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Soil moisture storage estimation based on steady vertical fluxes under equilibrium

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ABSTRACT

Soil moisture is an important variable for hillslope and catchment hydrology. There are various computational methods to estimate soil moisture and their complexity varies greatly: from one box with vertically constant volumetric soil water content to fully saturated-unsaturated coupled physically-based models. Different complexity levels are applicable depending on the simulation scale, computational time limitations, input data and knowledge about the parameters. The Vertical Equilibrium Model (VEM) is a simple approach to estimate the catchment-wide soil water storage at a daily time-scale on the basis of water table level observations, soil properties and an assumption of hydrological equilibrium without vertical fluxes above the water table. In this study VEM was extended by considering vertical fluxes, which allows conditions with evaporation and infiltration to be represented. The aim was to test the hypothesis that the simulated volumetric soil water content significantly depends on vertical fluxes. The water content difference between the no-flux, equilibrium approach and the new constant-flux approach greatly depended on the soil textural class, ranging between ~1% for silty clay and ~44% for sand at an evapotranspiration rate of 5 mm·d^{-1}. The two approaches gave a mean volumetric soil water content difference of ~1 mm for two case studies (sandy loam and organic rich soils). The results showed that for many soil types the differences in estimated storage between the no-flux and the constant flux approaches were relatively small.

1. Introduction

The unsaturated soil water content makes up a very small fraction of the global water storage, but plays a defining role in hydrological processes from hillslope to global scales. The soil water content and distribution affects soil aggregate formation (Denef et al., 2001), development and mobility of microbial communities (Fierer and Schimel, 2002), carbon mineralization processes (Tietema et al., 1992), soil organic matter concentration, and decomposition (Falloon et al., 2011; Siena et al., 2014), as well as weathering (Erlandsson et al., 2016). Plant roots live mostly in the unsaturated soil, and the water availability there controls the growth, carbon uptake and evapotranspiration (Borken and Matzner, 2009).

Soil moisture storage and its vertical variation are often represented by simplistic or very complex approaches. Simplistic approaches utilize vertically constant soil moisture, (e.g., Bergström, 1992; Milly, 1994; Jothityangkoon et al., 2001; Pathiraja et al., 2016; Nijzink et al., 2016). In complex approaches, the integrated soil water content (below referred to as unsaturated zone storage) is represented by layers in physically-based models, which resolve the fluxes and storage variation with depth (e.g., Brunner and Simmons, 2012; Šimůnek et al., 2008).

The Vertical Equilibrium Model (VEM) was introduced as an alternative between these simplistic and complex approaches, and considers a more realistic vertical distribution of soil moisture in a simple way. With VEM the volumetric soil water content is based on the water table position assuming a zero-flux equilibrium (Seibert et al., 2011). Under this assumption, the moisture profile above the water table should be in equilibrium and determined by the depth of the water table below the soil surface. While in simplistic approaches with a vertically constant water content the unsaturated water storage is linearly related to the depth of the groundwater table, this relationship is, at least for the storage above shallow groundwater tables, in reality strongly non-linear. VEM allows for consideration of this non-linear relationship. Thanks in part to the zero-flux equilibrium assumption, the input

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data requirements are relatively small (water table position, porosity and soil water retention curve) and no information on unsaturated hydraulic conductivities is needed. The model was developed for shallow groundwater systems, and in particular the moraine soils of the broad zone in the high latitude boreal and northern temperate zone where glaciers have shaped the landscape. The strength of VEM is that it not only takes highly heterogeneous profiles into account, but it also requires low computational time. However, the limitation of disregarding vertical fluxes will lead to the model overestimating the volumetric soil water content during dry periods, as soil moisture draw-down in the upper soil layers due to evapotranspiration is not accounted for. This was indeed noted in a test of the model against field observations (Seibert et al., 2011). VEM was used to calculate the unsaturated zone storage, which was incorporated in the calculation of turnover time at the Gårdsjön Covered Catchment, in southern Sweden (Bishop et al., 2011, Seibert et al., 2011), and at the Krycklan Study Catchment in northern Sweden (Amvrosiadi et al., 2017).

Here we extended VEM so that infiltration and evapotranspiration were taken into account as steady vertical fluxes. The aim of this study was to test the hypothesis that the modeled total volumetric soil water content stored in a soil profile varies significantly depending on the vertical flux assumption. For this, the volumetric soil water content of eleven soil textural classes were simulated and compared under various flux conditions with assumptions on vertical fluxes: 1) the zero flux assumption (VEM_0, which is the original VEM model) and 2) the constant flux assumption (VEM_F, which is the VEM extension developed in this study). The two models were compared to each other and also evaluated against measurements from two case studies.

2. Materials and methods

2.1. Model description

In the original version of VEM, the unsaturated water content is calculated as a function of the pressure potential. In the case of zero vertical flux ($F = 0$) and vertical equilibrium, the pressure potential equals the gravimetric potential, determined by the water table position (Seibert et al., 2011). The inputs to the model are water table depth (*WTD*) and soil properties (described by soil water retention curves).

In the extended version presented here, vertical fluxes were introduced ($F < 0$ for infiltration and $F > 0$ for evapotranspiration). The column was divided into 1 cm thick sublayers, for which the water content was quantified as a function of water table depth and vertical flux.

Effective saturation S_e [−], which is defined as in Eq. (1), can be also expressed as a function of matric potential ψ, (Eq. (2)), (van Genuchten, 1980).

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (1)$$

$$S_e = [1 + (a \cdot |\psi|)^n]^{-\lambda}, \quad \lambda = 1 - 1/n, \quad 0 < \lambda < 1 \quad (2)$$

where θ ($m^3 \cdot m^{-3}$) is the actual volumetric water content, θ_s ($m^3 \cdot m^{-3}$) is the saturation water content, θ_r ($m^3 \cdot m^{-3}$) is the residual water content, a [m^{-1}] is the inverse of air entry pressure, n [−] is an index for pore size distribution, and ψ(m) here is defined as the matric potential in the middle of each sublayer.

The effective saturation was linked to relative hydraulic conductivity K_r [$m \cdot d^{-1}$] following Mualem's model (Eq. (3)), (Mualem, 1976; van Genuchten and Nielsen, 1985).

$$K_r = \sqrt{S_e} \cdot \left[1 - \left(1 - S_e^{1/\lambda}\right)^{\lambda}\right]^2 \quad (3)$$

Here Mualem's model was preferred over Burdine's (Burdine, 1953), as the former can be used for more soil types while the latter is limited for the cases with $n < 2$ (van Genuchten and Nielsen, 1985).

Eqs. (2) and (3) were then substituted in the Buckingham – Darcy equation (Eq. (4)) (Buckingham, 1907).

$$F = -K \cdot \nabla H = -K_r \cdot K_s \cdot \frac{(\psi_{i+1} + z_{i+1}) - (\psi_i + z_i)}{z_{i+1} - z_i} \quad (4)$$

where F [$m \cdot d^{-1}$] is the specific vertical flux through the sublayer (hereafter referred to as vertical flux for the sake of brevity), K_s [$m \cdot d^{-1}$] is the saturated hydraulic conductivity, and z [m] is the gravimetric potential.

At the water table, where the bottom boundary of the deepest sublayer ($i = 1$) is located, the matric potential is ψ_i equal to zero. The matric potential of the top boundary of this sublayer was obtained by numerically solving Eq. (4) for ψ_{i+1}, for a pre-defined value of F (here we used values ranging from −5 to 5 $mm \cdot d^{-1}$). The matric potential for the next sublayer above was computed similarly, in an iterative manner keeping F constant through the entire column. This implies that all ET exits the soil column at the soil surface, when in fact the transpiration is extracted deeper in the column by roots, thus reducing the actual upward flux through the soil matrix. A numerical solution was required, as Eq. (4) is not analytically solvable, considering that K_r is also a function of ψ (see Eqs. (2) and (3)). For the numerical solution the *fzero* method in Matlab was employed, which uses a combination of bisection, secant, and inverse quadratic interpolation methods (Mathworks, 2016). This calculation process was then repeated iteratively to compute the soil moisture for each layer up to the soil surface. Depending on soil parameterization (i.e. depending on the assumed textural class), Eq. (4) was solvable up to different heights above water table. This height (which also depends on vertical flux rate) represents the position where the unsaturated hydraulic conductivity decreases more with decreasing water content than what can be compensated for by an increasing matric potential gradient. The thickness of the hydraulic continuity zone, i.e. the maximum height above water table where the upward flux rate does not exceed the hydraulic conductivity is referred to as D_{max} (Sadeghi et al., 2012; Sadeghi et al., 2014).

2.2. Simulation of example textural classes

The water content of eleven soil column scenarios (sand, loam, sandy loam, sandy clay loam, silt loam, silty clay loam, clay loam, silt, clay silty clay and sandy clay) were examined under the assumption of a series of steady state vertical fluxes at the soil surface, varying from −5 to 5 $mm \cdot d^{-1}$. The highest upward flux of 5 $mm \cdot d^{-1}$ used here was selected to match the highest estimated ET rate at the case study site, discussed in Section 2.3. The hydraulic parameters of these classes were adapted from Carsel and Parrish (1988). For each textural class and vertical flux assumption the water content was quantified from the bottom boundary up to D_{max}. For $z > D_{max}$ the above described method is not applicable; therefore, to treat the soil above D_{max}, the effective saturation between and soil surface was linearly interpolated, assuming $S_e = 0$ at the surface (i.e., residual water content).

The integrated water content difference W_{diff} between zero- and various vertical flux conditions was defined as in Eq. (5).

$$W_{diff} = \left|\frac{W_0 - W_F}{W_0}\right| \cdot 100\ (\%) \quad (5)$$

where W_0 and W_F are the integrated soil water contents (i.e. unsaturated zone storage) for $F = 0$ and $F \neq 0$ respectively.