Appendix

The UBMOD is a water balance model based on a hybrid of numerical and statistical methods. Comparing with the traditional ones, the model can simulate upward soil water movement in heterogeneous situations.

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 top to bottom if there is infiltration. The governing equation of layer i is,

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

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}]; $\theta_{\mathrm{s},i}$ 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 is the consumed infiltration water per unit area by upper layers [L]. 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. We leave out of consideration the partitioning of rainfall between infiltration and runoff by now. We are focusing on the subsurface hydrological processes in a large arid agricultural district. The surface runoff process is ignored. The partitioning of rainfall between infiltration and runoff will be added into our model afterwards.

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

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

where the vertical coordinate is positive downward. As shown in Fig. 1(b), the soil water content of the layers 1, 2 and 3 exceed the field capacity. The empirical formulas of $K(\theta)$ are of much concern in this procedure, and are referred as drainage functions. The commonly used drainage functions are listed in Table 1 in Mao et al. (2018).

Thirdly, the source/sink terms are used to account for soil evaporation and crop transpiration. 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,

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left(D(\theta)\frac{\partial\theta}{\partial z}\right), \tag{3}$$

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

$$D(\theta)=10^{a\times S(\theta)+b} \tag{4}$$

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. (4). Furthermore, we establish the relationship between the two intermediate parameters (a and b) and the saturated hydraulic conductivity K_s as,

$$\begin{cases} b=-3.55+0.55\times\log_{10}\left(K_s\right)-1.36\times\log_{10}\left(K_s\right)^2 \\ a=3.72+0.61\times\log_{10}\left(K_s\right)+1.52\times\log_{10}\left(K_s\right)^2 \end{cases}. \tag{5}$$

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,

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left(D(\theta)\left(\frac{\partial\theta}{\partial z}-\left(\frac{\partial\theta}{\partial\theta_s}\frac{\partial\theta_s}{\partial z}+\frac{\partial\theta}{\partial\theta_r}\frac{\partial\theta_r}{\partial z}+\frac{\partial\theta}{\partial\alpha}\frac{\partial\alpha}{\partial z}+\frac{\partial\theta}{\partial n}\frac{\partial n}{\partial z}\right)\right)\right), \tag{6}$$

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. A regression formula is developed to characteristic the relationship between n and the saturated hydraulic conductivity K_s. 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.

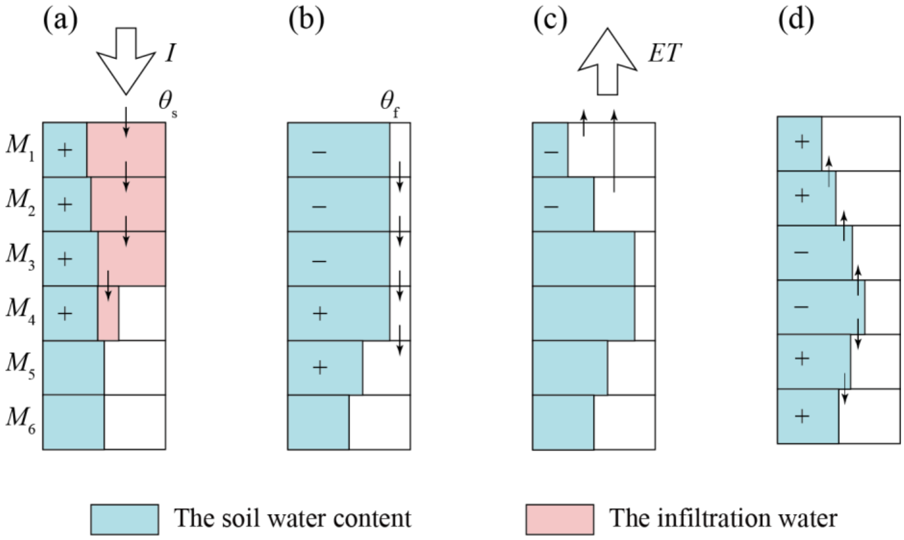

Fig. 1. The schematic procedures of UBMOD with the (a) the allocation of the infiltration water, (b) the soil water advective movement driven by the gravitational potential, (c) the source/sink terms and (d) the soil water diffusive movement driven by the matric potential.