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One-dimensional expression to calculate specific yield for shallow groundwater systems with microrelief

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Abstract

Although the importance to account for microrelief in the calculation of specific yields for shallow groundwater systems is well recognized, the microrelief influence is often treated very simplified, which can cause considerable errors. We provide a general one-dimensional expression that correctly represents the effect of a microrelief on the total specific yield that is composed of the soil and surface specific yield. The one-dimensional expression can be applied for different soil hydraulic parameterizations and soil surface elevation frequency distributions. Applying different van Genuchten parameters and a simple linear microrelief model, we demonstrate that the specific yield is influenced by the microrelief not only when surface storage directly contributes to specific yield by (partial) inundation but also when water levels are lower than the minimum surface elevation. Compared with a simplified representation of the soil specific yield, in which a mean soil surface is assumed for the calculation of soil specific yield, the correct representation can lead to lower as well as higher soil specific yields depending on the specific interaction of the soil water retention characteristics and the microrelief. The new equation can be used to obtain more accurate evapotranspiration estimates from water level fluctuations and to account for the effect of microtopographic subgrid variability on simulated water levels of spatially distributed hydrological models. © 2015 The Authors *Hydrological Processes* Published by John Wiley & Sons Ltd.

Key Words specific yield; surface storage; water table fluctuation; van Genuchten; microrelief

Introduction

Water table depth is one of the crucial state variables of shallow groundwater systems such as wetlands and riparian zones. Shallow groundwater ecosystems are highly dependent on the typical site-specific water table depth dynamics and react very sensitively to its disturbance (Dorrepaal *et al*., 2009; Jenerette *et al*., 2012). The water level monitoring, interpretation and modification in course of restoration projects are of crucial importance for nature conservation. For flood control, knowledge about the free water storage capacity and water release behaviour before and after heavy rainfall periods is essential for the prediction accuracy of forecasting models (De Roo *et al*., 2003). Furthermore, water table depth fluctuations are increasingly used for evapotranspiration and groundwater recharge estimates following the pioneering work of White (1932) (Loheide *et al*., 2005; Mould *et al*., 2010; Fahle and Dietrich, 2014; McLaughlin and Cohen, 2014; Wang and Pozdniakov, 2014). For these scenarios and applications, a detailed physical and quantitative understanding of the fluctuations and how they are related to the ability of the system to store water is a prerequisite.

For flat soil surfaces, the water table depth dynamics within the soil profile of shallow groundwater systems as a response to boundary fluxes is primarily controlled by the water retention characteristics of the soil in and above the range of the water level fluctuations. Figure 1a and 1b shows the integrals of two soil moisture profiles, $A_{zu,\mathrm{soil}}$ and $A_{zl,\mathrm{soil}}$, that are determined by the water retention characteristics of a soil at two hydrostatic equilibria of an upper (*zu*) and a lower water level (*zl*). Their difference ΔA_{soil} ($A_{zu,\mathrm{soil}} - A_{zl,\mathrm{soil}}$) is shown in Figure 1c. For the case of a decreasing water level, ΔA_{soil} is equal to the amount of water released by a soil, e.g. due to evaporation. In a normalization step, ΔA_{soil} is usually divided by the water level change (Δz), which results into a variable that is known as specific yield (S_y) (Childs, 1960). S_y is often used for the analysis and the modelling of water level fluctuations. For homogeneous zones of deeper groundwater systems, this value is constant. In contrast, for shallow groundwater systems with homogeneous soils, it changes with depth depending on the distance to the soil surface (Duke, 1972; Crosbie *et al*., 2005; Cheng *et al*., 2015; Wang and Pozdniakov, 2014), because the soil moisture profile above the water level is truncated by the soil surface before reaching residual water content. Because of the truncation, the soil volume that can release water is still increasing when water levels decrease; i.e. S_y is increasing with depth.

Following Figure 1 and the paragraph in the preceding text, the specific yield of the soil ($S_{y,\mathrm{soil}}$) for a certain depth increment between *zu* and *zl* can be calculated as the difference of the integrals of two soil moisture profiles ($\Delta A_{\mathrm{soil}} = A_{zu,\mathrm{soil}} - A_{zl,\mathrm{soil}}$) of two water levels divided by Δz with the following equation (e.g. Crosbie *et al*., 2005 and Cheng *et al*., 2015):

$$
\begin{aligned}
S_{y,\mathrm{soil}} &= \frac{1}{\Delta z}\cdot\left(A_{zu,\mathrm{soil}} - A_{zl,\mathrm{soil}}\right) \\
&= \frac{1}{\Delta z}\cdot\left(\underbrace{\Delta z\cdot\theta_s + \int_{zu}^{0}\theta(z)dz}_{A_{zu,\mathrm{soil}}} - \underbrace{\int_{zl}^{0}\theta(z)dz}_{A_{zl,\mathrm{soil}}}\right) \\
&= \theta_s - \frac{1}{\Delta z}\int_{zu}^{zl}\theta(z)dz \qquad (1)
\end{aligned}
$$

where *zl* is the lower and *zu* is the upper water level ($\Delta z = zu - zl$) with z being 0 at the soil surface (later in case of a microrelief, $z = 0$ corresponds to the mean elevation of the soil surface) and negative below the ground. $\theta(z)$ is the volumetric water content at pressure head $h = z$. It equals the saturated water content θ_s for pressure heads $h > 0$. Several authors gave analytical expressions for calculating S_y based on the parameterization of the water retention function by Brooks and Corey (1964) (Duke, 1972; Nachabe, 2002) and by van Genuchten (1980) (Crosbie *et al*., 2005; Cheng *et al*., 2015) in the following referred as *VG*. It should be noted that analytical expressions calculating S_y with *VG* as parameterization for θ are an approximation, e.g. by means of Taylor series in Cheng *et al*. (2015), with increasing errors for larger water level changes.

For periods of inundation, S_y is defined by the specific yield above the soil surface ($S_{y,\mathrm{surface}}$), which is here assumed to be 1, which corresponds to an open water surface. In some studies, a volume replacement by the plant material fraction (e.g. tree trunks) has been considered, which reduces $S_{y,\mathrm{surface}}$ accordingly (Sumner, 2007; McLaughlin and Cohen, 2014). For water level changes approaching the soil surface, changes in soil water content are small. According to Equation (1), this leads to S_y values near 0 for water levels close to the soil surface with an abrupt transition to 1 in case of inundation. It should be noted that the transition from surface to soil storage is, except for bare soil, not abrupt but continuous and successively influenced by plant material. The separation into soil and surface storage is a conceptual simplification that is commonly made to approximate this distinct change of S_y along this transition. Depending on the vegetation, part of the vegetation layer could also be attributed to the soil compartment when it acts like a porous system that significantly releases water in the range of the occurring matric potential fluctuations. This is, for example the case for the peat moss layer in bog ecosystems.

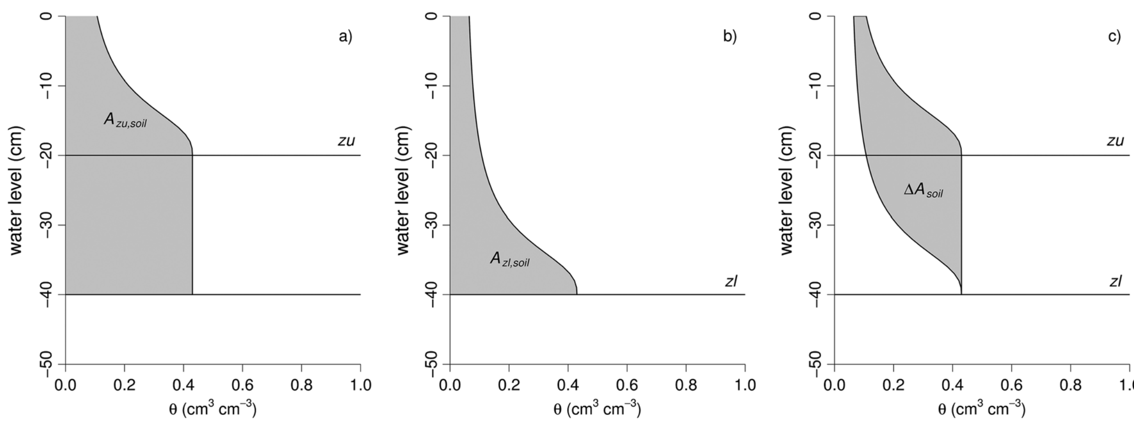

Figure 1. Integrals of the soil moisture profiles ($A_{zu,\mathrm{soil}}$, $A_{zl,\mathrm{soil}}$) of an upper water level (*zu*) (a), lower water level (*zl*) (b) and the difference (ΔA_{soil}) between $A_{zl,\mathrm{soil}}$ and $A_{zu,\mathrm{soil}}$ (c)

Many kinds of landscapes that (can) occur at shallow groundwater levels are characterized by a distinctive microrelief leading to a mosaic of inundated and non-inundated areas such as, e.g. pits and mounds in forests (Lyford and MacLean, 1966; McClellan *et al.*, 1990), heathlands (Myerscough *et al.*, 1996), ridge and slough environments (Sumner, 2007), hummocks and hollows in peatlands (Nungesser, 2003) and corrugated fields as relics of arable cultivation (Sittler, 2004). A schematic microrelief with an exemple water level at the mean surface height of the microrelief (μ) is shown in Figure 2. A microrelief can be described as cumulative frequency distribution ($F_{(s)}$) of the soil surface elevations. Traditional approaches would lead to very different S_y values for the two dip wells 1 and 2. For the water level given in Figure 2 at μ, dip well 1 would be completely flooded resulting in S_y of 1, and S_y of dip well 2 would only be influenced by the water retention characteristics of the soil (also indicated in Figure 2). However, as partly inundated areas around dip wells influence water level changes, S_y should be calculated as spatial average. Following this, for both dip wells, 50% of the microrelief is inundated in Figure 2 at the given water level at μ. Thus, S_y is a combination of $S_{y,\text{soil}}$ and $S_{y,\text{surface}}$ with a continuous transition from $S_{y,\text{soil}}$ to $S_{y,\text{surface}}$ for a rising water level depending on the distribution of soil surface elevations (Sumner, 2007).

Ignoring the transition leads to unrealistic low S_y values for shallow water level changes in areas with a microrelief. The importance to account for this transition is well recognized (McLaughlin and Cohen, 2014). However, the way it is accounted for often occurs in a simplified manner, in which a constant $S_{y,\text{soil}}$ is assumed. In this approach, S_y equals to $S_{y,\text{soil}}$ for water levels below the lowest height and to $S_{y,\text{surface}}$ above the highest height of the microrelief. In between, *Sy* is interpolated by the fraction of inundated area (McLaughlin and Cohen, 2014).

To our knowledge, the study by Sumner (2007) is the only study in which both the nonlinear specific yield of the soil (that approaches zero close to the soil surface) and the effect of the microrelief have been considered simultaneously. In his study, this was realized by averaging S_y over multiple soil columns of different surface elevations. In this paper, we revisit the simultaneous consideration of nonlinear $S_{y,soil}$ and microrelief effects for the calculation of S_y. There are two reasons for revisiting this topic. Firstly, the 'multi-column' approach of Sumner (2007) needs a high number of soil columns to achieve convergence for the mean *Sy* value, i.e. to achieve a proper integration about the microrelief. Albeit providing correct results, this approach is computationally inefficient. The inefficiency may become a relevant problem when a high number of these calculations are required either for a spatially distributed model or during inverse parameter estimation. Secondly, although Sumner (2007) presented a correct representation of a simultaneous consideration of nonlinear $S_{y,\text{soil}}$ and microrelief effects, the study failed to illustrate and discuss the important implications on S_y when water levels are below the soil surface. We believe that this is one reason that this approach has not been adopted in all subsequent publications on this topic.

In this paper, we present a new one-dimensional (1D) expression for the calculation of S_y that accounts for both the effect of a continuously increasing contribution of surface storage and the effect of the soil volume distribution around the mean soil surface on S_y. With the correct 1D representation, we demonstrate that S_y values are also affected by the microrelief when water levels are below the lowest soil surface elevation. Differences are illustrated by comparing total S_y values assuming a flat soil surface at the mean soil surface elevation ($S_{y,\text{flat}}$) (calculated according to Equation (1)) and soil specific yield values that are correctly calculated by accounting for microrelief effects ($S_{y,\text{uneven}}$).

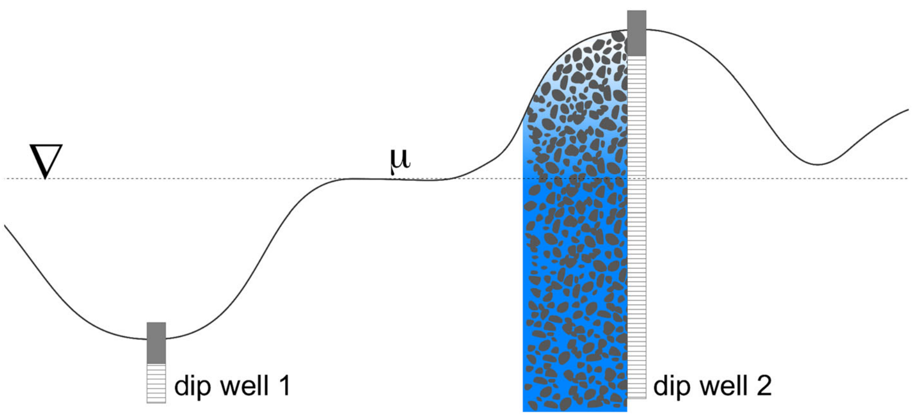

Figure 2. Exemplary microrelief with a water level at the mean surface elevation (μ), which here corresponds to 50% inundation. The saturated and unsaturated zones of the soil are illustrated to demonstrate the vertical distribution of air-filled pore space that is available for further water storage. Further, two dip wells are indicated at different surface elevations

Theory

In the following, we consider a 1D effective representation of a soil column with a flat or uneven soil surface. Accordingly, the total specific yield (S_y) for a certain depth increment is composed of the soil specific yield ($S_{y,\text{soil}}$) and the surface specific yield ($S_{y,\text{surface}}$).

$$S_y = S_{y,\text{soil}} + S_{y,\text{surface}} \tag{2}$$

Assuming $F_s(z)$ is the cumulative frequency distribution normalized between 0 and 1 of soil surface elevations, $S_{y,\text{surface}}$ can be calculated as

$$S_{y,\text{surface}} = \begin{cases} 1 & zl \geq z_{\text{elev,max}} \\ \frac{1}{\Delta z} \int_{zl}^{zu} F_s(z)dz & zl < z_{\text{elev,max}} \text{ and } zu > z_{\text{elev,min}} \\ 0 & zu \leq z_{\text{elev,min}} \end{cases} \tag{3}$$

with $S_{y,\text{surface}} = 0$ when zu is below the lowest elevation ($z_{\text{elev,min}}$) of the soil surface and $S_{y,\text{surface}} = 1$ when zl is above the highest elevation ($z_{\text{elev,max}}$) of the soil surface. For a flat surface, $S_{y,\text{surface}}$ abruptly changes from 0 to 1 at the soil surface, and for uneven surfaces, this transition is continuous.

In a 1D representation of $S_{y,\text{soil}}$ that includes any microrelief effects, the parameter $S_{y,\text{soil}}$ must be interpreted as a spatial average. For heights above the lowest surface elevation, the soil volume covers only parts of the total volume. Thus, to obtain the spatially averaged (effective) soil moisture, the soil moisture must be multiplied by the fraction that is actually covered by soil ($1 - F_s(z)$). This has to be performed for the whole soil moisture profile in dependence on the cumulative distribution of the surface elevations ($F_s(z)$). Besides the horizontal reduction of the soil moisture profiles, the soil moisture profiles need to be vertically extended to the maximum height of the surface elevation. This can easily be seen looking at Figure 2. The soil moisture profile of dip well 1 should be extended to the maximum height of the surrounding microrelief. The complete spatially averaged (effective) soil moisture profiles can then be used to calculate $A_{zl,\text{soil}}$ and $A_{zu,\text{soil}}$.

Including the correct representation of the microrelief in the calculation of the soil moisture profiles gives

$$A_{zl,\text{soil}} = \int_{zl}^{\infty} (1 - F_s(z))\theta(z - zl)dz \tag{4}$$

$$A_{zu,\text{soil}} = \int_{zl}^{\infty} (1 - F_s(z))\theta(z - zu)dz \tag{5}$$

The bounds of the integrals are set to infinity because the cumulative frequency distribution reaches 1 at the highest surface elevation. At this point, the effective soil moisture is 0, which results from the term $(1 - F_s(z))$.

Following section on Introduction, $S_{y,\text{soil}}$ is given by ΔA_{soil} ($A_{zu,\text{soil}} - A_{zl,\text{soil}}$) divided with Δz. Substituting Equations (4) and (5) into Equation (1) leads to

$$\begin{aligned} S_{y,\text{soil}} &= \frac{1}{\Delta z} \cdot \left(\int_{zl}^{\infty} (1 - F_s(z))\theta(z - zu)dz - \int_{zl}^{\infty} (1 - F_s(z))\theta(z - zl)dz \right) \\ &= \frac{1}{\Delta z} \cdot \int_{zl}^{\infty} (1 - F_s(z))[\theta(z - zu) - \theta(z - zl)]dz \end{aligned} \tag{6}$$

For a flat soil surface, Equation (6) simplifies to Equation (1).

Discussion and Conclusions

Microrelief influence on effective soil moisture profile and specific yield

In the following, the influence of the microrelief on the effective 1D soil moisture profile is demonstrated (Figure 3). For demonstration, we assume a linear surface elevation model (corresponding to a uniform frequency distribution) in the calculation of the effective soil moisture profiles and specific yields. The linear model requires two microrelief parameters, i.e. the lowest and highest surface elevation. The contribution of the linear surface storage starts at −20 cm and ends at 20 cm (Figure 3b). The linear model can be replaced by more complex frequency distributions when adequate data are available. The influence is illustrated with van Genuchten parameters of two sands that are well documented in ROSETTA (Schaap *et al.*, 2001) implemented in HYDRUS-1D (Šimůnek *et al.*, 2013), which is a frequently used soil hydraulic parameter catalogue. For ‘sand 1’, we used soil hydraulic parameters (*VG*) of the default sand from HYDRUS-1D (θ_s: 0.43, θ_r: 0.045, α: 0.145, n: 2.68). For ‘sand 2’, soil hydraulic parameters (*VG*) were derived by ROSETTA (Schaap *et al.*, 2001) for a pure (100%) sand (θ_s: 0.376, θ_r: 0.0507, α: 0.0344, n: 4.4248). The parameters indicate that both sands, 1 and 2, are unimodal sands that start to dewater substantially at matric potentials of about −7 cm (=1/α) and −30 cm, respectively.

Figure 3a shows the effective soil moisture profiles for a water level change from −30 to −10 cm for ‘sand 1’ for (i) a flat surface and (ii) an uneven surface. The effective soil moisture profile for case (ii) is extended in dependence on the distribution of the surface elevations (in our case up to 20 cm above the mean surface elevation). Below the mean surface elevation, the effective soil moisture is linearly reduced in dependence on the surface storage starting from −20 cm. The resulting integrals of the moisture profiles of the two cases ($\Delta A_{\text{soil,flat}}$ and $\Delta A_{\text{soil,uneven}}$) thus clearly differ in their vertical distribution.

To illustrate the implication for S_y, Figure 4 shows S_y values of water level changes of 1 cm between −100

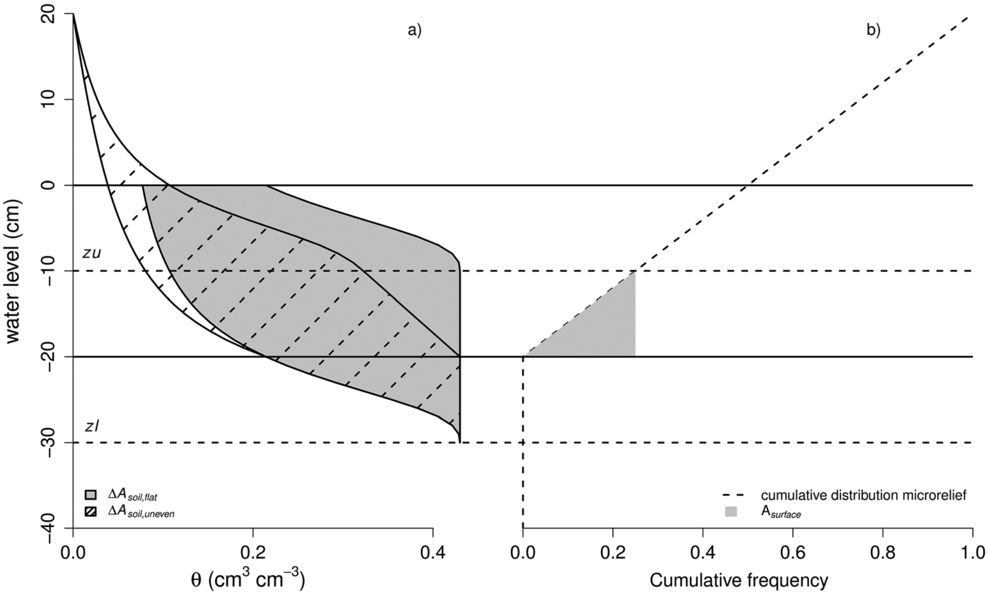

Figure 3. Influence of the soil surface elevation distribution on the effective soil moisture (θ) profiles for a water level change from $zl = -30$ cm to $zu = -10$ cm. (a) Effective soil moisture profiles of a flat surface ($\Delta A_{\mathrm{soil,flat}}$) (grey area) and uneven surface ($\Delta A_{\mathrm{soil,uneven}}$) (hatched area). Retention characteristic is described with *VG* parameters for 'sand 1'. (b) Cumulative linear surface elevation distribution (F_s) (dashed line) and the integral of the surface storage (A_{surface}) (grey area)

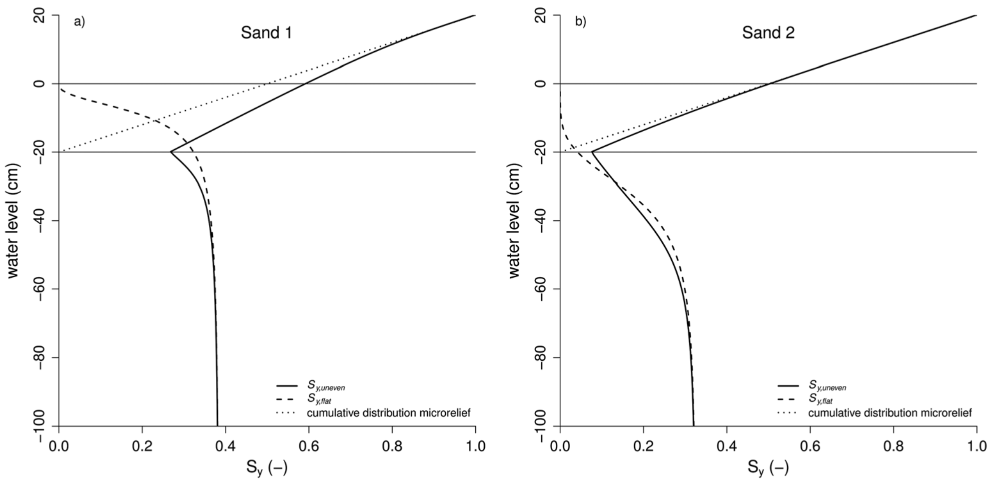

Figure 4. S_y values of water level changes of 1 cm between -100 and 20 cm for a simplified flat surface representation ($S_{y,\mathrm{flat}}$) and for an uneven surface ($S_{y,\mathrm{uneven}}$). Illustrated for 'sand 1' (a) and 'sand 2' (b)

and 20 cm. S_y values that were calculated assuming a flat soil surface at the mean surface elevation are referred as $S_{y,\mathrm{flat}}$, and S_y values that were calculated by taking into account the microrelief effect are referred as $S_{y,\mathrm{uneven}}$. As expected from the soil water retention function, $S_{y,\mathrm{flat}}$ decreases with lower water levels approaching 0 towards the flat soil surface. In contrast, $S_{y,\mathrm{uneven}}$ between -20 and 20 cm water level height is strongly controlled by the surface storage with S_y reaching 1 at $z = 20$ cm. This effect of the increasing inundated fraction on S_y is well recognized and accounted for in previous studies (McLaughlin and Cohen, 2014). However, when the microrelief effect on S_y has been accounted for in previous studies, the specific yield contribution of the soil was only accounted for as a constant value that is simply reduced by the fraction of the inundated area. We emphasize that this differs from Equation (6) in which $S_{y,\mathrm{soil}}$ is not a constant value but the microrelief affects the full soil moisture integral. It can be noted from Figure 4 that the microrelief has a considerable influence on S_y even for water levels below the lowest surface elevation, i.e. before the direct storage contribution of the microrelief to S_y. Figure 4a shows S_y values for 'sand 1'. Note the reduced S_y values between -40

and −20 cm. It results from the reduced soil volume in the pressure range in which the soil water capacity (i.e. the first derivative of the water retention function) of 'sand 1' is highest. The contrary effect, with higher S_y values just below −20 cm, is shown in Figure 4b for 'sand 2'. This sand has the highest capacity in the soil volume above the mean elevation; i.e. S_y values are increased by this additional soil volume compared with the flat surface reference. The two examples demonstrate the interaction of soil hydraulic parameters and microrelief and its effect on vertical distribution of S_y.

The difference between $S_{y,\mathrm{uneven}}$ and $S_{y,\mathrm{flat}}$ depends on the frequency distribution of the soil surface elevations and the retention characteristics of the soil. Above the lowest surface elevation, $S_{y,\mathrm{uneven}}$ is mainly controlled by $S_{y,\mathrm{surface}}$, i.e. by the range ($z_{\mathrm{elev,max}}$–$z_{\mathrm{elev,min}}$) and the type of the microrelief frequency distribution (uniform, normal, etc.). Below the lowest surface elevation, we noticed that varying the type of the microrelief frequency distributions has a minor effect on $S_{y,\mathrm{soil}}$. It is rather the range of the microtopographic height variation in combination with the retention characteristics of the soil that determines whether a strong effect can be expected or not. As a thumb rule, stronger effects occur when the soil releases relevant portions of its capillary water at matric potentials that are within the range of heights of the microtopographic variation. In the examples in the preceding text, this corresponds to matric potentials between 0 and −40 cm. Thus, stronger effects can be expected for coarse substrates.

We emphasize that in our examples, we assumed soil homogeneity for demonstration purpose, i.e. an effective parametric description of the soil profile, but soil moisture profiles of layered soils could equally be considered with the presented approach.

Possible applications of the equation

Here, we provided a simple 1D equation for calculating $S_{y,\mathrm{uneven}}$ that is valid for small and large water level changes and can be applied with any parameterization of θ and frequency distribution of surface elevations. The proposed equation can make a significant improvement in several applications, in which the effect of microtopographic variability on S_y must be represented with a 1D model conceptualization. In general, the resulting S_y depth distributions can be used to obtain more accurate estimates of water level fluctuations for regions with shallow groundwater levels.

As an application example, we here highlight the relevance of our study for the various recent papers that focus on calculating evapotranspiration from water level fluctuations with the method of White (1932). In these studies, S_y is the most crucial parameter. It became obvious in our discussion in the preceding text that the consideration of its depth dependence will be important to derive reliable evapotranspiration estimates for different water table depths. Here, we provide the necessary equation to obtain physically correct vertical S_y profiles from site-specific soil and microrelief characteristics. To our knowledge, in all recent studies on the estimation of evapotranspiration from water level fluctuations (Cheng *et al*., 2015; McLaughlin and Cohen, 2014; Wang and Pozdniakov, 2014), either $S_{y,\mathrm{flat}}$ or constant $S_{y,\mathrm{soil}}$ was used without taking into account the full microrelief effect on $S_{y,\mathrm{soil}}$. In the case of uneven surfaces, this may lead to considerable errors.

As a second application example, we want to highlight the possible use of the equation in spatially distributed models. Because of computational limitations, spatially distributed catchment (or larger scale) models are often computed on spatial grids that are much coarser than the typical microtopographic variation. Thus, an effective parameterization is needed to account for the subgrid (i.e. within a grid cell) height variability of the soil surface. Similar to Manning's roughness coefficient (Manning *et al*., 1890) that accounts for the resistance of microrelief and vegetation to open channel or overland flow, our approach can be used to obtain the S_y depth distributions for each grid cell from the information about the subgrid microtopographic variability. With the increasing availability of detailed digital elevation models from laser scanning data, it is easily possible to account for subgrid variability for each grid cell individually. Our simple equation ensures a computationally efficient application. In coupled hydrological models, in which the unsaturated zone is modelled dynamically with Richards' equation, the soil model domain needs to be reduced by the cumulative frequency distribution of the surface elevations similar to that we proposed in our derivation of Equation (6). A discussion of the implementation of our approach in such fully coupled hydrological models is beyond the scope of this paper.

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