The Report of UBMOD

- **Overview**

Since 1970s, various numerical methods have been developed to simulate unsaturated soil water movement at various temporal and spatial scales Among them, the two major approaches are numerical solutions of the Richards' equation and the reservoir cascade scheme. Based on the principle of mass conservation and the Darcy-Buckingham law, the Richards' equation is the fundamental governing equation that describes the unsaturated flow, and its numerical solutions have been implemented in many public-domain and commercial software, such as HYDRUS, SWIM, FEFLOW. The Richards' equation has solid theoretical foundation, and its numerical solutions have been widely used. However, using Richards' equation requires intensive input data and model parameters, which are not always available in practice due to spatial heterogeneity. In addition, the computational cost for large-scale modeling is high caused by the highly nonlinearity of the Richards' equation.

The water balance models, which, also known as conceptual models, are physically based on water mass balance. In water balance models, simplified or empirical expressions, rather than the Darcy-Buckingham law, are used to describe the movement of soil water. Many water balance models are currently in use because of their computational efficiency and stability, especially in large-scale modelling where data and fundamental understanding of the factors and processes of soil water movement are lacking. The widely used water balance models include SWAT, INFIL

3.0, SoilWat, DSSAT.

Many water balance models take the assumption that the gravitational potential dominates over matric potential, and therefore neglect matric potential and only simulate downward flux of soil water driven by gravitational potential. As a result, the "tipping-bucket" method has been used to describe the infiltration, redistribution and drainage processes. This is a reasonable assumption, when groundwater recharge is the major concern and when the errors introduced by neglecting matric potential is insignificant. However, when the errors alter soil water movement and the salt accumulation at the top soil due to the upward flux especially in agricultural areas with strong evapotranspiration, the assumption of neglecting matric potential becomes invalid.

- **Model development**

The UBMOD is a water balance model based on a hybrid of numerical and statistical methods.

There are four major components to describe the soil water movement in UBMOD model, as shown in Fig. 1. Firstly, the vertical soil column is divided into a cascade of "buckets" and each "bucket" corresponds to a soil layer. The "buckets" will be filled to saturation from the top layer to the bottom layer if there is infiltration, which is referred as the allocation of infiltration water. Specifically speaking, the infiltration water first fills the top "bucket", then the excessive infiltration water moves downward to the next "bucket", until all the infiltration water is allocated in the "buckets", as shown in Fig.

1(a). The governing equation of layer i is,

$$q_i = \min\left(M_i \times \left(\theta_{s,i} - \theta_i\right), I - I_{d,i-1}\right), \tag{1}$$

where i indicates the vertical soil layer, i = 1, … ,j; q_i is the amount of allocated water per unit area of layer i [L]; M_i is the thickness of layer i [L]; θ_i is the initial soil water content of layer i [L^3L^{-3}]; $\theta_{s,i}$ is the saturated soil water content of layer i [L^3L^{-3}]; I is the quantity of infiltration water per unit area [L]; $I_{d,\,i\text{-}1}$ is the consumed infiltration water per unit area by upper layers for the specific layer i [L]; I - $I_{d,\,i\text{-}1}$ is the infiltration water applied to the upper boundary of soil layer i [L]. The infiltration rate I is an input data in the model, and the partitioning of rainfall between infiltration and runoff has not been considered by now. As shown in Fig. 1(a), the first three layers are filled to saturation, and the fourth layer is filled with the residual infiltration water.

Secondly, when the soil water content exceeds the field capacity, the soil water will move downward driven by the gravitational potential. The governing equation is,

$$\frac{\partial \theta}{\partial t} = -\frac{\partial K(\theta)}{\partial z}, \tag{2}$$

where t is the time [T]; $K(\theta)$ is the unsaturated hydraulic conductivity [LT^{-1}] as a function of soil water content; z is the elevation in the vertical direction [L]. The vertical coordinate is positive downward. The unsaturated hydraulic conductivity $K(\theta)$ in Eq. 2 is a function of soil water content θ. The relationship between $K(\theta)$ and θ is characterized by empirical formulas for the purpose of simplifying calculation and eliminating the soil hydraulic parameters. These empirical formulas are referred to as drainage functions. The commonly used equations are listed in Table 1.

Table 1 Empirical drainage functions representing the relationship between the unsaturated hydraulic conductivity $K(\theta)$ and soil water content θ.

Name	Function	Parameters	Application
Linear equation	$K(\theta)=K_s\times\frac{\theta-\theta_f}{\theta_s-\theta_f}$	K_s, θ_s, θ_f	SWAT (Arnold et al., 2012), SoilWat (Holzworth et al., 2014; Verburg, 1995)
Exponential equation	$K(\theta)=K_s\times\exp\left(-\alpha\times\frac{\theta-\theta_w}{\theta-\theta_w}\right)$	K_s, θ_s, θ_f, θ_w, α	Kendy (Kendy et al., 2003), Jiang (Jiang et al., 2008)
Power equation	$K(\theta)=K_s\times\left(\frac{\theta}{\theta_s}\right)^{\beta}$	K_s, θ_s, θ_f, β	SWRRB (Merritt et al., 2003), DPM (Vaccaro, 2007), INFIL 3.0 (FILL, 2008), EPIC (Wang et al., 2012), CREAMS (Adnan et al., 2017)
Exponential approximation equation	$K(\theta)=K_s\times\frac{\exp(\theta-\theta_f)-1}{\exp(\theta_s-\theta_f)-1}$	K_s, θ_s, θ_f,	BUDGET (Raes, 2002), Aquacrop (Abedinpour et al., 2014)
Square equation	$K(\theta)=K_s\times\left[\frac{\theta-\theta_f}{\theta_s-\theta_f}\right]^2$	K_s, θ_s, θ_f,	BOWET (Sluiter, 1998), BEACH (Sheikh et al., 2009)

Note: The parameters K_s, θ_s and θ_f are the saturated hydraulic conductivity (LT^{-1}), the saturated water content (L^3L^{-3}) and the field capacity (L^3L^{-3}); θ_w is the soil water content at wilting point (L^3L^{-3}); α in the exponential equation is a site-specific parameter determined mainly from soil characteristics and it has an inverse relationship with K_s, and the value ranges between 10 to 30 (Jiang et al., 2008); The parameter β in the power equation ensures $K(\theta)$ to approach zero when θ approaches to θ_f, and Arnold et al. (1990) proposed an empirical formula as $\beta=-2.655/\log(\theta_f/\theta_s)$.

Thirdly, the source/sink terms are used to account for soil evaporation and crop transpiration. The governing equation is as follows,

$$\frac{\partial\theta}{\partial t}=-W\,, \tag{3}$$

where W is the source/sink term [T^{-1}]. The Penman-Monteith formula and Beer's law (also known as Ritchie-type equation) are adopted in UBMOD to estimate the potential soil evaporation E_p and potential crop transpiration T_p. Then E_p and T_p are distributed to each layer based on the evaporation cumulative distribution function and the root density function. The actual soil evaporation and crop transpiration are obtained by discounting E_p and T_p with the soil water stress coefficient.

Lastly, we calculate the diffusive movement driven by the matric potential. The governing equation is,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta) \frac{\partial \theta}{\partial z} \right), \tag{4}$$

where $D(\theta)$ is the hydraulic diffusivity [L^2T^{-1}], $D(\theta) = K(\theta) \times {\partial h}/{\partial \theta}$, where h is the matric potential [L]. The finite difference method is used to solve the governing equation. A new empirical formula is presented to describe the hydraulic diffusivity $D(\theta)$. The expression formula of $D(\theta)$ has an exponential form, as

$$D(\theta) = 10^{a \times S(\theta) + b} \tag{5}$$

where $S(\theta)$ is the effective saturation (-); a and b are two intermediate parameters. In order to eliminate the parameters, we calculate the hydraulic diffusivity $D(\theta)$ of different soils by van Genuchten model firstly, and then fit the hydraulic diffusivity $D(\theta)$ by Eq. 5. Furthermore, as shown in Fig. 2, we establish the relationship between the two intermediate parameters (a and b) and the saturated hydraulic conductivity K_s as,

$$\begin{cases} b = -3.55 + 0.55 \times \log_{10}(K_s) - 1.36 \times \log_{10}(K_s)^2 \\ a = 3.72 + 0.61 \times \log_{10}(K_s) + 1.52 \times \log_{10}(K_s)^2 \end{cases}. \tag{6}$$

By following the steps above, the hydraulic diffusivity $D(\theta)$ of a specific soil type can be estimated with three physical meaning parameters (K_s, θ_s, and θ_r).

Soil water content is discontinuous at the material interface when a soil profile is heterogeneous. When adopting van Genuchten model to represent the soil water characteristics, the Eq. (4) can be expressed as,

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left(D(\theta)\left(\frac{\partial\theta}{\partial z}-\left(\frac{\partial\theta}{\partial\theta_s}\frac{\partial\theta_s}{\partial z}+\frac{\partial\theta}{\partial\theta_r}\frac{\partial\theta_r}{\partial z}+\frac{\partial\theta}{\partial\alpha}\frac{\partial\alpha}{\partial z}+\frac{\partial\theta}{\partial n}\frac{\partial n}{\partial z}\right)\right)\right), \tag{7}$$

where α and n are two parameters in van Genuchten model. The two terms, $\partial\theta/\partial\theta_s$ and $\partial\theta/\partial\theta_r$ can be easily calculated. The value of $\partial\theta/\partial\alpha$ is close to zero, which can be ignored, as shown in Fig. 3. A regression formula is developed to characteristic the relationship between n and the saturated hydraulic conductivity K_s. The specific equations are shown as follows,

$$\begin{cases}\dfrac{\partial\theta}{\partial\theta_s}=S(\theta)\\ \dfrac{\partial\theta}{\partial\theta_r}=1-S(\theta)\\ \dfrac{\partial\theta}{\partial n}=(\theta_s-\theta_r)S(\theta)\left[\dfrac{\ln(S(\theta))}{n(n-1)}-\dfrac{n-1}{n^2}\left(S(\theta)^{n/(1-n)}-1\right)\ln\left(S(\theta)^{n/(1-n)}-1\right)S(\theta)^{-n/(1-n)}\right]\\ n=0.9505+0.8883e^{0.7751\times\log_{10}(K_s)}\end{cases} \tag{8}$$

Therefore, the diffusive term of the heterogeneous soil can be calculated. With the help of the diffusive term, the UBMOD can consider upward soil water movement, which is ignored by most water balance models.

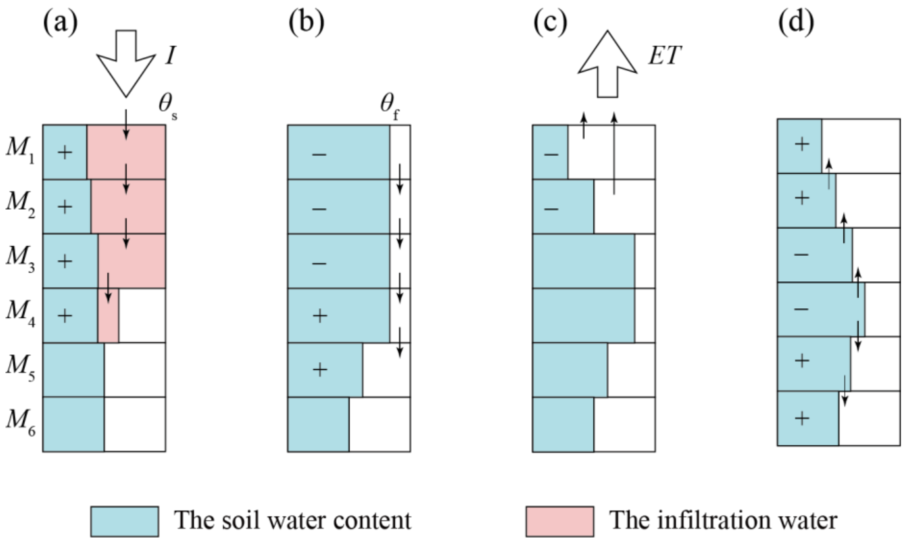

Fig. 1. The schematic procedures of UBMOD with the (a) the allocation of the infiltration water, (b) the soil water advective movement driven by the gravitational potential, (c) the source/sink terms and (d) the soil water diffusive movement driven by the matric potential.

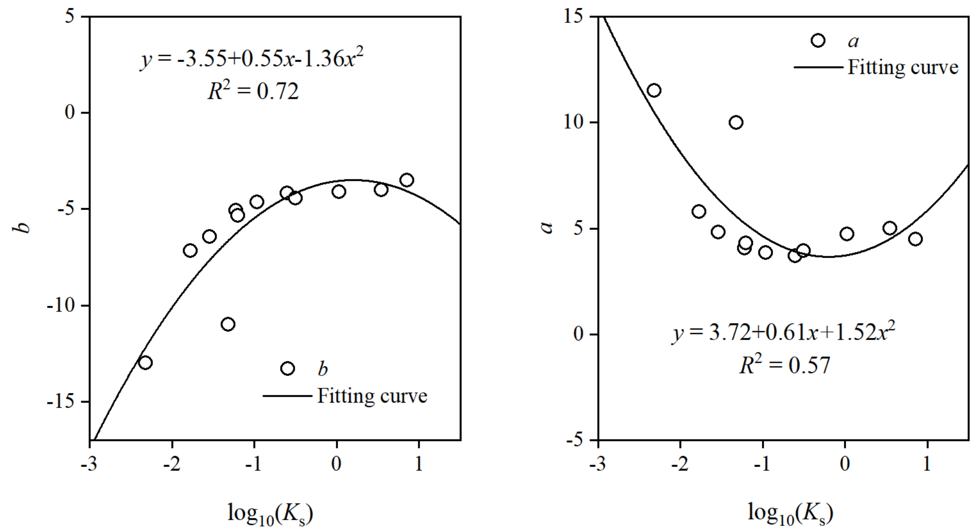

Fig. 2 The relationship between the logarithmic saturated hydraulic conductivity K_s and the two parameters of two piecewise lines obtained by fitting the hydraulic diffusivity curves of van Genuchten model in a semi-logarithmic coordinate system.

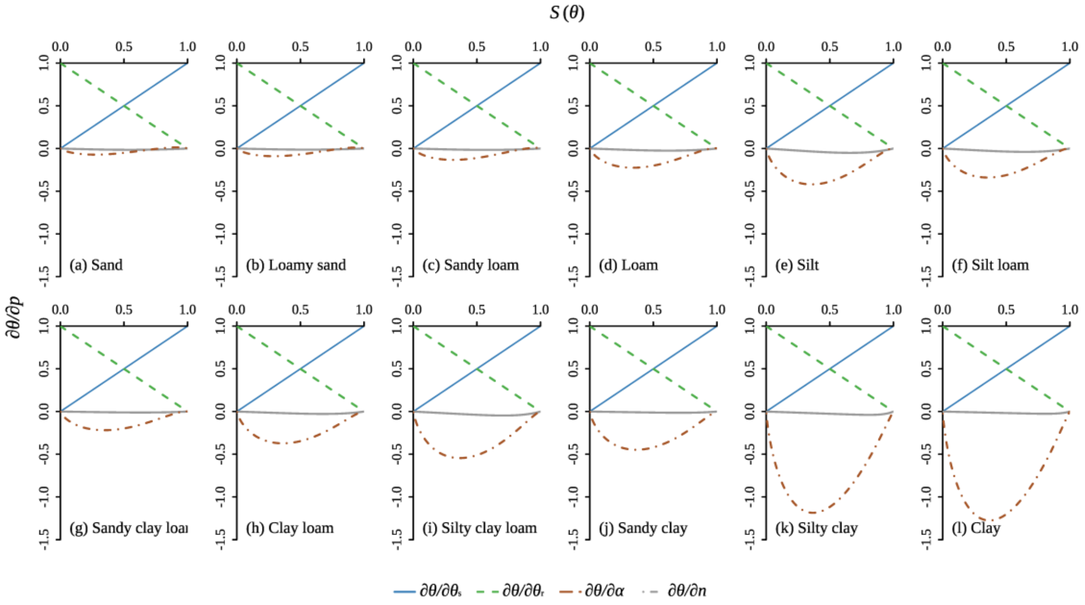

Fig. 3 The partial derivative of each parameter in the correction term for heterogeneous soils.

- **Demo**

1. Demo 1

The soil column is 2 m in length and the profile is homogeneous, with both the upper and bottom boundaries being impermeable. The initial soil water content of the top half profile is set as 0.1, and the bottom half profile as 0.4.

The soil water content in the top half profile increases over time. The increased soil water content is driven by the matric potential, since the water movement under gravitational potential is downward.

2. Demo 2

The soil column is 2 m in length, and there is no crop and the lower boundary is impermeable. The upper boundary condition includes the daily precipitation and the soil evaporation. The annual precipitation is 650 mm, and the annual soil evaporation is 756 mm. The initial water table is in the depth of 0.48 m, and the soil water content changes linearly from 0.2 at the surface to saturation at the water table. The soil is loam.

3. Demo 3

The soil column is 2 m in length, filled with alternate two types of soil (each 0.4 m thick). The two soil types are sandy loam and silt loam, and begin with the silt loam. The upper boundary is the atmospheric boundary, and the lower boundary is impermeable. The annual precipitation is 650 mm, and the annual soil evaporation is 672.01 mm. The initial soil water content is uniform with the value of 0.25. The square drainage function is used in the water balance model.

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