficient for many applications, or can be used in calibrations if data are available. Currently examples of evaluating PTFs as model inputs are scarce. Accumulation of such examples is a precondition to a progress in site-specific PTF selection.

The emerging transdisciplinary research field of hydropedology attracts a substantial attention because of its promise to bridging pedology and hydrology. Such interaction is desirable because the wealth of pedological information can advance understanding and predicting water distribution in soils and landscapes, whereas advances of hydrology can enrich interpretation of spatial distributions of soil properties. One possible approach to the hydropedology agenda is to consider it from the standpoint of relations between structure and function. Hydrologic functioning of soils and landscapes is defined by the structure of pathways and voids available for water to move and to be stored. In turn, structure of soil pore space and hydrological units is substantially affected by the functioning of soils and landscapes in hydrological cycles. This relationship has a multitude of feedbacks that modify the function according to changes in structure and vice versa, and introduce the non-linearity that may manifest itself in chaotic behavior. One immediate consequence of this relationship is the need to seek structure-related inputs for PTF.

Using geophysical, remote-sensing and topographic information to infer soil variability is a promising research direction that presents a challenging exercise in searching a trade-off between quantity and quality of data and demonstrates the need for and value of integrative studies. Systematic coupling measurements of basic soil properties, soil hydraulic properties, and geophysical measurements adds value to all of those measurements as pedotransfer relationships can be derived to be used in a wide variety of applications. Both existing pedotransfer pathways, i.e. 'geophysical data \rightarrow soil basic properties' and 'geophysical data \rightarrow soil hydraulic properties', are of interest.

Change of scale practically means change of the model type and change of representation of soil hydraulic properties in models. No direct scaling relationship is possible across the hierarchy of scales because of differences in the type of information that we obtain about the SVA system, differences in variables that we use to characterize the system, and differences in observed variability of the system. Structural features that are rare at fine scale tend to control flow and transport at coarser scales. The coarse-scale hydraulic properties have to be simulated using an exhaustive representation of variability and relevant physical processes at the fine scale.

Comparison of performance for several models requires criteria that would take into account differences both in model complexity and in data quality. Currently such criteria are used rarely and have never been tested in vadose-zone studies. Poorly defined measurements should not allow model discrimination, and quality of measurements should be reflected in uncertainty of parameter estimates. Presenting modeling results with their uncertainty creates another challenge, as the probabilistic approach is not necessarily familiar to end-users.

Experience with models in a wide variety of hydrologic settings and contexts indicates that, regardless of the amount and quality of data, it is generally neither possible nor justifiable to describe all relevant aspects by a unique model. Given existing trends, we shall need to learn how to generate and use multiple predictions from multiple models on top of overcoming difficulties to populate a single model with parameters using data from multiple sources.

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