Chapter 4 Mathematical modeling of soil water flow

4.1 Soil profile partitioning

Rather than treating the whole soil profile as one large and homogenous soil layer, it is better to divide the soil profile into two or more soil layers and then use Darcy's law (Eq. 3.5) to model the flow of water from one soil layer to the next, taking into account the physical properties of each soil layer (Fig. 4.1).

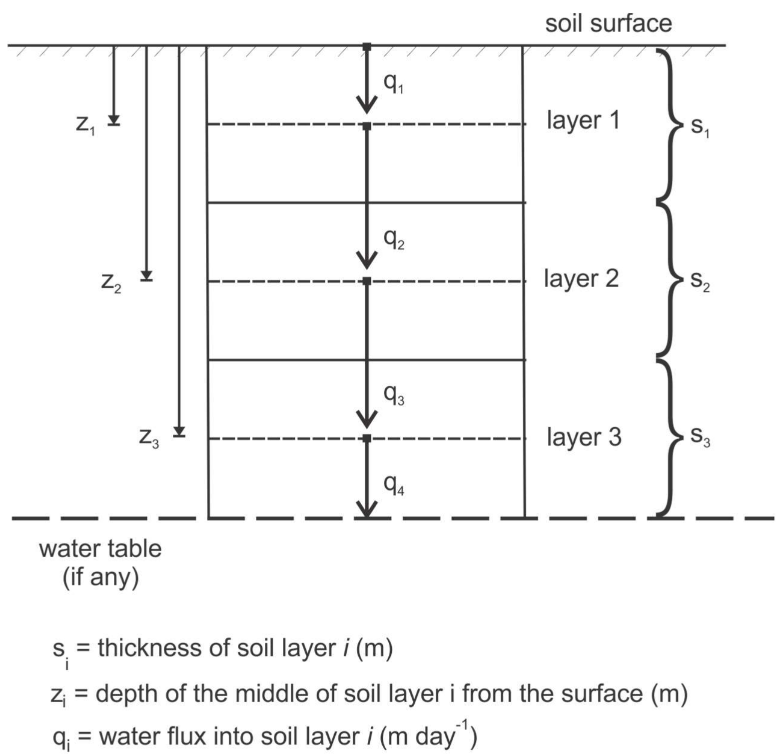

Fig. 4.1. Water flow in a soil profile that is divided into three successive layers, with the presence of a water table just beneath the third soil layer.

This method of modeling soil water flow is known as the 'tipping bucket' system because water flow is treated in a sequential manner, moving from one soil layer to the next, where water flow begins in the first soil layer, then moves successively down through the soil profile until to the last soil layer.

It is recommended to divide a soil profile into two or more consecutive layers, where soil layer i (i = 1 to n) has a thickness of s_i (m), and the depth from the soil surface to the middle of layer i is z_i (m). Water flux into soil layer i is denoted as q_i (m day^{-1}). We will further use the downward positive coordinate system (Fig. 3.2), so that downward flow of water is taken as a positive value, and the reference level is taken as the soil surface level.

How many soil layers should we establish for our soil profile? Preferably, the soil profile should be divided into sufficient number of layers such that each layer represents a distinct set of physical properties of the soil profile. The presence of a compacted layer or laterites within the soil profile, for example, should be represented as one soil layer to distinguish this layer from the others. But even if the entire soil profile was homogenous, it is still better to divide the soil profile into two or more layers. The more layers we establish, the more accurate the modeling of soil water flow. However, establishing increasingly more soil layers will increasingly slow down simulation runs because more calculations are required, but with increasingly less gain in simulation accuracy.

As stated earlier, it is recommended to establish at least two soil layers, with the first layer being a much thinner layer (about 20 mm or less thick). This first layer is unique because this is the soil layer that interacts with the atmosphere and from where evaporation of water from the soil surface only occurs. The next and second soil layer should then at least encompass the maximum rooting zone of the crop.

Recall that the soil water balance for a given soil profile (Fig. 2.1) is given by Eq. 2.1 as

$$\Delta\Theta = (P_n + I + RI + CR) - (ET + RO + P)$$

where $\Delta\Theta$ is the change in the soil water content (Θ); P_n is the net rainfall; I is the irrigation; RI and RO are run-in and runoff, respectively; CR is capillary rise from the groundwater table below; ET is the evapotranspiration; and P is the deep percolation.

In rainfed agriculture, no irrigation is supplied; thus, $I = 0$. Furthermore, we will assume no surface flow of water occurs (RI and $RO = 0$), or even if it did, $RI = RO$, so there is no net change due to surface water flow. The groundwater, if present, is assumed to have a constant depth from the soil surface. But if the groundwater is absent or located too deep, we will assume that the soil below the last soil layer is uniformly wet, and it has the same water content as the last soil layer. This means that water flows out of the last soil layer (*e.g.*, q_4 in Fig. 4.1) due to gravitational pull alone (*i.e.*, no matric suction gradient).

4.2 Soil moisture characteristics

For soil layer i, the volumetric soil water content at saturation, field capacity, and permanent wilting point are estimated based on clay, sand, and organic matter contents. Soil water characteristics (water content at permanent wilting point, field capacity, and saturation) are estimated based from Saxton and Rawls (2006):

$$\theta_{1500,i} = \theta_{1500t,i} + \left(0.14\theta_{1500t,i} - 0.02\right) \tag{4.1a}$$

$$\theta_{1500t,i} = -0.024S_i + 0.487C_i + 0.006OM_i + 0.005(S_i \times OM_i) \quad (4.1b)$$

$$-0.013(C_i \times OM_i) + 0.068(S_i \times C_i) + 0.031$$

$$\theta_{33,i} = \theta_{33t,i} + \left(1.283\theta_{33t,i}^2 - 0.374\theta_{33t,i} - 0.015\right) \quad (4.2a)$$

$$\theta_{33t,i} = -0.251S_i + 0.195C_i + 0.011OM_i + 0.006(S_i \times OM_i) \quad (4.2b)$$

$$-0.027(C_i \times OM_i) + 0.452(S_i \times C_i) + 0.299$$

$$\theta_{s,i} = \theta_{33,i} + \theta_{(S-33),i} - 0.097S_i + 0.043 \quad (4.3a)$$

$$\theta_{(S-33),i} = \theta_{(S-33)t,i} + 0.636\theta_{(S-33)t,i} - 0.107 \quad (4.3b)$$

$$\theta_{(S-33)t,i} = 0.278S_i + 0.034C_i + 0.022OM_i - 0.018(S_i \times OM_i) \quad (4.3c)$$

$$-0.027(C_i \times OM_i) - 0.584(S_i \times C_i) + 0.078$$

where for soil layer *i*, $\theta_{1500,i}$, $\theta_{33,i}$, and $\theta_{s,i}$ are its volumetric soil water content at permanent wilting point, field capacity, and saturation, respectively (all in m^3 m^{-3}); S_i and C_i its the sand and clay contents, respectively (fraction); and OM_i is its organic matter content (%).

The above estimated soil water content at permanent wilting point, field capacity, and saturation, however, needs to calibrated for greater accuracy for Malaysian mineral soils (Teh and Iba, 2010) as

$$\hat{\theta}_{1500,i} = 1.528\theta_{1500,i}\left(1 - \theta_{1500,i}\right) \quad (4.4)$$

$$\hat{\theta}_{33,i} = 1.605\theta_{33,i}\left(1 - \theta_{33,i}\right) \quad (4.5)$$

$$\hat{\theta}_{s,i} = 2.225\theta_{s,i}(1 - \theta_{s,i}) \tag{4.6}$$

where $\hat{\theta}_{1500,i}$, $\hat{\theta}_{33,i}$, and $\hat{\theta}_{s,i}$ are the calibrated volumetric soil water content at permanent wilting point, field capacity, and saturation for soil layer i, respectively (m^3 m^{-3}).

4.3 Soil layer depth and cumulative thickness

Soil depth of layer i is calculated by

$$z_i = \sum_{i=1}^{n} 0.5(s_i + s_{i-1}) \tag{4.7}$$

where z_i is the depth of soil layer i from the soil surface (m), taken from the middle of that soil layer to the soil surface; n is the number of soil layers (taken as 3 in Fig. 4.1); and s_i and s_{i-1} are the thickness of soil layer i and i-1, respectively (m). Note: $s_0 = 0$.

The cumulative thickness of a given soil layer i is

$$S_i = \sum_{j=1}^{i} s_j \tag{4.8}$$

where S_i is the cumulative thickness of soil layer i (m); that is, the sum of the thickness of layer i and all its preceding layers.

4.4 Root extraction of water

The amount of water in the root zone is the summation of water content from the first soil layer (i = 1) until the rooting depth. The algorithm to determine the total water content in the root zone is as follows:

$$\theta_{root} = \frac{1}{d_{root}} \times \sum_{i=1}^{n} MAX[0, \theta_i(s_i - m_i)] \quad (4.9a)$$

$$m_i = MAX(0, S_i - d_{root}) \quad (4.9b)$$

where θ_{root} is the volumetric soil water content within the rooting depth (m^3 m^{-3}); d_{root} is the rooting depth (m); s_i is the thickness of soil layer i (m); S_i is the cumulative thickness of soil layer i (m); n is the number of soil layers; and *MAX*() is the maximum of the enclosed values.

The amount of water extracted by roots in each soil layer follows the water uptake algorithm by Miyazaki (2005):

$$T_{a,i} = T_a(\varphi_i - \varphi_{i-1}) \quad (4.10a)$$

$$\varphi_j = 1.8c_j - 0.8c_j^2 \quad (4.10b)$$

$$c_j = MIN\left(1, \frac{S_j}{d_{root}}\right) \quad (4.10c)$$

where $T_{a,i}$ is the amount of water extracted by roots in soil layer i (m day^{-1}); T_a is the daily actual transpiration (m day^{-1}); d_{root} is the rooting depth (m); S_j is the cumulative thickness of soil layer *j* (m); and *MIN*() is the minimum of the enclosed values.

Eq. 4.10 is formulated in such a way that if we divide the total rooting depth into a succession of four layers of equal thickness, the proportion of water extracted by the roots is 40% from the first soil layer, 30% from the second, 20% from the third, and 10% from the last layer.

4.5 Hydraulic conductivity

The method by Saxton and Rawls (2006) is followed to estimate a soil's hydraulic conductivity. The saturated hydraulic conductivity in soil layer i (K_{si}, m day^{-1}) is determined by

$$K_{s,i} = 1930\left(\theta_{s,i} - \theta_{33,i}\right)^{3-\lambda_i} \tag{4.11a}$$

$$\lambda_i = \frac{1}{B_i} \tag{4.11b}$$

$$B_i = \frac{ln1500 - ln33}{ln\theta_{33,i} - ln\theta_{1500,i}} \tag{4.11c}$$

where for soil layer i, $\theta_{1500,i}$, $\theta_{33,i}$, and $\theta_{s,i}$ are its volumetric soil water content at permanent wilting point, field capacity and saturation, respectively (m^3 m^{-3}); and λ_i is its slope of the logarithmic suction-soil moisture curve (also known as the pore-size distribution).

The unsaturated hydraulic conductivity in soil layer i (K_i, m day^{-1}) is determined by

$$K_{\theta,i} = K_{s,i}\left(\frac{\theta_i}{\theta_{s,i}}\right)^{3+2/\lambda_i} \quad (4.12)$$

where for soil layer i, $K_{\theta,i}$ and $K_{s,i}$ are its unsaturated and saturated hydraulic conductivity, respectively (m day^{-1}); θ_i is its current volumetric soil water content (m^3 m^{-3}); $\theta_{s,i}$ is its volumetric soil water content at saturation (m^3 m^{-3}); and λ_i is its slope of the logarithmic suction-soil moisture curve, as determined from Eq. 4.11b and c.

4.6 Matric suction and gravity heads

The soil matric suction for soil layer i is determined by

$$H_{m,i} = \begin{cases} 3.3 - \left[\dfrac{(33-\Psi_{e,i})(\theta_i - \theta_{33,i})}{10(\theta_{s,i}-\theta_{33,i})}\right] & \theta_i \geq \theta_{33,i} \\ \dfrac{A_i}{10}\theta_i^{-B_i} & \theta_i < \theta_{33,i} \end{cases} \quad (4.13a)$$

$$A_i = exp(ln33 + B_i ln\theta_{33,i}) \quad (4.13b)$$

$$\Psi_{e,i} = \Psi_{et,i} + (0.02\Psi_{et,i}^2 - 0.113\Psi_{et,i} - 0.70) \quad (4.13c)$$

$$\begin{aligned}\Psi_{et,i} = & -21.674S_i - 27.932C_i - 81.975(\theta_{s,i} - \theta_{33,i}) \\ & +71.121S_i(\theta_{s,i} - \theta_{33,i}) + 8.294C_i(\theta_{s,i} - \theta_{33,i}) \\ & +14.05S_iC_i + 27.161\end{aligned} \quad (4.13d)$$

where for soil layer i, $H_{m,i}$ is its soil matric suction (m); θ_i is its volumetric soil water content (m^3 m^{-3}); $\theta_{33,i}$ and $\theta_{s,i}$ are its volumetric soil water content at field capacity and saturation, respectively (m^3 m^{-3}); S_i and C_i are its sand and clay contents, respectively (fraction); $\psi_{e,i}$ is its air entry suction (kPa) (Saxton and Rawls, 2006); and the intermediary variable B_i is determined from Eq. 4.11c.

The gravity head for soil layer i is determined by

$$H_{g,i} = z_i \tag{4.14}$$

where $H_{g,i}$ is the gravity head for soil layer i (m); and z_i is the depth of the middle of soil layer i from the soil surface (m).

Consequently, the total head for soil layer i is

$$H_{t,i} = H_{m,i} + H_{g,i} \tag{4.15}$$

where for soil layer i, $H_{t,i}$, $H_{m,i}$, and $H_{g,i}$ are its total head, matric suction head, and gravity head, respectively (m).

4.7 Water content

Darcy's law (Eq. 3.5) is used to describe the water flow in the soil. Water flow is taken to occur from the middle of layer i-1 to the middle of layer i. The method based on Hillel (1977) is followed. Water flux into soil layer i is governed by the following set of equations:

$$q_i = \begin{cases} MIN\left(K_{s,i},\ P_{net}\right) - E_a - T_{a,i} & i = 1 \\ -\overline{K}_{\theta,i}\dfrac{\left(H_{t,i-1} - H_{t,i}\right)}{\left(z_{i-1} - z_i\right)} - T_{a,i} & 1 < i \le n \\ K_{\theta,n} & i = n + 1 \end{cases} \tag{4.16a}$$

$$\overline{K}_{\theta,i} = \frac{K_{\theta,i-1} - K_{\theta,i}}{lnK_{\theta,i-1} - lnK_{\theta,i}} \tag{4.16b}$$

where subscripts i-1 and i denote soil layer i-1 and i, respectively; q is the water flux (m day^{-1}); P_{net} is the net daily rainfall (m day^{-1}); E_a is the actual daily soil evaporation (occurs only from the first soil layer) (m day^{-1}); T_a is the daily extraction of water by roots (actual plant transpiration) (m day^{-1}); $\overline{K}_{\theta,i}$ is the logarithmic mean of the hydraulic conductivities of layer i and i-1 (m day^{-1}); $K\theta$ and z are the soil layer's hydraulic conductivity and thickness, respectively (m); and H_t is the total head (sum of matric suction and gravity head) (m). Note that both E_a and $T_{a,i}$ must be expressed in unit m day^{-1}.

In Eq. 4.16, the mean hydraulic conductivity of two soil layers is calculated because water flows across two soil layers that may have different hydraulic conductivities. Moreover, the logarithmic not arithmetic mean of hydraulic conductivity is used because hydraulic conductivity, as shown in Fig. 3.5, is sensitive to soil water content, varying by large degrees even over a small change in the soil water content. Bittelli *et al*. (2015) found that using logarithmic mean of hydraulic conductivity produced more stable and reliable simulation results than when using geometric or harmonic means.

Recall that the positive downward coordinate system (Fig. 3.2) is used, so a positive q flux denotes water flowing downward and conversely, a negative q denotes an upward flow, against gravity.

For the first soil layer, water entry is via net rainfall, P_{net}, whose entry into the soil is limited by the first soil layer's saturated hydraulic conductivity $K_{s,1}$.

In addition, water flux out of the last soil layer ($i = n$) is denoted by q_{n+1}, and it is merely equal to the hydraulic conductivity of the last soil layer, $K_{\theta,n}$, because of the assumption that the soil below the last layer is uniformly wet and it has the same water content as the last soil layer. Consequently, water flux is only due to gravity gradient (no matric suction gradient). In this case, $q_{n+1} = K_{\theta,n}$.

The difference between water entering and exiting a soil layer is the net flux, or the change in soil water content, which is determined simply by subtraction:

$$\Delta\Theta = q_i - q_{i+1} \tag{4.17}$$

where $\Delta\Theta$ is the net flux in soil layer i (m day^{-1}) which is the difference between water flux entering soil layer i (q_i) and that exiting the layer (q_{i+1}) (both in m day^{-1}). Since a positive water flux q_i means a downward water flow, a positive net flux $\Delta\Theta$ denotes more water entering than exiting the soil layer; thus, the soil layer is wetting.

The soil water content in a soil layer is thus:

$$\Theta_{i,t+1} = \Theta_{i,t} + \Delta\Theta \tag{4.18}$$

where $\Theta_{i,t}$ and $\Theta_{i,t+1}$ are the water content in soil layer i (m) at time step t and t+1, respectively; and $\Delta\Theta$ is the net flux in soil layer i (m day^{-1}).

4.8 Scaling potential to actual evapotranspiration

Limited soil water availability could reduce potential evapotranspiration to a lower level, known as actual evapotranspiration (Fig. 2.6 and 2.7). Both potential evaporation and transpiration are reduced to their respective actual counterparts by a reduction factor:

$$E_a = E_p \times R_E \tag{4.19a}$$

$$R_E = \frac{1}{1 + \left(3.6073\, \theta_1 / \theta_{s,1}\right)^{-9.3172}} \tag{4.19b}$$

$$T_a = T_p \times R_T \tag{4.20a}$$

$$R_T = \begin{cases} 1 & \theta_{root} \geq \theta_{cr,root} \\ \dfrac{\theta_{root} - \theta_{1500,root}}{\theta_{cr,root} - \theta_{1500,root}} & \theta_{1500,root} < \theta_{root} < \theta_{cr,root} \\ 0 & \theta_{root} \leq \theta_{1500,root} \end{cases} \tag{4.20b}$$

$$\theta_{cr,root} = \theta_{1500,root} + p\left(\theta_{s,root} - \theta_{1500,root}\right) \tag{4.20c}$$

where E and T are evaporation and transpiration, respectively (m day^{-1}), and their subscripts a and p indicate their actual and potential values, respectively; R_E and R_T are the reduction factor for potential evaporation and potential transpiration, respectively (0 to 1); θ_{root}, $\theta_{1500,root}$, and $\theta_{s,root}$ are the current soil water content, permanent wilting point, and saturation in the rooting zone, respectively (m^3 m^{-3}); $\theta_{cr,root}$ is the critical soil water content in the rooting zone, below which plant suffers from the effects of water stress (m^3 m^{-3}); and p is 0.5 and 0.3 for C3 and C4 crops, respectively (Fig. 2.6). Note that soil evaporation occurs only at the first soil layer, where potential evaporation is scaled down to actual evaporation by a reduction factor (R_E) that is calculated using information about the first soil layer's current soil water content (θ_1) and soil saturation ($\theta_{S,1}$) (both in m^3 m^{-3}). Lastly, Eq. 4.19b describes the R_E curve in Fig. 2.7.

4.9 Water table (ground water)

The water table, if present, is assumed to have a constant water table level or depth and is located just beneath the last soil layer. For instance, if three soil layers are specified (such as in Fig. 4.1), with a total soil layer thickness of 2 m, then the water table is located at a constant depth of 2 m below the soil surface. This water table is located just beneath the third (the last) soil layer. Water flow from the water table follows Darcy's law as described earlier, where water flows upward (negative water flux), against the gravity, from the saturated water table into the drier soil layers above.

4.10 Net rainfall

Net rainfall refers to the amount of rain reaching the ground as both throughfall and stemflow. As discussed in section 2.2, there is a strong linear relationship between net rainfall and gross rainfall. However, their linear regression coefficients vary, depending on crop or plant types. We will assume that net rainfall is no more than 80% of gross rainfall for full canopies, and full canopies is achieved when leaf area index is 3 m^2 leaf m^{-2} ground. Consequently, net rainfall is linearly related with gross rainfall and a function of leaf area index, and their relationship can de described as

$$P_{net} = P_g \times MAX(0.8, 0.267L) \tag{4.21}$$

where P_{net} is the daily net rainfall (m); P_g is the daily gross rainfall (rainfall above the canopies, m); and L is the leaf area index (m^2 leaf m^{-2} ground). Eq. 4.21 is applicable for full, partial, or zero canopy cover. At full canopy (achieved when $L \geq 3$), net rainfall is no more than 80% of gross rainfall.

Note: P_{net} must be in unit m before it is used in the soil water balance model.

4.11 Model information to be provided by user

Modeling the soil water flow requires several information to be known. Some of these information can be estimated, such as the relationship between soil hydraulic conductivity and soil water content, as shown in section 4.5.

Some model information, however, cannot be estimated and need to be known or measured, and these user-provided model information are:

a) The physical soil properties of each soil layer in the soil profile. The physical properties are: sand, clay, and organic matter distribution (all in % by weight). Also needed is the initial soil water content in each soil layer (m^3 m^{-3}).
b) Initial plant rooting depth (m)

c) Daily data: amount of rain (mm), leaf area index (m^2 leaf m^{-2} ground), potential evaporation (mm), and potential transpiration (mm).

The plant's leaf area index and the potential evaporation and transpiration are often simulated in modeling work. These information are required to determine the amount of water entering the soil profile via net rainfall and the amount of water lost from the soil and plant via evapotranspiration. Nonetheless, discussions and modeling the crop growth and energy balance are beyond the scope of this book. Thus, in the absence of any crop growth and energy balance model components, the information about leaf area index and potential evapotranspiration must be provided in this book for the soil water model.

The next chapter will further discuss these model inputs.

4.12 A note of time step for modeling soil flow

Hydraulic conductivity is sensitive to soil water content, where a small change in soil water content causes a large change to hydraulic conductivity (Fig. 3.5). Consequently, it is vital that the water fluxes are calculated using very small time steps because using too large a time step (*e.g.*, 1 day) may cause unrealistically large fluctuations or changes in the soil water content over a short period.

The size of the time step would depend on the soil profile physical characteristics. The more sensitive hydraulic conductivity is to the changes in the soil water content, the smaller the time step should be. As a guide, the time step should not be more than 15 mins (or less than about 100 time steps a simulation day). For instance, if we set the time step at 15 mins, but if this interval produces large, erratic fluctuations in the simulated soil water content, the time step should be shorted by about half to 7 mins (about 200 time steps a simulation day), and the simulation should be repeated. The time step should be shortened until the simulated soil water content follows a stable and steady trend. Although using a very small time step will produce more accurate estimates than that using a large time step, setting a time step that is too small would considerably slow down simulations run but with little returns in greater estimation accuracy.

Consequently, there is some trial-and-error involved in setting the suitable time step interval. The interval for the time step should be small enough for simulations to produce steady and stable trends in soil water content but not too small that simulation runs become unnecessarily too time-consuming or intensive.