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Dynamical process upscaling for deriving catchment scale state variables and constitutive relations for meso-scale process models

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Abstract

In this study we propose an uspcaling approach for the assessment of (a) subcatchment/REW scale state variables, and (b) of catchment/REW scale soil hydraulic functions which embed/reflect the effects of critical subscale soil heterogeneities in the unsaturated zone on parameterizations of water flow at the next higher scale. The test area for this investigation is the well observed and studied Weiherbach catchment, which is located in a Loess area in south-west Germany. The approach adopted is to use the spatially averaged outputs and internal state variables generated by a highly detailed physically based numerical model that represents the dominant heterogeneities which are typical for this Loess area, and which has been previously shown to closely portray the dynamics of various state variables and fluxes within the study catchment. For these reasons, this detailed numerical model is deemed to be landscape and process compatible. By running this landscape and process compatible model with boundary and initial conditions observed in the Weiherbach catchment, and different assumed structures for soil heterogeneities, we generated time series of catchment-scale average soil saturations in the unsaturated zone by averaging the corresponding distributed model outputs. Due to the differences in assumed spatial patterns of soil heterogeneities and of macropores, the resulting different model structures yield clearly different time series of catchment scale average soil saturation values. The time series of catchment-scale average soil saturation values generated in this way from the landscape and process compatible model structure are, therefore, deemed as best estimates of the actual time series of average catchment scale soil saturation within the study catchment since the model embeds the fingerprints of typical patterns of soils and macropores and is shown to be physically consistent with a distributed set of soil moisture and discharge observations inside the catchment. Finally, we also derive hillslope scale soil hydraulic functions from simulated hillslope scale drainage experiments for the different assumed hillslope model structures. Different patterns of soil and macroporosity within the hillslope yield clearly different hillslope scale soil hy-

draulic functions, and these differences are consistent with the REV soil pore spectra of the soils. Assuming simple parametric functions for the soil water retention curve and the hydraulic conductivity curve we then obtain different parameters characterizing these soil hydraulic functions for the different assumed model structures. The different parameters obtained for these different model structures thus embed within them fingerprints of the assumed subscale soil patterns and structures on water flow in the unsaturated zone at the next higher scale, in the sense of Vogel and Roth (2003). The ultimate motivation for this analysis is that the so derived, hillslope or sub-catchment scale soil hydraulic functions will become intrinsic components of physically based numerical models, which use subcatchments as building blocks. Lee et al. (2006; this issue) have utilized hillslope scale soil hydraulic functions, derived similarly with the use of the same landscape and process compatible model, for the parameterisation of the CREW model, which is a numerical implementation of the REW approach (Reggiani et al., 1998, 1999), and showed that these lead to successful implementation of the model in the Weiherbach catchment. Their findings show clearly that the presented upscaling approach does indeed yield useful constitutive relations and target state variables for development and validation of meso-scale hydrological models based on the REW approach, embedding within them the fingerprints of the dominant within-catchment heterogeneities on simulated subsurface flow dynamics at the REW-scale.

1 Introduction

Solving the problem of “predictions in ungauged basins” (PUB) is clearly one of the biggest contemporary challenges in hydrological science. Predictions in ungauged or poorly gauged catchments for water resources planning, but also predictions of global change impact even in gauged catchments, seem hardly possible with the kind of predictive tools or models that we currently have that rely so much on calibration (Sivapalan et al., 2003). Meso-scale hydrological models of the conceptual variety only mimic hydrological behaviour a posteriori, i.e., after calibration to precipitation and stream flow data that are available for catchment states that we are interested in. These models are not capable of predicting hydrological response for catchment states outside the range for which precipitation and stream flow data are available. Fully physically based, distributed hydrological models such as MIKE SHE (Refsgaard and Storm, 1995) or CATFLOW (Zehe et al., 2001) may, in principle, be used to extrapolate beyond this "range of experience", because they are based on appropriate formulations of universal conservations laws, which essentially means that state variables and model parameters must be measurable quantities. Furthermore, such models may be able to explicitly resolve spatial patterns of key variables, which allows us, (a) to test/improve our perception of how spatial patterns control hydrological processes of interest, and consequently (b) may be adopted to support the design of field experiments. However, the application of distributed, physically based hydrological models is only reasonable if spatially highly resolved data sets, with detailed information on the patterns of surface and subsurface hydraulic properties, are available, and for this reason is restricted to the hillslope and small catchment scales for which such data sets may be available in only a limited number of catchments worldwide.

Therefore, solving the PUB problem requires that we:

- develop a new generation of hydrological models for the meso-scale, that are, on the one hand, based on conservation principles, meaningful state variables and parameters that may be derived from field observations using appropriate upscaling. On the other hand, these models have to be less complex than traditional physically based distributed models, so that parameter estimation remains a tractable problem.

- change our modelling attitude from ad hoc model modifications, when and if models do not fit the data, and more towards model development that is oriented towards rigorous testing of hypotheses, to increase the understanding or explanations of why our models fail.

The Representative Elementary Watershed (REW) approach (Reggiani et al., 1998, 1999, 2000) offers an appropriate theoretical and numerical framework for developing meso-scale hydrological models with the key characteristics that were highlighted above. The "heart" of the REW approach is a set of coupled mass and momentum balance equations for "different zones" represented within the appropriately chosen representative elementary watershed or REW, which are the unsaturated zone (u-zone), saturated zone (s-zone), concentrated overland flow zone (c-zone), saturated overland flow zone (o-zone), and channel zone. Mass and momentum fluxes between these different zones within the REW, and the corresponding fluxes between different REWs within a larger watershed, are generally unknown. Closing this set of model equations in order to make them determinate (i.e., same number of equations as the unknowns), essentially means, to assess reasonable process formulations for these mass exchanges as functions of REW scale state variables and catchment characteristics so that the set of balance equations becomes mathematically tractable. A second problem which is closely related to this "closure problem" is the assessment of model parameters and REW scale constitutive relations which connect different state variables that are associated with each of these REW-scale subregions, e.g. the relationship between REW-scale capillary pressure and REW-scale saturation in the unsaturated zone, which incorporate within them the effects of spatial patterns of associated variables within the REW at a lower level of scale (Reggiani et al., 2005; Zehe et al., 2005b).

The approaches that we propose in this paper for the assessment of closure relations and constitutive relations is essentially based on the disaggregation-aggregation approach of Sivapalan (1993) and Viney and Sivapalan (2004), and more specifically the "scale-way" idea of Vogel and Roth (2003). The latter authors argue that upscaling in environmental modelling, in general, has to deal alternatively with both "texture" and "structures". Texture is not explicitly resolved in the model and associated processes are described by means of continuum mechanics. Structures, on the other hand, can and have to be explicitly spatially resolved in the model. Structures at the next lower spatial scale or "subscale" determine partly the dynamics in the "texture" and hence the textural properties at the higher spatial scale. Employing these ideas for physically based, distributed hydrological models, the soil matrix is the texture, described by Richards-equation and suitable soil hydraulic relations that represent the effects of subscale structure such as the pore size distribution as well as the topology and connectivity of the pore space on water fluxes at the REV scale. Structures, on the other hand, refer to the spatial patterns of soil heterogeneities, layering and any preferential pathways, when they exist. Moving on from the REV scale to the REW scale it is obvious that structures i.e. spatial patterns of soils and preferential pathways in a catchment will strongly determine average mass exchange fluxes in the "texture" at the REW scale. Thus, it is essential to assess REW scale textural properties and parameters which embed the effects of these subscale structures on the average mass fluxes at the REW scale, which are again described using methods of continuum mechanics. Due to the non-linear nature of subsurface hydrological processes this is not a simple task!

In an ideal world we would derive constitutive relations based on measurements of average flows and soil moisture dynamics at the catchment scale. However, with current measurement techniques such data are far out of reach. The key objectives of the present study are to propose a dynamical upscaling approach for (a) generating the time series of REW scale state variables that may assist towards eventual model validation, as well as (b) deriving REW scale "soil hydraulic functions" which help parameterize and embed within them the net effects of subscale soil and macroporosity patterns that exist at the sub-REW scale. The proposed upscaling approach is implemented in the well observed and well studied Weiherbach catchment in south-western Germany. This dynamical upscaling approach employs the structure and averaged output of a detailed distributed and physically based, hydrological model, which has been previously shown to portray well the hydrological dynamics in the study catchment (Zehe et al., 2001, 2005a; Zehe and Blöschl, 2004), including reflecting the distributed small scale observations available within the catchment. Thus, the model is used as virtual landscape in order to simulate measurements of average flow and soil moisture dynamics at the catchment scale!

In an accompanying paper that appears in this special issue, Lee et al. (2006) present a successful application of a numerical model, CREW, that is based on the REW approach, to the Weiherbach catchment. The derivation of closure relations is described in detail in the paper of Lee et al. (2006). These authors used REW-scale soil hydraulic relations of the same functional form as proposed in this study, however these relations were manually calibrated. Based on the upscaling approach presented here we succeeded in deriving REW scale hydraulic relations with almost identical values as those calibrated from Lee et al. (2006) but a priori without calibration. Furthermore the REW-scale state variables obtained from the present study, and were used as target measures for validating the CREW model.

This paper is organized as follows. After explaining the dynamical upscaling methodology in Sect. 2 we will introduce the study area and the available database; the details of the model and the model setup are presented in Sect. 3. The derived REW scale state variables and constitutive relations are presented in Sect. 4. Finally, we will close with a discussion of results and conclusions in Sect. 5.

2 Concepts of the dynamical upscaling approach

2.1 Basic idea

The proposed approach is similar in principle to the perturbation methods proposed by Dagan (1989) and Gelhar (1993) for assessing first and second moments of tracer plumes in groundwater, and the volume averaging and homogenization techniques proposed by Attinger (2003) and Lunati et al. (2002) to derive effective process descriptions and parameterizations for an equivalent homogeneous medium at larger spatial scales. The work of these authors is focused on groundwater modelling and is based on assuming log-normally distributed random transmissivities, which allowed them to successfully employ analytical techniques. In the unsaturated zone within a catchment context, however, subsurface water fluxes are determined by patterns of vegetation, soil layering and preferential pathways, which interact amongst each other in a nonlinear way. Analytical averaging techniques are therefore not appropriate because they (a) cannot account for the nonlinear interactions of this multitude of spatial patterns, and (b) the spatial variability of key soil parameters is only partially of a statistical type, and a large part of variability is of the structural type.

The principal difference between the above listed approaches and the upscaling approach presented here is to use the spatially averaged output of a numerical process model for dynamic upscaling, since a detailed numerical model does naturally account for the nonlinear multiple influences of different patterns on the subsurface fluxes. Zehe et al. (2001) showed furthermore for the Weiherbach catchment, which is situated in a loess area in Germany, that a model structure which only incorporates typical (not actual) spatial patterns of soils, vegetation and preferential pathways in that loess landscape, and neglects local scale statistical variability, is sufficient to explain a large part of the observed variability of hydrological processes, i.e. the dynamics of runoff, soil moisture and evapotranspiration (ET) within a long term simulation. In the following study this “landscape and process compatible” model structure is employed for the implementation of the dynamical upscaling approach.

2.2 Derivation of catchment scale average state measures

The basic idea of the methodology is to use the landscape and process compatible model structure of the Weiherbach catchment as a virtual landscape because such a model structure:

– explicitly represents the dominant spatial patterns of soils, vegetation and preferential pathways inside the study catchment, and

– has been shown to portray the catchment behaviour in comparisons of model predictions from a long term continuous simulation to a distributed set of observations of different state variables and fluxes, such as soil moisture time series at 61 locations, discharge at the catchment outlet, and evapotranspiration (ET) at one meteorological station (Zehe et al., 2001, 2005a).

If we employ this model structure, as well as observed boundary conditions, for simulating space-time- fields of soil moisture θ_{sim}(x,y,z,t) and matric potential ψ_{sim}(x,y,z,t), we can suppose with confidence that these represent the best approximation to the real, unknown patterns of soil moisture θ_{real}(x,y,z,t) and matric potential ψ_{real}(x,y,z,t) that will evolve in this catchment under the given boundary conditions. By integrating the model output over the total catchment volume and dividing by the catchment volume, we can obtain the time series of catchment-scale average soil moisture?θ(t) [L^3L^{-3}] and catchment-scale average matric potential Ψ(t) [L]:

$$\begin{aligned}\overline{\theta}(t) &= \frac{1}{V_{\text{Catchment}}} \int\int\int_{\text{Catchment}} \theta_{\text{sim}}(x,y,z,t)\,dx\,dy\,dz \\ \Psi(t) &= \frac{1}{V_{\text{Catchment}}} \int\int\int_{\text{Catchment}} \psi_{\text{sim}}(x,y,z,t)\,dx\,dy\,dz\end{aligned} \qquad (1)$$

where x, y, z denote the Cartesian coordinates and t the time.

We consider these state variables, derived from the landscape and process compatible model structure, as physically consistent with local observations, i.e. time series of soil moisture at 61 locations within the catchment, and thus represent the dominant patterns within the catchment. Consequently, we postulate that the simulated time series of catchment-scale average soil moisture and matric potential may be used as additional target measures for validation of meso-scale models developed for this area. In Sect. 4.1 we will show that model structures different from the landscape and process compatible one will yield clearly different dynamics of the catchment-scale average soil moisture and matric potential. Hence these measures can be deemed to embed the fingerprints of the dominant patterns inside the catchment at the next larger scale.

2.3 Derivation of constitutive relations for the unsaturated zone of the CREW model

As the focus of this study is on the unsaturated zone, we will only discuss the corresponding mass balance equation here, the balance equations and closure relations for the remaining four zones in a typical REW may be found in Lee et al. (2005; 2006). If we assume no exchanges between neighbouring REWs, the mass balance equation for the unsaturated zone is given as follows (Lee et al., 2006):

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\rho \varepsilon y^u s^u \omega^u\right) = \underbrace{e^{uA}}_{\text{evapotranspiration}} + \underbrace{e^{us}}_{\substack{\text{recharge or}\\ \text{capillary rize}}} + \underbrace{e^{uc}}_{\text{infiltration}} \tag{2}$$

where y^u [L] is the average thickness of the unsaturated zone, s^u [–] is the average saturation ranging from zero to one, ω^u [L^2] is the area fraction of the unsaturated zone in the REW/catchment, ε^u [L^3L^{-3}] is the porosity, and ρ [ML^{-3}] is the mass density of water. The flux densities e^{uA}, e^{us}, e^{uc} denote the mass exchange rates at the interface to the atmosphere, saturated zone and concentrated overland flow zone, respectively.

We focus on the exchange term e^{us}, which denotes groundwater recharge or capillary rise. The most fundamental assumption we make here is that capillary forces and gravity are still the major drivers for groundwater recharge and capillary rise at the REW scale. We assume furthermore that e^{us} is still driven by average gradients of matric potential and gravity, that catchment-scale average water saturation s^u in the unsaturated zone is related to catchment-scale average capillary pressure? ψ by an average water retention function, and that the average flow resistance may be described by an average catchment-scale unsaturated hydraulic conductivity $\overline{k}$, which is also a function of average saturation s^u. Hence, e^{us} is given by (Lee et al., 2006):

$$\begin{aligned} e^{us} &= \alpha^{us} s^u w^u v_z^u \\ v_z^u &= \frac{\overline{k}}{s^u y^u}\left[\frac{1}{2}\left|\Psi\right| - y^u\right] \end{aligned} \tag{3}$$

$\Psi = f(s^u)$

where α^{us} is a dimensionless scaling parameter. The basic idea now is to derive $\overline{k}(s^u)$ and $\Psi=f(s^u)$ from simulated drainage experiments carried out with the landscape and process compatible model. In this sense, the detailed numerical model represents a REW/catchment scale measurement instrument. To this end, we start at an initially saturated catchment and impose an increasing suction head at the lower boundary of the catchment. The boundary conditions at the remaining boundaries are of the zero flux type. The simulated outflow $q(x,y,z_B,t)$ at the lower boundary, i.e. at a defined depth in the soil z_B, is averaged over the whole catchment area for each time step.

$$e^{su}(t) = \frac{1}{A_{\text{Catchment}}} \iint\limits_{\text{Area}} q(x, y, z_B, t)\, \mathrm{d}x\, \mathrm{d}y \tag{4}$$

Additionally, the simulated saturation and the matric potential are averaged over the whole catchment volume, as defined in Eq. (1). This way we obtain series of values of average outflows e^{su} as a function of average saturation s^u, and if Eq. (3) is now solved for $\overline{k}$ we end up with $\overline{k}$ as a function of s^u. We can also obtain, in a similar manner, the relationship between average matric potential Ψ and average saturation s^u. By fitting particular functional forms to the numerically obtained relationships, the relationships can be analytically represented in terms of REW-scale effective parameters. In this work, as a first step, we have assumed the parametric relationships of the type given in Eq. (5) below:

$$\begin{aligned} \overline{k}(s^u) &= \overline{k}_s \left(s^u\right)^{\beta_k} \\ \Psi\left(s^u\right) &= \Psi_b \left(s^u\right)^{\beta_\Psi} \\ s^u &= \frac{\overline{\theta}}{\overline{\theta}_s} \end{aligned} \tag{5}$$

Given the assumed functional forms, the next step is to estimate the associated the REW scale effective parameters in Eq. (5), namely, hydraulic conductivity $\overline{k}_s$, bubbling pressure Ψ_b, and the exponents β^k and β^Ψ.

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This approach to deriving REW scale constitutive relations presented above will be exemplified in the next sections through application to the Weiherbach catchment. In Sect. 4.2 we will also show that model structures different from the landscape and process compatible one yield clearly different parameter values for Eq. (5), thus demonstrating that these parameters do indeed robustly embed, at the REW scale, the fingerprints of the dominant patterns inside the catchment.

3 Application to a micro-scale catchment

3.1 Study catchment and data base

3.1.1 Weiherbach catchment

The application of the proposed theory is based on detailed laboratory data and field observations that were conducted in the Weiherbach valley (Zehe et al., 2001). The Weiherbach is a rural catchment of 3.6 km^2 size situated in a loess area in the south-west of Germany. Geologically it consists of Keuper and Loess layers of up to 15 m thickness. The climate is semi-humid with an average annual precipitation of 750–800 mm $year^{-1}$, average annual runoff of 150 mm $year^{-1}$, and annual potential evapotranspiration of 775 mm $year^{-1}$.

More than 95% of the total catchment area is used for cultivation of agricultural crops or pasture, 4% is forested and 1% is paved area. Crop rotation is usually once a year. Typical main crops are barley or winter barley, corn, sunflowers, turnips and peas; typical intermediate crops are mustard or clover. Ploughing is usually to a depth of 30 to 35 cm in early spring or early fall, depending on the cultivated crop. A few locations in the valley floor are tile drained to a depth of approximately 1 m. However, the total portion of catchment area that is under tile drains is less than 0.5% of the total catchment.

Most of the Weiherbach hillslopes exhibit a typical loess catena with moist but drained Colluvisols located at the foothills and dryer Calcaric Regosols located at the top and mid-slope sectors. Preferential pathways in the Weiherbach soils are very apparent. The thickness of the Loess cover ranges from 15 to 30 m. Preferential flow pathways are mainly a result of up to 1.5 m deep earthworm burrows and their spatial pattern is closely related to the typical hillslope soil catena (Zehe and Flühler, 2001; Ehrmann, 1996). Detailed field observations (Zehe et al., 2001) in the Weiherbach catchment indicated that storm runoff is produced by infiltration excess overland flow. As the average depth of the macropore system is small compared to the thickness of the Loess cover and due to the absence of lateral preferential pathways or strata, macropores enhance infiltration and decrease storm runoff in this type of landscape.

3.1.2 Experimental database

Figure 1 presents a map view of the observational network in the northern part of Weiherbach catchment. Rainfall input was measured in a total of 6 rain gauges and streamflow was monitored at two stream gauges, all at a temporal resolution of 6 min, and for a period of over 10 years. The gauged catchment areas are 0.32 and 3.6 km^2. Soil moisture was measured at up to 61 locations at weekly intervals using two-rod TDR equipment that integrates over the upper 15, 30, and 45 cm of the soil. A soil map was compiled from texture information that was available on a regular grid of 50 m spacing. As expected for this Loess area, the catchment scale pattern of soil types turned out to be highly organized. The typical Loess soil catena at a hillslope is Calcaric Regosol in the top and mid slope sector and Colluvisol in the valleys. The soil hydraulic properties of Weiherbach soils after van Genuchten (1980) and Mualem (1976) were measured in the laboratory using undisturbed soil samples along transects at several hillslopes, up to 200 samples per slope (Table 1, Schäfer, 1999). The topography was represented by a digital elevation model of 12.5 m grid spacing.

The macropore system, i.e. the number of earth worm burrows, was mapped at 15 sites in the catchment, each 1 m^2 large plot was subdivided into 0.5 m^2 raster elements and a horizontal soil profile was prepared. For each element, macropores that were connected to the soil surface were counted and their depths and diameters were measured using a Vernier caliper and a wire. The spatial pattern of soil macroporosity turned out to be closely related to the soil catena. The macroporosities tend to be small in the dry Calcaric Regosols located at the top and mid-slope regions, and larger in the moist and drained Colluvisols located at the foot hills (Zehe and Flühler, 2001; Zehe, 1999). This form of spatial organization may be explained by the habitat preferences of *Lumbricus terrestris* which is the dominant earthworm species in that landscape (Ehrmann, 1996).

Curves representing the temporal development of LAI, plant height, biomass production, and root length were determined based on visual inspections of the main crops such as corn, wheat, oats, sunflowers, sugar beets, peas, mustard, and turnips as the basis for the evaporation module of CATFLOW. Further details on the measurement program are given in Zehe et al. (2001).

3.2 Hydrological model, and process and landscape compatible model structure

3.2.1 Model structure and process formulation

For the dynamical upscaling methodology presented in this paper we employ the physically based, distributed hydrological model, CATFLOW (Maurer, 1997; Zehe et al., 2001). The model subdivides a catchment into a number of hillslopes and a drainage network. Each hillslope is discretized along the main slope line into a 2-dimensional vertical grid using curvilinear orthogonal coordinates. Each surface model element extends over the width of the hillslope. The widths of the surface elements may vary from the top to the foot of the hillslope. For each hillslope, evapotranspiration is represented using an advanced SVAT approach based on Penman-Monteith equation, which accounts for plant growth, albedo as a function of soil moisture, and the impact of local topography on wind speed and radiation. Soil water dynamics and solute transport are simulated based on the Richards equation in the mixed form, as well as a transport equation of the convection diffusion type. These equations are numerically solved using an implicit mass conservative "Picard iteration" (Celia and Bouloutas, 1990) and a random walk (particle tracking) scheme. The simulation time step is dynamically adjusted to achieve an optimal change of the simulated soil moisture per time step, which assures fast convergence of the Picard iteration. The hillslope module can simulate infiltration excess runoff, saturation excess runoff, reinfiltration of surface runoff, lateral water flow in the subsurface, return flow and solute transport.

However, in the Weiherbach catchment only infiltration excess runoff contributes to storm runoff and lateral subsurface flow does not play a major role at the event scale. What is important is the redistribution of near surface soil moisture in controlling infiltration and surface runoff. Surface runoff is routed on the hillslopes, fed into the channel network and routed to the catchment outlet based on the convection diffusion approximation to the 1-dimensional Saint-Venant equation. For reasons of brevity the model equations, which are now standard ones for most physically based models, are not presented here; for more details readers may refer to Maurer (1997) and Zehe et al. (2001, 2005b).

Preferential flow is important for infiltration and generation of surface runoff in the Weiherbach catchment. In CATFLOW preferential flow is represented by an effective threshold approach, which is motivated by experimental findings of Zehe and Flühler (2001). Macropore flow starts when the relative saturation S [–] at a macroporous grid point at the soil surface exceeds the threshold S_0. As the effect of active macropores in a model element is to increase the infiltration capacity, the hydraulic conductivity, k^B, of the element is increased as follows:

$$\begin{aligned}
&k^B(x,z) = k_S(x,z) + k_S(x,z) f_m(x,z)\frac{S-S_0}{1-S_0} && \text{if } S \geq S_0 \\
&k^B(x,z) = k_S(x,z) && \text{otherwise} \\
&S(x,z) = \frac{\theta(x,z)-\theta_r(x,z)}{\theta_s(x,z)-\theta_r(x,z)}
\end{aligned} \tag{6}$$

where k_s [l/t] is the saturated hydraulic conductivity of the soil matrix, θ_s [$l^3 l^{-3}$] and θ_r [$l^3 l^{-3}$] are saturated and residual soil moisture content, respectively, θ [$l^3 l^{-3}$] is the soil moisture, x and z are the coordinates along the slope line and the vertical. The macroporosity factor, f_m[–], is defined as the ratio of the water flow rate in the macropores, $Q_m[l^3/t]$, in a model element of area A and the saturated water flow rate in the soil matrix $Q_{matrix}[l^3/t]$. It is therefore a characteristic soil property reflecting the maximum influence of active preferential pathways on saturated soil water movement:

$$f_m(x,z) = \frac{Q_m(x,z)}{Q_{matrix}(x,z)} \tag{7}$$

For the Weiherbach soils we chose the threshold S_0 to be equal to 0.8, which corresponds to a soil moisture value of 0.32 in the Colluvisol. This is a plausible value as it is in the order of the field capacity for the soils in the Weiherbach catchment. For relative saturation values above this threshold, free gravity water is present in the coarse pores of the soil, and this free water may percolate into macropores and thus may help start preferential flow. This plausible value of S_0 has been corroborated through model simulations performed at a number of space-time scales in the Weiherbach catchment. Using the hillslope module of CATFLOW Zehe and Blöschl (2004) simulated preferential flow and tracer transport at several field plots in the Weiherbach catchment which were in good agreement with observations. The two-dimensional f_m pattern in the macroporous medium that Zehe and Blöschl used for their study was computed using Eq. (2), based on a statistical generation of macropores of different sizes, and assigned macropore flow rates for each macropore. Simulations of tracer transport and water dynamics over an entire hillslope over a period of two years matched well the corresponding observations of a long term tracer experiment at the hillslope scale (Zehe et al., 2001).

3.2.2 Landscape and process compatible model structure for the Weiherbach catchment

For the catchment scale simulations the Weiherbach catchment was subdivided into 169 hillslopes and an associated drainage channel network, and each of the slopes was discretized into a 2-dimensional finite difference grid along the slope line. The surface model elements are 5–20 m wide (depending on the position on the hillslope) and 10 m long. The width of the finite difference grid in the vertical direction varies from 5 cm close to the surface, to 25 cm at the lower boundary. The total soil depth represented by the model was 2 m. The Manning roughness coefficients for the hillslopes and the channels were taken from a number of irrigation experiments performed in the catchment, as well as from the literature based on the current crop pattern (see Gerlinger et al., 1998; Zehe et al., 2001). For the hillslopes the following boundary conditions were chosen: free drainage at the bottom, seepage boundary conditions at the interface to the stream, atmospheric conditions at the upper boundary, and no flux boundary at the watershed boundary.

Due the existence of a "typical hillslope" with a typical soil catena and spatially organized macroporosity patterns in the Weiherbach catchment, we selected a simplified model structure that accounted only for the typical characteristics of the hillslope, and neglected details of individual hillslopes. Thus, all hillslopes in the model catchment were given the same relative catena, with Calcaric Regosol in the upper 80% and Colluvisol in the lower 20% of the hill. The corresponding van Genuchten-Mualem parameters are listed in Table 1. Furthermore, all hillslopes were given the same spatial patterns of macroporosity. Measurements of macroporosity at 15 sites with 1 m^2 sampling area in the Weiherbach catchment suggested high macropore volumes, typically of 1.5×10^{-3} m^3 in the moist Colluvisols at the hill foot, and low values of 0.6×10^{-3} m^3 at the top and mid-slope sectors (Zehe, 1999, cf. his Fig. 4.1). We chose the macroporosity factor to be $0.6\times f_m$ at the upper 70% of the hillslope, $1.1\times f_m$ at the mid-sector ranging from 70 to 85% of the hillslope, and $1.5\times f_m$ at the lowest 85 to 100% of the slope length. The depth of the macroporous layer was assumed to be constant throughout the whole catchment and set at 0.5 m. The unknown macroporosity factor, f_m, of the hillslopes was estimated by matching model predictions against observations from the largest observed rainfall-runoff event on record, where a value of 2.1 turned out to be optimal (cf. Sect. 4.1 later for details).

Based on this model structure the water cycle in the Weiherbach catchment was simulated continuously over the period 21 April 1994 to 15 September 1995. During the simulation we accounted for plant growth and related changes in LAI, plant height and root depth, as well as seasonal changes in the crop pattern. Meteorological input data were taken from the meteorological station located at the centre of the catchment, wind speed and radiation were regionalized to the catchment scale, as described in Zehe et al. (2001). After an initialization phase of approximately 30 days the model yielded, simultaneously, reasonable predictions of discharge with a Nash-Sutcliffe efficiency of 0.82, and good predictions of evapotranspiration (ET) with a correlation of R=0.91. Furthermore, the model yielded reasonable predictions of soil moisture dynamics at 61 sites within the catchment. The average correlation between observed and simulated soil moisture was 0.64 at hilltop locations and 0.74 at the mid-slope and valley floor sectors. For reasons of brevity we omit figures on simulated and observed discharge, ET as well as on simulated and observed soil moisture values. Interested readers are referred to Zehe et al. (2005b) for these additional details.

Readers should keep in mind that the model structure presented here only accounts for typical variability exhibited within the catchment, i.e. representative hillslope soil catena and related structured patterns of macroporosity, as outlined in the previous section. Small-scale variability of soil hydraulic properties and the deviations in individual hillslopes from the assumed idealized soil pattern, have been neglected. Nevertheless, a major part of the variability of soil moisture, discharge and ET may already be explained by this landscape and process compatible model structure.

3.3 Derivation of catchment scale state variables and constitutive relations

3.3.1 Catchment scale state variables

As outlined in Sect. 2.2 we postulate that we may employ the process and landscape compatible model structure introduced in the last section for deriving realistic estimates of the space-time patterns of soil moisture that will develop in the Weiherbach catchment, under the given boundary conditions. By volumetric averaging, as defined in Eq. (1), we end up with a time series of catchment scale average soil moisture which embeds the fingerprint of the dominant patterns of soils and macropores inside the catchment, at the next larger scale. To test this hypothesis we compare the following model structures during a simulation with observed boundary conditions covering the period from the 21 April 1994 to 15 September 1995:

- Landscape and process compatible model structure as described in Sect. 3.2.2: Calcaric Regosols in the upper 80% and Colluvisols in the lower 20% of the hillslope (see Table 1 for the soil hydraulic parameters). Macroporosity is increasing downhill as follows: $0.6\times f_m$ at the upper 70%, $1.1\times f_m$ from 70–85%, and $1.5\times f_m$ for 85–100% of the total hillslope length, average macroporosity value was f_m=2.1.

- No macropores: same soil pattern as in the landscape and process compatible model structure but with f_m=0

- Disturbed macroporosity pattern: same soil pattern as in the landscape and process compatible model structure, but a flipped macro-porosity pattern: $0.6\times f_m$ at the lower 70% of the hillslope, $1.1\times f_m$ from 15 to 30%, and $1.5\times f_m$ at the upper 15% of the total hillslope length. The value of f_m remains equal to 2.1.

- Disturbed macroporosity and soils patterns: in addition to the macroporosity pattern the soil pattern was flipped in the same sense. The value of f_m remained equal to 2.1.

- Sand on Loess: completely different model structure consisting of a sand layer of 1 m depth extending over the complete hillslope length, followed by Calcaric Regosol while macropores were neglected. The soil hydraulic parameters of the sand were taken from the pedotransfer function proposed by Carsel and Parrish (1988; see their Table 1).

For each of these model structures the average catchment-scale soil saturation and the average catchment-scale matric potential were derived after the 1.5 year long simulation using Eq. (1).

3.3.2 Catchment scale constitutive relations

As outlined in Sect. 2.3 we derive REW scale soil hydraulic properties that embed the effect of dominant subscale soil and macroporosity patterns from simulated REW scale drainage experiments with the process and landscape compatible model structure. In the case of the Weiherbach catchment the characteristic building block of the distributed model was the typical hillslope characterised in Sect. 3.2.2. For assessing the REW scale soil hydraulic functions we simulated a drainage experiment for a single hillslope from the landscape and process compatible model structure (Fig. 2). To this end we start at an initially saturated hillslope and impose an increasing suction head at the lower boundary. The boundary conditions at the remaining boundaries are of the zero flux type. The total depth of the simulation domain was 2 m, and the simulation period was 2 years. Hillslope topography was taken from a typical hillslope in the Weiherbach catchment.

Of course a simple rearrangement of soil patterns without changing their area fraction does not affect the simulated drainage at the lower boundary. To demonstrate that hillslopes different from that of the landscape and process compatible model structure yield clearly different REW scale soil hydraulic functions, the drainage experiment was carried out for the hillslope structures different from those introduced in Sect. 3.3.1:

1. Landscape and process compatible hillslope.
2. Hillslope with deep macropores: the hillslope has the same soil and macroporosity patterns as in the case of the landscape and process compatible hillslope, but the depth of the macroporous layer equals the depth of the simulation domain.
3. Hillslope with Loess soil: the entire hillslope consists of Calcaric Regosol, f_m was

set to 1.6.

4. Hillslope with Colluvisol soil: the entire hillslope consists of Colluvisol, f_m was set to 1.6.

5. Hillslope with sandy soil: the entire hillslope consists of sand, f_m was set to 0.

For each simulated case we computed the REW scale hydraulic conductivity from the average flow from across the lower boundary using Eq. (3). By computing the average hillslope scale soil moisture and matric potential we end up with the hillslope scale hydraulic conductivity as a function of the average hillslope scale water saturation as well as the hillslope scale water saturation as a function of the average hillslope scale matric potential. In the last step parametric functions defined in Eq. (5) were fitted to the data using the curve fitting toolbox of MATLAB.

4 Results and discussion

4.1 Catchment scale state variables

As can be seen in Fig. 3 (left panels), for the largest rainfall event from 27 June 1994, the different model structures cause clear differences in runoff responses. Sand on top of the loess soil yields a retarded and reduced runoff response, which stems from subsurface storm flow on the loess horizon that exists at 1 m depth. It is remarkable that the rearrangement, i.e. the flipping of the spatial soil and/or macroporosity patterns, is already sufficient to yield significantly different rainfall–runoff behaviour. Flipping the macroporosity pattern causes a stronger runoff response as the infiltration capacity of soils near the stream is now, even in the case of active macropores, lower than in the case of the landscape and process compatible model structure. Flipping both the spatial soil and macroporosity patterns yields an even stronger runoff response, as the saturated hydraulic conductivity of the Calcaric Regosol is only one tenth of the saturated hydraulic conductivity of the Colluvisol.

Figure 4 (upper panel) shows the time series of the catchment-scale average soil saturation. The time series derived from the landscape and process compatible model structure clearly differs from those derived from the remaining model structures. Major differences occur during stronger rainfall events, e.g. on day 67 (27 June 1994), and persist for more than 100 days. But there are also smaller differences between the time series with flipped spatial patterns of soils and/or macroporosity. As expected, the catchment scale soil saturation for the sand on loess catchment exhibits the lowest values throughout the simulation period. These series of averaged soil saturation values show clearly and unambiguously that the fingerprint of within-catchment heterogeneities of soils and macropores on soil moisture dynamics does not vanish when we move to the next higher scale.

Furthermore, Fig. 4 also shows (lower panel) that the time series of catchment-scale average soil moisture θ_{av} simulated by the landscape and process compatible model structure falls in the range of the observed soil moisture values, measured with from 45 cm long TDR rods at up to 61 measurement locations. As θ_{av} is averaged over a depth of 2 m, the time series is, as expected, smoother than the observations. It should be noted here that the time series of the upscaled catchment scale soil moisture are not just simply the arithmetic averages of the observations.

4.2 Catchment scale constitutive relations

Figure 5 presents the results of the simulated hillslope scale drainage experiments for the landscape and process compatible hillslope (left column) and the case of long macropores (right column). In addition, Table 2 lists the 95% confidence limits of the estimated hydraulic parameters (according to Eq. 5), which are clearly different for the different hillslope structures. The landscape and process compatible hillslope and the one with long macropores yield similar hillslope scale water retention curves (according to Eqs. 3 and 5). However, since the longer macropores that reach continuously to the lower boundary of the model domain cause a faster drainage at saturations larger than 0.8, the bubbling pressure Ψ_b is therefore 50% smaller in this case. The faster drainage results also in a hillslope scale saturated hydraulic conductivity, which at 1.61×10^{-5} ms^{-1}, is twice as high as for the landscape and process compatible hillslope. However, the fit of the hillslope hydraulic conductivity curve, in the case of the long macropores, with an R^2 of 0.51, is not really satisfactory. This is due to the very fast drop of the hydraulic conductivity at high saturations, because of the threshold approach adopted for the onset of macropore flow in CATFLOW (Eq. 6).

It is interesting to note that the catchment scale saturated hydraulic conductivity estimated for the landscape and process compatible hillslope is, at 8.1×10^{-6} ms^{-1}, close to the area weighted average of the average REV scale values given in Table 1 (note the this hillslope has 80% Calcaric Regosol and 20% Colluvisol). Similarly, the hillslope scale saturated hydraulic conductivities estimated for the Loess and the Colluvisol soil (Fig. 6) are, at 3.98×10^{-6} ms^{-1} and 3.2×10^{-5} ms^{-1} respectively, close to the average REV scale values given in Table 1. The exponent β^{Ψ} of the water retention function is a measure of the amount of fine pores and therefore for the capillary forces that act on water in the upscaled textural medium. The higher clay content and the larger amount of fine pores in Colluvisol are therefore reflected in a value of β^{Ψ} which is 4 times larger than that of the Loess hillslope. As expected β^{Ψ} of the landscape and process compatible hillslope, at 3.65, falls between the values derived for the Loess and the Colluvisol hillslopes.

5 Summary and conclusions

The main findings of the present study may be condensed into the following three points: firstly, the representation of the dominant spatial patterns of soil heterogeneity and macroporosity in the process model CATFLOW, which are typical for in a Loess area of Germany, is sufficient to explain the major aspects of the observed discharge-, ET- and soil moisture dynamics in a typical catchment in this region. We want to stress here in this context that, to achieve this result, it was not necessary to account for the exact soil catena and the small-scale variability of soil properties at the individual hillslopes. The model is nevertheless landscape specific since it only accounts for the dominant heterogeneities that are and typical for this Loess area, and process compatible, since it explains a large part of the observed dynamics of the different state variables.

Secondly, we derived the time series of catchment-scale average soil saturation by averaging the output of the landscape and process compatible model. The fingerprints of the within-catchment heterogeneity of soils and macropores on the average soil moisture dynamics do not vanish when we move to the next higher scale. The time series of catchment-scale average soil moisture is physically consistent with a distributed set of observations inside the catchment. This state variable is therefore capable of reflecting and embedding within it the fingerprints of the dominant within-catchment heterogeneities on subsurface dynamics at the REW-scale, and therefore represents a suitable target data set for testing subsurface components of meso-scale hydrological models, as shown in the accompanying paper by Lee et al. (2006). We consider this approach of dynamical upscaling to be much more appropriate for the upscaling of local observations than, for example, geo-statistical approaches, because it maximises the use of all available physically-based process understanding and landscape specific information through the application of spatially explicit process models for interpolations within the catchment.

Thirdly, within simulated hillslope scale drainage experiments, we derived hillslope-scale soil hydraulic functions for different model structures. Different patterns of soil and macroporosity within the hillslope yielded clearly different hillslope scale soil hydraulic functions, and these differences were consistent with the REV scale soil pore size spectra. Assuming simple two-parameter functions for the soil water retention curve and the hydraulic conductivity curve at the REW scale, we obtained clearly different parameters for the different model structures. As expected, in homogeneous soils the average saturated hydraulic conductivity determined from a sufficiently large sample of point measurements is a good estimate for the hillslope scale/REW scale saturated hydraulic conductivity. The different parameters obtained for the different model structures embed within them the fingerprints of subscale soil patterns and structures on water flow in the unsaturated zone to the next higher scale, in the sense of Vogel and Roth (2003).

Lee et al. (2005) proposed a similar approach for deriving constitutive relations for the Weiherbach catchment. However, within there approach the authors used the complete catchment and the observed boundary conditions instead. The authors simply averaged the unsaturated hydraulic conductivity of the model structure to obtain a catchment scale hydraulic conductivity curve. The parameters obtained with the latter approach did not yield a reasonable I performance of the CREW model, which represents a numerical implementation of the REW approach, in the Weiherbach catchment as shown by Lee et al. (2006). In their study the authors had to calibrate the constitutive relations for a model structure consisting of just one REW which resulsted in a simulated discharge time series with a Nash-Sutcliffe efficiency of 0.82. The reader should note that the calibrated parameter values obtained by Lee et al. (2006) are almost identical to the values we obtained a priori for the landscape and process compatible model. At the same time, the time series of the unsaturated zone saturation simulated with the CREW model matched very well the time series of catchment-scale average soil saturation derived from the landscape and process compatible model structure. This correspondence shows clearly that the presented upscaling approach yields useful constitutive relations and target measures for meso-scale hydrological models based on the REW approach. Furthermore, the 95% confidence intervals derived within the parameter fitting (Table 2) allowed, quite naturally, the assessment of predictive model uncertainty within a Monte Carlo framework. Thus, we propose something like a frame work for dynamical upscaling i.e. a scaleway of process models for deriving constitutive relations and closure relations for the REW approach by simulating experiments at the catchment scale as long as we cannot not assess such data in real world. The nice thing about the framwork idea is, that it can be maintained in the sense the better process desicriptions e.g. for preferential we might obtain at the REV scale may be included in this framework. The framework is not restricted to a specific model!

But even if we succeed in deriving closure relations and setting up the CREW model for a catchment of interest such as the Weiherbach catchment, the crucial question is: To which extent are these closure relations unique and only valid in the particular catchment they were derived for? Beven (2000) argues, each catchment is an "individual" due to individual details in subsurface structures. So do we have to repeat this very laborious derivation of closure relations at each individual catchment? Or do the closure relations capture the typical hydrological functioning of landscape compartments. In this case a REW with a certain set of closure relations would be a characteristic building block for meso-scale models in a landscape, which allow the setup of models that need less calibration and assure realistic dynamics of state variables and stream flow at the same time, as long as we stay within the same landscape. To support the second point of view we employ the pattern-process paradigm and the idea of potential natural states from theoretical ecology (Watt, 1947; Turner, 1989; Turner and Gardner, 2001). The essence of the pattern-process paradigm is that similarity of patterns (e.g. in soils, vegetation and subsurface structures), in for example, two different catchments of a specific landscape, is an indicator of similarity of processes (Underwood et al., 2000; Grayson and Blöschl, 2000).

Furthermore, the potential natural state of a landscape is an equilibrium state due to a balance of "external" disturbances and "internal" forces. This balance is reflected in typical, spatially organized patterns of vegetation, soils and subsurface structures. Since these patterns had been formed by hydro-climatic processes in a specific geological environment and climate, we argue that these typical patterns in turn cause similarity of hydrological processes. We postulate, therefore, the existence of a typical process spectrum/hydrological functioning to be a generic feature of a landscape. We believe therefore that a set of typical closure relations exists for each landscape that may encapsulate this typical hydrological functioning, in the sense similar to typical soil hydraulic functions being applicable for different soil types. However, this hypothesis remains to be tested within a future application of the CREW model with the closure relations derived within this study and the study of Lee et al. (2006) to a larger catchment such as the SULM catchment in the same Loess area in Germany. This exploration is currently in progress and results are expected in the near future.

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Table 1. Average hydraulic properties for typical Weiherbach soils, determined from 200 undisturbed soil samples. The definition of parameters is after van Genuchten (1980) and Mualem (1976). Saturated hydraulic conductivity k_s, porosity θ_s, residual water content θ_r, air entry value α, and shape parameter n.

Soil	k_s [m/s]	θ_s[–]	θ_r[–]	α [1/m]	n[–]
Calcaric Regosol	$(3.4\pm1.5)\times10^{-6}$	0.46	0.06	1.5	1.36
Colluvisol	$(4.1\pm2)\times10^{-5}$	0.43	0.11	1.2	1.20

Table 2. Parameters of the REW scale soil hydraulic functions (compare Eq. 5) derived for the different model structures (defined in Sect. 3.3.2): Average hydraulic conductivity $\overline{k_s}$, exponent of the unsaturated hydraulic conductivity curve β^k, average REW scale bubbling pressure Ψ^b as well as the exponent of the water retention function β^Ψ. The values in brackets give the 95% confidence limits.

Parameter	1	2	3	4	5
$\overline{k_s}$	8.1	16.1	3.98	31.7	70.8
[10^{-6} m/s]	[3.76, 11.2]	[2.2, 26.0]	[2.01, 5.99]	[3.27, 60.2]	[63.6, 71,1]
β^k	4.31	4.35	3.26	8.57	2.67
[–]	[1.05, 7.57]	[1.21, 9.86]	[3.40, 7.92]	[2.32, 14.8]	[2.60, 2.93]
R^2_k	0.82	0.5	0.78	0.81	0.81
Ψ^b	0.206	0.121	0.071	0.0031	$4.3\ 10^{-5}$
[m]	[0.197, 0.220]	[0.11, 0.133]	[0.062, 0.080]	[0.0023, 0.0032]	[3.9, 4.8]$\times10^{-5}$
$t\beta^\Psi$	3.65	4.03	2.73	9.28	5.15
[–]	[3.70, 3.50]	[4.10, 3.97]	[2.79, 2.07]	[9.34, 9.28]	[5.18, 5.12]
R^2_Ψ	0.89	0.98	0.97	0.99	0.99

1. Landscape and process compatible hillslope
2. Hillslope with deep macropores
3. Hillslope with Loess soil
4. Hillslope with Colluvisol soil
5. Hillslope with loamy sandy

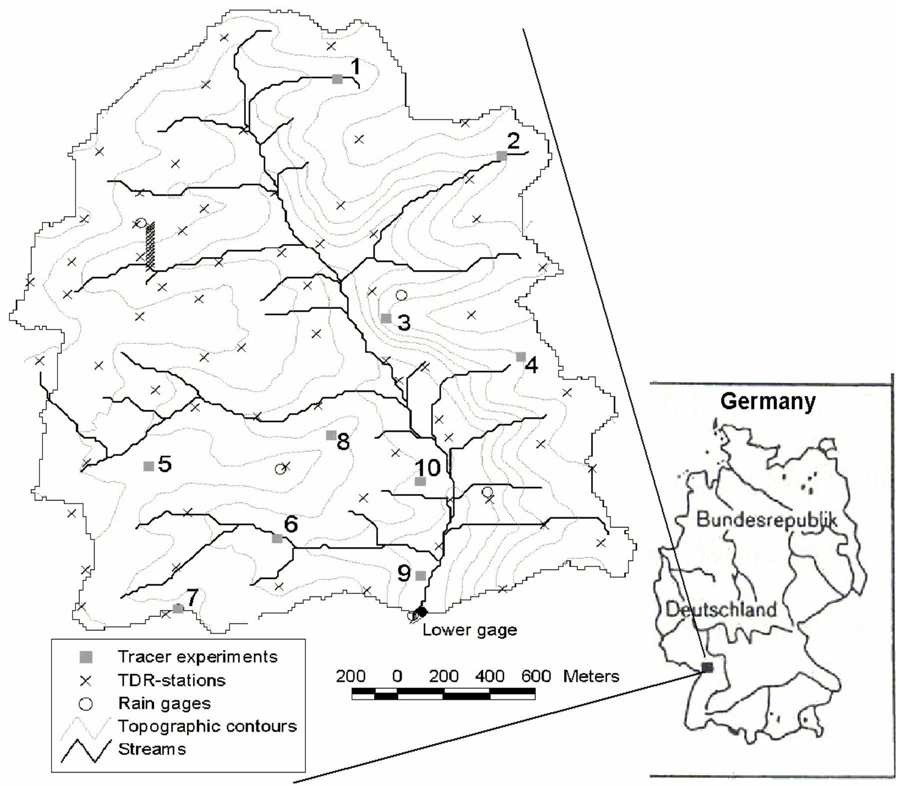

Fig. 1. Observational network of the Weiherbach catchment. Soil moisture was measured at 61 TDR stations at weekly intervals (crosses). Triangle indicates the stream gage. Topographic contour interval is 10 m.

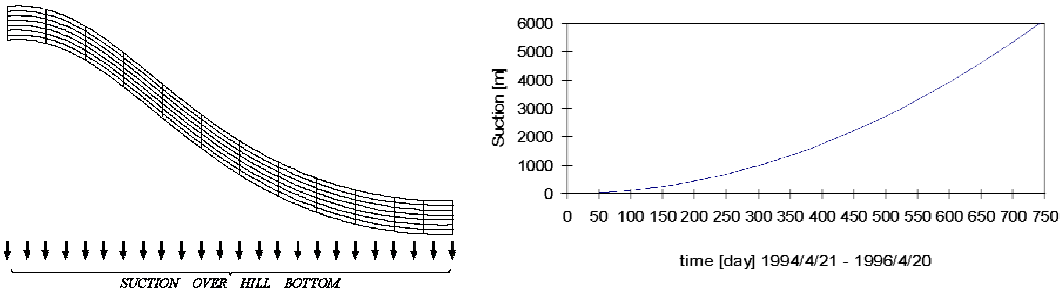

Fig. 2. Numerical setup for simulated hillslope scale drainage experiments, left panel shows the finite difference grid, right panel shows suction head imposed to the lower boundary as a function of time. The boundary conditions at the remaining boundaries were set to zero flux, the initial state was full saturation and the vertical extent of the domain is 2 m.

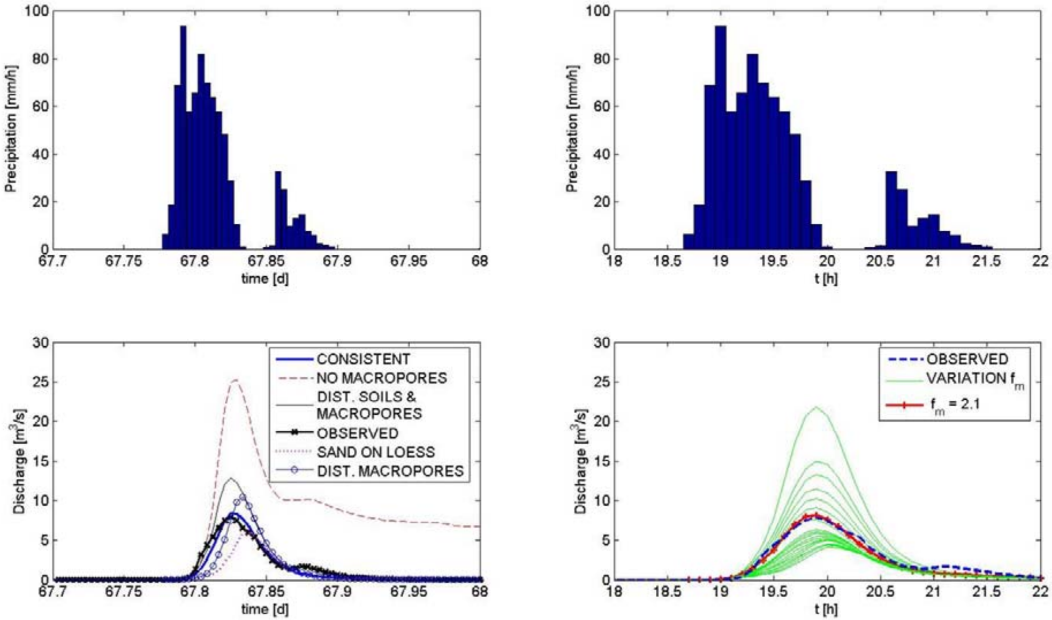

Fig. 3. The lower right panel shows simulated discharges (thin solid lines) for the largest rainfall runoff event (27 June 1994) that was selected for model calibration for macroporosity factors ranging from f_m=0.1 to 3. Increasing values of f_m correspond to decreasing runoff. The best fit to the observed hydrograph is obtained for f_m=2.1. The lower left panel show the runoff response for different model structures even small modifications cause a clear difference in runoff production. Hillslope topography was taken from a typical hillslope in the Weiherbach catchment.

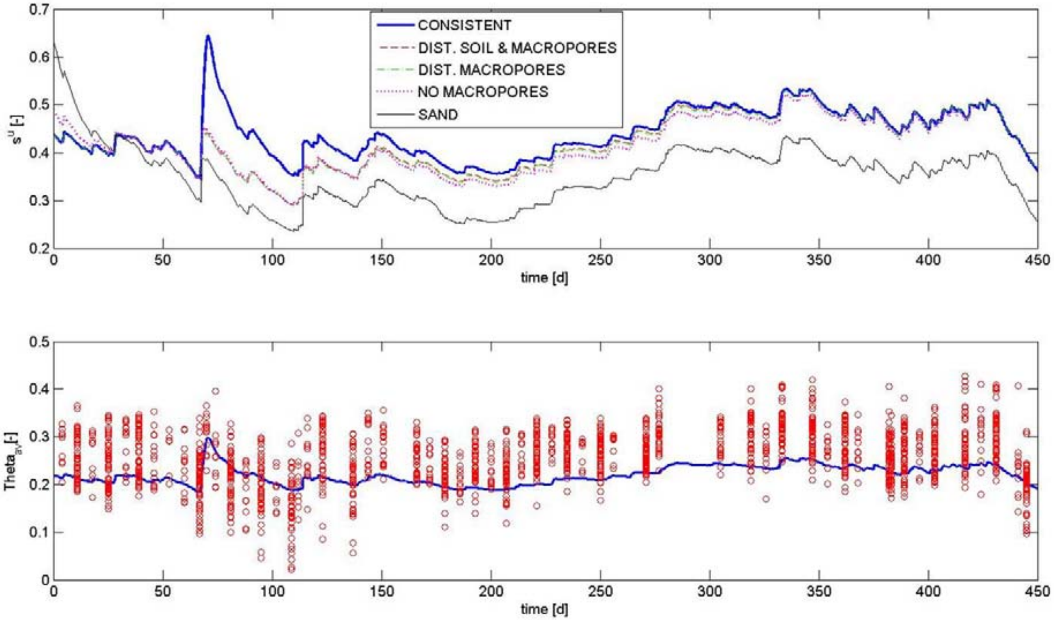

Fig. 4. Average catchment-scale soil saturation (top panel) for the different model structures. The lower panel shows the average catchment scale soil moisture (according to Eq. 1) simulated with the landscape and process compatible model structures as well as the observed soil moisture values from 45 cm TDR rods available at up to 61 locations.

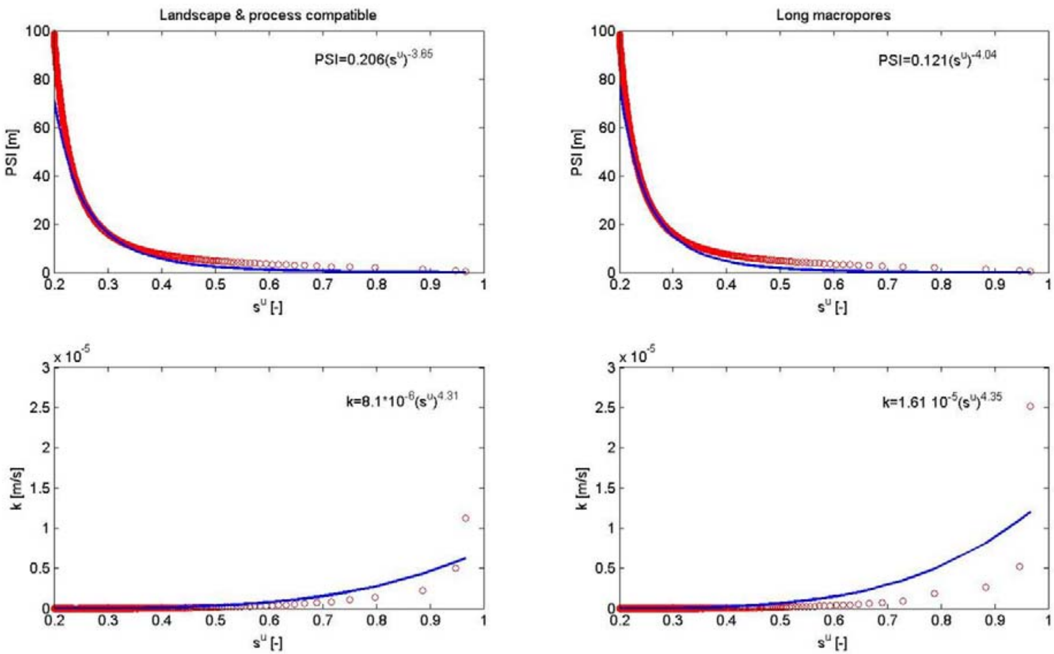

Fig. 5. Hillslope/REW scale soil hydraulic functions derived from simulated drainage experiments for the landscape and process compatible hillslope (left panels) and a hillslope with same spatial pattern of soils and macropores, but where the macropores reach continuously to the lower boundary of the modelling domain (right panels). The 95%-confidence limits as well as the R^2 of the fits are given in Table 2.

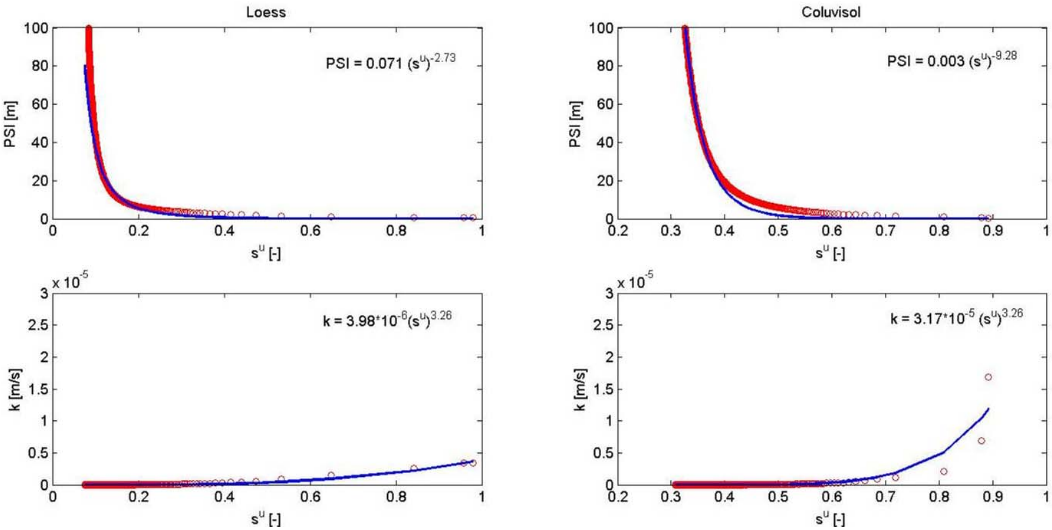

Fig. 6. Hillslope/REW scale soil hydraulic functions derived from simulated drainage experiments for a homogeneous hillslope with a loess soil (left panels, REV scale hydraulic parameters given in Table 1) and a homogeneous hillslope with a Colluvisol soil (right panels). The 95%-confidence limits as well as the R^2 of the fits are given in Table 2.

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