Tree Hydrodynamic Modelling of Soil Plant Atmosphere Continuum (SPAC-3Hpy)

Supplementary Material

This document provides details on the derivation of the system of partial differential equations describing the water flow through the soil and root, and stem xylem, and a description of the numerical scheme used to solve these equations. The explanation of the numerical scheme is also meant to provide a user manual for the code developed in Python.
After the numerical scheme, details on the calculation of the transpiration rates, conductance and capacitances in the soil, root and stem xylem are presented. These refer to the formulations used in the examples presented in the article and can be easily modified in the code in different subroutines.

S.1 Governing equations

The water flow within the soil, and root and stem xylem is described as flow in porous media. Equations for the mass conservation are combined with the Darcy's equation extended to unsaturated porous media to derive an equation for the water potential in the soil, roots, and stem.

S.1.1 Soil

According to the schematic shown in Fig. 1 in the main text, for mass conservation, considering a volume of soil with an infinitesimal depth over an area A_s, $dV_s = A_s dz$, changes of the mass of water, M_s (kg), over time within this volume are due to the difference between the water fluxes entering, F_{in} (kg s^{-1}), and exiting, F_{out} (kg s^{-1}), the volume, and the water exchanged with the roots. This can be expressed as

$$\frac{\partial M_s}{\partial t} = F_{in} - F_{out} - \rho S dV_s, \tag{S.1}$$

where $dM_s = \rho\theta_s dV_s$, ρ is the density of water (kg m^{-3}), θ_s is the soil volumetric water content, and S (s^{-1}) is the rate at which water is extracted from the soil per unit of mass of water contained in dV_s. The term F_{out} can be written as

$$F_{out} = F_{in} + \frac{\partial F}{\partial z} dz, \tag{S.2}$$

which, substituting Eq. (S.2) into Eq. (S.1), yields

$$\rho \frac{\partial \theta_s}{\partial t}\ A_s dz = -\frac{\partial F}{\partial z} dz - \rho S\ A_s dz. \tag{S.3}$$

The flux F can be written as

$$F = \rho\ v_s\ A_s, \tag{S.4}$$

where v_s is the Darcy's velocity (m s^{-1}), expressed as

$$v_s = -K_s \left(\frac{\partial \Phi_s}{\partial z} + \rho g \right), \tag{S.5}$$

K_s being the hydraulic conductance of the soil (m^2 s^{-1}Pa^{-1}), g the gravitational constant, and Φ_s the soil water potential (Pa).
Eq. (S.3) thus can be simplified into

$$C_s \frac{\partial \Phi_s}{\partial t} = \frac{d\theta_s}{d\Phi_s} \frac{\partial \Phi_s}{\partial t} = \frac{\partial}{\partial z} \left[K_s \left(\frac{\partial \Phi_s}{\partial z} + \rho g \right) \right] - S. \tag{S.6}$$

S.1.2 Roots

Following the same procedure as the soil, the conservation of water mass in the roots, with $dM_r = \rho\theta_r A_r dz$, results in

$$\rho \frac{\partial(\theta_r A_r)}{\partial t} dz = \frac{\partial}{\partial z} \left[K_r A_r \left(\frac{\partial \Phi_r}{\partial z} + \rho g \right) \right] dz + \rho S A_s dz. \tag{S.7}$$

Dividing Eq. (S.7) by $\rho A_s dz$ leads to

$$C_r \frac{\partial \Phi_r}{\partial t} = \frac{d}{d\Phi_r} \left(\frac{\theta_r A_r}{A_s} \right) \frac{\partial \Phi_r}{\partial t} = \frac{\partial}{\partial z} \left[K_r \frac{A_r}{A_s} \left(\frac{\partial \Phi_r}{\partial z} + \rho g \right) \right] + S, \tag{S.8}$$

where A_r/A_s (m$^2_{root}$ m$^{-2}_{ground}$) is the root cross area index, representing the total root cross-sectional area at a given elevation per unit of ground area.

S.1.3 Stem

The conservation of water mass in the stems, with $dM_x = \rho\theta_x A_x dz$, results in

$$\rho\frac{\partial(\theta_x A_x)}{\partial t}dz = \frac{\partial}{\partial z}\left[K_x A_x\left(\frac{\partial\Phi_x}{\partial z} + \rho g\right)\right]dz - \rho S_x dz, \tag{S.9}$$

where S_x ($m^2\ s^{-1}$) is the flow of water leaving the stems per unit of vertical length.
Dividing Eq. (S.9) by $\rho A_s dz$, such that water fluxes across soil, roots, and stem are expressed in terms of ground area, one obtains

$$C_x\frac{\partial\Phi_x}{\partial t} = \frac{d}{d\Phi_x}\left(\frac{\theta_x A_x}{A_s}\right)\frac{\partial\Phi_x}{\partial t} = \frac{\partial}{\partial z}\left[K_x\frac{A_x}{A_s}\left(\frac{\partial\Phi_x}{\partial z} + \rho g\right)\right] - \frac{S_x}{A_s}, \tag{S.10}$$

where A_x/A_s ($\mathrm{m}^2_{xylem}\mathrm{m}^{-2}_{ground}$) is the stem xylem cross area index, representing the total sapwood area per ground area.

S.2 Numerical scheme

The water flow across the soil-plant-atmosphere continuum is lumped along the vertical direction. The domain of the model can be idealized as the combination of the vertical extent of the soil and the tree (root and stem) xylem, with exchange of water between the soil and the roots (Fig. S.1).
Each of Eqs. (S.6), (S.8), and (S.10) can be written as

$$C\frac{\partial\Phi}{\partial t} = -\frac{\partial F}{\partial z} \pm S^*, \tag{S.11}$$

where C is a capacitance, Φ is the water potential, F is the flux, and S^* is a source or sink term accounting for either the exchange of water between soil and roots or the water loss due to transpiration for the stem xylem.
Eq. (S.11) is discretized using constant intervals, Δz, with values of Φ calculated at the nodes and fluxes, F, calculated between nodes. Eq. (S.11) is approximated using a fully implicit backward Euler method, and its discretized form for a generic node i reads

$$C_i^{n+1}\frac{\Phi_i^{n+1} - \Phi_i^n}{\Delta t} = -\frac{F_{i+1/2}^{n+1} - F_{i-1/2}^{n+1}}{\Delta z} \pm S_i^{*,n+1}, \tag{S.12}$$

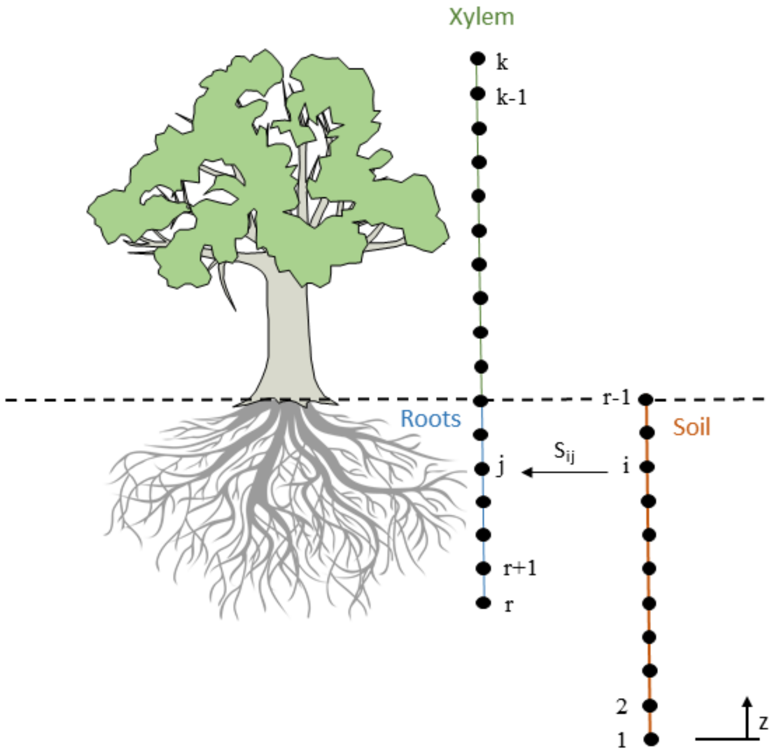

Figure S.1: Representation of the model domain

where n and $n+1$ indicate values of the variables at two consecutive times, with $\Delta t = t^{n+1} - t^n$. The fluxes can be then expressed as

$$F_{i+1/2}^{n+1} = -K_{i+1/2}^{n+1} \frac{\Phi_{i+1}^{n+1} - \Phi_i^{n+1}}{\Delta z} - K_{i+1/2}^{n+1} \rho g \tag{S.13}$$

$$F_{i-1/2}^{n+1} = -K_{i-1/2}^{n+1} \frac{\Phi_i^{n+1} - \Phi_{i-1}^{n+1}}{\Delta z} - K_{i-1/2}^{n+1} \rho g, \tag{S.14}$$

where K is the hydraulic conductance (including the ratio of the areas appearing in Eqs. S.8 and S.10).

In the following, a full detailed description of the numerical approximation of the system of equations and the implementation of initial and boundary conditions are presented.

S.2.1 Discretization

Eqs. (S.6), (S.8), and (S.10) are approximated as in Eq. (S.11), and are then combined and solved at the same time with the standard fully implicit Picard method following the scheme in Celia et al. (1990).

With m denoting the number of the Picard iteration, and the subscript i denoting a generic node, Eq. (S.12) reads

$$C_i^{n+1,m}\frac{(\Phi_i^{n+1,m+1}-\Phi_i^n)}{\Delta t} = +K_{i+1/2}^{n+1,m}\frac{(\Phi_{i+1}^{n+1,m+1}-\Phi_i^{n+1,m+1})}{(\Delta z)^2} - K_{i-1/2}^{n+1,m}\frac{(\Phi_i^{n+1,m+1}-\Phi_{i-1}^{n+1,m+1})}{(\Delta z)^2} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z}\rho g - \frac{K_{i-1/2}^{n+1,m}}{\Delta z}\rho g \pm S_i^{*,n+1}, \quad \text{(S.15)}$$

with the hydraulic conductance calculated in the middle of two neighbouring nodes as

$$K_{i-1/2}^{n+1,m} = \frac{1}{2}(K_{i-1}^{n+1,m}+K_i^{n+1,m}) \quad \text{(S.16)}$$

$$K_{i+1/2}^{n+1,m} = \frac{1}{2}(K_i^{n+1,m}+K_{i+1}^{n+1,m}). \quad \text{(S.17)}$$

The terms in Eq. (S.15) can be rearranged as

$$\begin{aligned}
&\frac{C_i^{n+1,m}}{\Delta t}\left(\Phi_i^{n+1,m+1}-\Phi_i^{n+1,m}\right) + \frac{C_i^{n+1,m}}{\Delta t}\left(\Phi_i^{n+1,m}-\Phi_i^n\right) = +\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_{i+1}^{n+1,m+1}-\Phi_{i+1}^{n+1,m}\right)\\
&+\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_{i+1}^{n+1,m}\right) - \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_i^{n+1,m+1}-\Phi_i^{n+1,m}\right) - \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_i^{n+1,m}\right) + \frac{K_{i+1/2}^{n+1,m}}{\Delta z}\rho g\\
&-\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_i^{n+1,m+1}-\Phi_i^{n+1,m}\right) - \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_i^{n+1,m}\right) + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_{i-1}^{n+1,m+1}-\Phi_{i-1}^{n+1,m}\right)\\
&+\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_{i-1}^{n+1,m}\right) - \frac{K_{i-1/2}^{n+1,m}}{\Delta z}\rho g \pm S_i^{*,n+1}, \quad \text{(S.18)}
\end{aligned}$$

which, defining the increment $\delta\Phi^{n+1,m} = \Phi^{n+1,m+1}-\Phi^{n+1,m}$, yields

$$\frac{C_i^{n+1,m}}{\Delta t}\left(\delta\Phi_i^{n+1,m}\right)+\frac{C_i^{n+1,m}}{\Delta t}\left(\Phi_i^{n+1,m}-\Phi_i^{n}\right)=+\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}\left(\delta\Phi_{i+1}^{n+1,m}\right)+\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_{i+1}^{n+1,m}\right)$$
$$-\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}\left(\delta\Phi_i^{n+1,m}\right)-\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_i^{n+1,m}\right)+\frac{K_{i+1/2}^{n+1,m}}{\Delta z}\rho g-\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\left(\delta\Phi_i^{n+1,m}\right)$$
$$-\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_i^{n+1,m}\right)+\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\left(\delta\Phi_{i-1}^{n+1,m}\right)+\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\left(\Phi_{i-1}^{n+1,m}\right)-\frac{K_{i-1/2}^{n+1,m}}{\Delta z}\rho g\pm S_i^{*,n+1}. \quad \text{(S.19)}$$

Reorganizing Eq.(S.19), one obtains

$$\left(\frac{-K_{i-1/2}^{n+1,m}}{\Delta z^2}\right)\delta\Phi_{i-1}^{n+1,m}+\left(\frac{C_i^{n+1,m}}{\Delta t}+\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2}+\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2}\right)\delta\Phi_i^{n+1,m}+\left(\frac{-K_{i+1/2}^{n+1,m}}{\Delta z^2}\right)\delta\Phi_{i+1}^{n+1,m}=$$
$$\frac{1}{\Delta z^2}\left[K_{i+1/2}^{n+1,m}\left(\Phi_{i+1}^{n+1,m}-\Phi_i^{n+1,m}\right)-K_{i-1/2}^{n+1,m}\left(\Phi_i^{n+1,m}-\Phi_{i-1}^{n+1,m}\right)\right]+\frac{K_{i+1/2}^{n+1,m}}{\Delta z}\rho g-\frac{K_{i-1/2}^{n+1,m}}{\Delta z}\rho g$$
$$-\frac{C_i^{n+1,m}}{\Delta t}\left(\Phi_i^{n+1,m}-\Phi_i^{n}\right)\pm S_i^{*,n+1}. \quad \text{(S.20)}$$

For the soil, $S_i^{*,n+1}$ is a sink of water (i.e., the sign '-' applies to Eq. (S.20))

$$S_i^{*,n+1}=k_{e,rad_i}(z,t)\cdot f(\theta_i^{n+1,m+1})(\Phi_{s_i}^{n+1,m+1}-\Phi_{r_j}^{n+1,m+1}), \quad \text{(S.21)}$$

where the subscripts s and r refer to soil and roots, and j is a node of the roots corresponding to the same elevation z as i for the soil (Figure S.1).

Introducing the increments $\delta\Phi^{n+1,m}$ for the water potentials, the expression for $S^{*,n+1}$ in the soil (with the sign '-' in Eq. S.19) and root xylem (with the sign '+' in Eq. S.19) is

$$S_i^{*,n+1}(z,t)=k_{e,rad_i}f(\theta_i^{n+1,m+1})(\delta\Phi_{s_i}^{n+1,m}-\delta\Phi_{r_j}^{n+1,m}-\Phi_{s_i}^{n+1,m}+\Phi_{r_j}^{n+1,m}). \quad \text{(S.22)}$$

Reorganizing the equation in the same form of Eq. (S.20), and substituting the expression for the sink term (Eq. S.22), the numerical approximation for the soil nodes becomes:

$$
\begin{aligned}
&-\frac{K^{n+1,m}_{s_i-1/2}}{\Delta z^2}\delta\Phi^{n+1,m}_{s_i-1} + \left[\frac{C^{n+1,m}_{s_i}}{\Delta t} + \frac{K^{n+1,m}_{s_i+1/2}}{\Delta z^2} + \frac{K^{n+1,m}_{s_i-1/2}}{\Delta z^2} + k_{e,rad_i} f(\theta_i^{n+1,m+1})\right]\delta\Phi^{n+1,m}_{s_i} \\
&\quad - \frac{K^{n+1,m}_{s_i+1/2}}{\Delta z^2}\delta\Phi^{n+1,m}_{s_i+1} - k_{e,rad_i} f(\theta_i^{n+1,m+1})\delta\Phi_{r_j} = \frac{1}{\Delta z^2}\left[K^{n+1,m}_{s_i+1/2}\left(\Phi^{n+1,m}_{s_i+1} - \Phi^{n+1,m}_{s_i}\right)\right. \\
&\qquad \left. - K^{n+1,m}_{s_i-1/2}\left(\Phi^{n+1,m}_{s_i} - \Phi^{n+1,m}_{s_i-1}\right)\right] + \frac{K^{n+1,m}_{s_i+1/2}}{\Delta z}\rho g - \frac{K^{n+1,m}_{s_i-1/2}}{\Delta z}\rho g \\
&\qquad - \frac{C^{n+1,m}_{s_i}}{\Delta t}\left(\Phi^{n+1,m}_{s_i} - \Phi^{n}_{s_i}\right) - k_{e,rad_i} f(\theta_i^{n+1,m+1})\left(\Phi^{n+1,m}_{s_i} - \Phi^{n+1,m}_{r_j}\right).
\end{aligned}
\tag{S.23}
$$

Likewise, the numerical approximation for the nodes of the root xylem becomes

$$
\begin{aligned}
&-\frac{K^{n+1,m}_{r_i-1/2}}{\Delta z^2}\delta\Phi^{n+1,m}_{r_i-1} + \left[\frac{C^{n+1,m}_{r_i}}{\Delta t} + \frac{K^{n+1,m}_{r_i+1/2}}{\Delta z^2} + \frac{K^{n+1,m}_{r_i-1/2}}{\Delta z^2} + k_{e,rad_i} f(\theta_i^{n+1,m+1})\right]\delta\Phi^{n+1,m}_{r_i} \\
&\quad - \frac{K^{n+1,m}_{r_i+1/2}}{\Delta z^2}\delta\Phi^{n+1,m}_{r_i+1} - k_{e,rad_i} f(\theta_i^{n+1,m+1})\delta\Phi_{s_j} = \frac{1}{\Delta z^2}\left[K^{n+1,m}_{r_i+1/2}\left(\Phi^{n+1,m}_{r_i+1} - \Phi^{n+1,m}_{r_i}\right)\right. \\
&\qquad \left. -K^{n+1,m}_{r_i-1/2}\left(\Phi^{n+1,m}_{r_i} - \Phi^{n+1,m}_{r_i-1}\right)\right] + \frac{K^{n+1,m}_{r_i+1/2}}{\Delta z}\rho g - \frac{K^{n+1,m}_{r_i-1/2}}{\Delta z}\rho g \\
&\qquad - \frac{C^{n+1,m}_{r_i}}{\Delta t}\left(\Phi^{n+1,m}_{r_i} - \Phi^{n}_{r_i}\right) + k_{e,rad_i} f(\theta_i^{n+1,m+1})\left(\Phi^{n+1,m}_{s_i} - \Phi^{n+1,m}_{r_j}\right).
\end{aligned}
\tag{S.24}
$$

A similar approximation can be written for the stem xylem, where the sink term is simpler than for the soil and root xylem, because it does not include interactions between nodes at different elevations.

Considering, for example, that both soil and roots have the same depth (i.e, roots are present from the bottom to the top of the soil column), the system of partial differential equations can be approximated by a system of algebraic equations for each iteration within each time step. In matrix format, this system of equations can be written as

$$
\infty \qquad
\begin{pmatrix}
b_1 & c_1 & 0 & 0 & ... & K_{rad,1} & 0 & 0 & ... & & & & & & & \\
a_2 & b_2 & c_2 & 0 & ... & 0 & K_{rad,2} & 0 & ... & & & & & & & \\
0 & a_3 & b_3 & c_3 & ... & 0 & 0 & K_{rad,3} & ... & & & & & & & \\
... & & & & & & & & & & & & & & & \\
K_{rad,1} & 0 & ... & & & 0 & b_r & c_r & 0 & ... & & & & & & \\
0 & K_{rad,2} & 0 & ... & & 0 & a_{r+1} & b_{r+1} & c_{r+1} & 0 & ... & & & & & \\
0 & 0 & K_{rad,3} & 0 & ... & 0 & 0 & a_{r+2} & b_{r+2} & c_{r+2} & 0 & ... & & & & \\
... & & & & & & & & & & & & & & & \\
... & & & & & & & & & & & ... & a_{k-2} & b_{k-2} & c_{k-2} & 0 \\
... & & & & & & & & & & & ... & 0 & a_{k-1} & b_{k-1} & c_{k-1} \\
... & & & & & & & & & & & ... & 0 & 0 & a_k & b_k
\end{pmatrix}
\cdot
\begin{pmatrix}
\delta_1^{n+1,m} \\
\delta_2^{n+1,m} \\
\delta_3^{n+1,m} \\
\\
\delta_r^{n+1,m} \\
\delta_{r+1}^{n+1,m} \\
\delta_{r+2}^{n+1,m} \\
\\
\delta_{k-2}^{n+1,m} \\
\delta_{k-1}^{n+1,m} \\
\delta_k^{n+1,m}
\end{pmatrix}
=
\begin{pmatrix}
d_1^{n+1} \\
d_2^{n+1} \\
d_3^{n+1} \\
\\
d_r^{n+1} \\
d_{r+1}^{n+1} \\
d_{r+2}^{n+1} \\
\\
d_{k-2}^{n+1} \\
d_{k-1}^{n+1} \\
d_k^{n+1}
\end{pmatrix},
$$

where the subscripts r and k denote the bottom of the roots and top of the canopy, respectively, and the node 1 represents the bottom of the soil (Figure S.1).

The matrix coefficients for a generic node within the soil read

$$a_i = -\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \tag{S.25}$$

$$b_i = \left(\frac{C_i^{n+1,m}}{\Delta t} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_i} f(\theta_i^{n+1,m+1}) \right) \tag{S.26}$$

$$c_i = -\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} \tag{S.27}$$

$$K_{rad,i} = -k_{e,rad_i} f(\theta_i^{n+1,m+1}) \tag{S.28}$$

$$d_i = \frac{1}{\Delta z^2} \left[K_{i+1/2}^{n+1,m} (\Phi_{i+1}^{n+1,m} - \Phi_i^{n+1,m}) - K_{i-1/2}^{n+1,m} (\Phi_i^{n+1,m} - \Phi_{i-1}^{n+1,m}) \right] \tag{S.29}$$

$$+\rho g \frac{(K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m})}{\Delta z} - \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) - k_{e,rad_i} f(\theta_i^{n+1,m+1}) \left(\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m} \right). \tag{S.30}$$

The coefficients for a generic node associated with the roots are

$$a_i = -\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \tag{S.31}$$

$$b_i = \left(\frac{C_i^{n+1,m}}{\Delta t} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_i} f(\theta_i^{n+1,m+1}) \right) \tag{S.32}$$

$$c_i = -\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} \tag{S.33}$$

$$K_{rad,i} = -k_{e,rad_i} f(\theta_i^{n+1,m+1}) \tag{S.34}$$

$$d_i = \frac{1}{\Delta z^2} \left[K_{i+1/2}^{n+1,m} (\Phi_{i+1}^{n+1,m} - \Phi_i^{n+1,m}) - K_{i-1/2}^{n+1,m} (\Phi_i^{n+1,m} - \Phi_{i-1}^{n+1,m}) \right] \tag{S.35}$$

$$+\rho g \frac{(K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m})}{\Delta z} - \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) + k_{e,rad_i} f(\theta_i^{n+1,m+1}) \left(\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m} \right). \tag{S.36}$$

The coefficients for a generic node of the stem read

$$a_i = -\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \tag{S.37}$$

$$b_i = \left(\frac{C_i^{n+1,m}}{\Delta t} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \right) \tag{S.38}$$

$$c_i = -\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} \tag{S.39}$$

$$d_i = \frac{1}{\Delta z^2} \left[K_{i+1/2}^{n+1,m} (\Phi_{i+1}^{n+1,m} - \Phi_i^{n+1,m}) - K_{i-1/2}^{n+1,m} (\Phi_i^{n+1,m} - \Phi_{i-1}^{n+1,m}) \right] \tag{S.40}$$

$$+\rho g \frac{(K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m})}{\Delta z} - \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) - S_{x,i}^{n+1}/A_{s,i}, \tag{S.41}$$

with details on the expression of S_x provided in Section S.3.

The system of algebraic equations is solved to find the values of $\delta\Phi_i^{n+1}$; this is then added to $\Phi_i^{n,m}$ to calculate $\Phi_i^{n+1,m+1}$, which is then used to calculate the new values of the coefficients for the calculation of a new value of $\delta\Phi_i$. These iterations proceed until the difference of two successive calculated water potentials in each node approaches a predefined tolerance, δ, such that

$$\left| \Phi^{n+1,m+1} - \Phi^{n+1,m} \right| \leq \delta. \tag{S.42}$$

S.2.2 Initial and boundary conditions

The initial condition needs to be a known function $\Phi_0 = \Phi(z, 0)$ across the soil, roots and stem. A common choice is to assume that soil and both root and stem xylem are in hydrostatic conditions (i.e., $\Phi_0 = -\rho g z$), without water fluxes occurring across the system. Boundary conditions are required at the bottom of the roots, at the top of the stem, and at the bottom and top of the soil. No-flux boundary conditions are the default conditions for the bottom of the roots and top of the stem. No flux boundary conditions can be imposed at the bottom of the soil and a specific flux can be imposed at the top of the soil as infiltration. Conditions at the bottom of the soil can be also provided as a given value of water potential or as free drainage.

No flux boundary conditions can be specified by imposing the flux at the corresponding nodes to be zero. For example, in the case of the bottom of the soil, for $i = 1$, a no flux condition is obtained by imposing $F^{n+1}_{1-1/2} = 0$ in Eq. (S.12).
Accordingly, the terms in the matrix summarizing the system of equation for node 1 are

$$b_1 = \frac{C_1^{n+1,m}}{\Delta t} + \frac{K_{1+1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_1} f(\theta_i^{n+1,m+1}),$$
$$c_1 = -\frac{K_{1+1/2}^{n+1,m}}{\Delta z^2},$$
$$K_{rad,1} = -k_{e,rad_1} f(\theta_i^{n+1,m+1})$$
$$d_1 = \frac{1}{\Delta z^2}\left[K_{1+1/2}^{n+1,m}(\Phi_2^{n+1,m} - \Phi_1^{n+1,m})\right] + \rho g \frac{K_{1+1/2}^{n+1,m}}{\Delta z}$$
$$-\frac{C_1^{n+1,m}}{\Delta t}(\Phi_1^{n+1,m} - \Phi_1^{n}) - k_{e,rad_1} f(\theta_i^{n+1,m+1})\left(\Phi_1^{n+1,m} - \Phi_{r_j}^{n+1,m}\right).$$

The conditions at the bottom of the roots and top of the stem can be obtained in a similar way.
In the case of a specified water potential boundary condition (Dirichlet), the potential at the bottom of the soil is a series of known values, such that $\phi(1,t) = \Phi_{b_i}$. This leads to the following expression for $\Phi_2^{n+1,m+1}$:

$$\left(\frac{-K_{2-1/2}^{n+1,m}}{\Delta z^2}\right)\delta\Phi_{b_i} + \left(\frac{C_2^{n+1,m}}{\Delta t} + \frac{K_{2+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{2-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_2} f(\theta_2^{n+1,m+1})\right)\delta\Phi_2^{n+1,m} +$$
$$\left(\frac{-K_{2+1/2}^{n+1,m}}{\Delta z^2}\right)\delta\Phi_3^{n+1,m} - k_{e,rad_2} f(\theta_2^{n+1,m+1})\delta\Phi_{s_i} =$$
$$\frac{1}{\Delta z^2}\left[K_{2+1/2}^{n+1,m}\left(\Phi_3^{n+1,m} - \Phi_2^{n+1,m}\right) - K_{2-1/2}^{n+1,m}\left(\Phi_2^{n+1,m} - \Phi_{b_i}^{n+1,m}\right)\right] + \frac{K_{2+1/2}^{n+1,m}}{\Delta z}\rho g$$
$$-\frac{K_{2-1/2}^{n+1,m}}{\Delta z}\rho g - \frac{C_2^{n+1,m}}{\Delta t}\left(\Phi_2^{n+1,m} - \Phi_2^{n}\right) - k_{e,rad_2} f(\theta_2^{n+1,m+1})(\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m}) \quad \text{(S.43)}$$

Reorganizing in the form of the matrix yields

$$a_2 = \frac{-(K_{2-1/2}^{n+1,m})}{\Delta z^2} \tag{S.44}$$

$$b_2 = \left(\frac{C_2^{n+1,m}}{\Delta t} + \frac{K_{2+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{2-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_2} f(\theta_2^{n+1,m+1}) \right) \tag{S.45}$$

$$c_2 = \frac{-(K_{2+1/2}^{n+1,m})}{\Delta z^2} \tag{S.46}$$

$$K_{rad,2} = -k_{e,rad_2} f(\theta_2^{n+1,m+1}) \tag{S.47}$$

$$d_2 = \frac{1}{\Delta z^2} \left[K_{2+1/2}^{n+1,m} (\Phi_3^{n+1,m} - \Phi_2^{n+1,m}) - K_{2-1/2}^{n+1,m} (\Phi_2^{n+1,m} - \Phi_{b_i}^{n+1,m}) \right] \tag{S.48}$$

$$+\rho g \frac{(K_{2+1/2}^{n+1,m} - K_{2-1/2}^{n+1,m})}{\Delta z} - \frac{C_2^{n+1,m}}{\Delta t} (\Phi_2^{n+1,m} - \Phi_2^n) - k_{e,rad_2} f(\theta_2^{n+1,m+1}) \left(\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m} \right) \tag{S.49}$$

In the case of soil profile with deep groundwater levels, the water flux at the bottom of the soil is only due to gravity; therefore, the pressure gradient is equal to zero:

$$F_{1-1/2}^{n+1} = -K_{1-1/2}^{n+1} \left(0 + \rho g\right), \tag{S.50}$$

$$C_1^{n+1} \frac{\Phi_1^{n+1} - \Phi_1^n}{\Delta t} = -\frac{F_{1+1/2}^{n+1} - (-K_{1-1/2}^{n+1} \rho g)}{\Delta z} - S(\Phi_1^n). \tag{S.51}$$

Reorganizing in matrix format, one obtains

$$b_1 = \frac{C_1^{n+1,m}}{\Delta t} + \frac{K_{1+1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_1} f(\theta_1^{n+1,m+1}),$$

$$c_1 = -\frac{K_{1+1/2}^{n+1,m}}{\Delta z^2},$$

$$K_{rad,1} = -k_{e,rad_1} f(\theta_1^{n+1,m+1})$$

$$d_1 = \frac{1}{\Delta z^2} \left[K_{1+1/2}^{n+1,m} (\Phi_2^{n+1,m} - \Phi_1^{n+1,m}) \right] + \rho g \frac{K_{1+1/2}^{n+1,m}}{\Delta z} - \frac{C_1^{n+1,m}}{\Delta t} (\Phi_1^{n+1,m} - \Phi_1^n)$$
$$- \frac{K_{1-1/2}^{n+1,m} \rho g}{\Delta z} - k_{e,rad_1} f(\theta_1^{n+1,m+1}) \left(\Phi_1^{n+1,m} - \Phi_{r_j}^{n+1,m} \right).$$

For the top of the soil column, considering inputs from infiltration, the flux at the node $i = s$ is known as $F_{s+1/2}^{n+1} = q_{inf}$, resulting in

$$C_s \frac{\Phi_s^{n+1} - \Phi_s^n}{\Delta t} = -\frac{q_{inf} - F_{s-1/2}^{n+1}}{\Delta z} - S, \tag{S.52}$$

$$q_{inf}^{n+1,m+1} = max\left(-q, -\left(\theta_{sat} - \theta_s^{n+1,m+1}\right) \cdot \left(\frac{\Delta z}{\Delta t}\right)\right), \tag{S.53}$$

where q is the precipitation rate.

Reorganizing in matrix format leads to

$$a_s = -\frac{K_{s-1/2}^{n+1,m}}{\Delta z^2},$$

$$b_s = \frac{C_s^{n+1,m}}{\Delta t} + \frac{K_{s-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_s} f(\theta_s^{n+1,m+1}),$$

$$K_{rad_s} = -k_{e,rad_s} f(\theta_s^{n+1,m+1}),$$

$$d_s = \frac{1}{\Delta z^2}\left[-K_{s-1/2}^{n+1,m}(\Phi_s^{n+1,m} - \Phi_{s-1}^{n+1,m})\right] - \rho g \frac{K_{s-1/2}^{n+1,m}}{\Delta z} - \frac{C_s^{n+1,m}}{\Delta t}(\Phi_s^{n+1,m} - \Phi_s^n)$$
$$-k_{e,rad_s} f(\theta_s^{n+1,m+1})\left(\Phi_s^{n+1,m} - \Phi_{r_j}^{n+1,m}\right) + \frac{q_{inf}}{\Delta z}.$$

S.3 Transpiration

Transpiration is calculated in a subroutine and can thus be defined according to the formulation assigned by the user. Here, we present how transpiration was calculated in Sections 3.2 and 3.3, following the formulation implemented in (Verma et al., 2014).

The water that the trees lose to the atmosphere via transpiration (S_x/A_s) is calculated as

$$\frac{S_x}{A_s} = T \cdot l(z), \tag{S.54}$$

where T is the transpiration rate per unit of ground area (m s^{-1}). Transpiration is distributed throughout the canopy height using the leaf area density (LAD) ($l(z)$, m^2 m^{-2} m^{-1}), which is the leaf area index (LAI) distributed along the canopy height z.

Transpiration is calculated through the Penman Monteith formulation (Allen et al., 1998; Verma et al., 2014):

$$T = \left[\frac{Q_n \Delta + C_p D g_a}{\lambda[\Delta g_c + \gamma(g_c + g_a)]}\right] g_c, \tag{S.55}$$

where Q_n (W m^{-2}) is the net radiation, Δ (kg m^{-1}s^{-2}K^{-1}) is the slope of the saturation vapor pressure curve for a given temperature, C_p (kg m^{-1}s^{-2}K^{-1}) is the specific heat of air, D is the vapour pressure deficit (VPD) (Pa), λ (kg m^{-1} s^{-2}) is the latent heat of vaporisation, g_a (m s^{-1}) is the aerodynamic conductance, γ (kg m s^{-2}K^{-1}) is the psychrometric constant, and g_c (m s^{-1}) is the canopy conductance. In this study, Q_n is assumed to be 60% of incoming solar radiation; this is different from Verma et al. (2014), where this term was calculated as 70% of solar radiation .Δ is calculated as

$$\Delta = \left[\frac{4098}{(T_a - 35.85)^2}\right] e_{sat}, \tag{S.56}$$

where e_{sat} (Pa) is the saturation vapour pressure for a given temperature (T_a), given as

$$e_{sat} = 611 \exp\left[\frac{17.27(T_a - 273.15)}{T_a - 35.85}\right]. \tag{S.57}$$

The canopy conductance, g_c, is calculated as

$$g_c = \left[\frac{g_s g_b}{g_s + g_b}\right] LAI, \tag{S.58}$$

where LAI is the leaf area index, g_b (m s^{-1}) is the leaf boundary layer conductance per m^2 of leaf area and g_s (m s^{-1}) is the stomatal conductance, which depends on both plant physiology and environmental factors. In the present model, g_s is modeled as (Jarvis, 1976),

$$g_s = g_{smax} \cdot f(S_{in}) \cdot f(T_a) \cdot f(D) \cdot f(\Phi_x), \tag{S.59}$$

where g_{smax} (m s^{-1}) is the maximum stomatal conductance, and $f(S_{in})$, $f(T_a)$, $f(D)$, and $f(\Phi_x)$ are empirical functions [-], representing the behavior of g_s according to variations in solar radiation, temperature, VPD, and leaf water potential, respectively. These functions vary between 0 and 1, and are calculated as

$$f(S_{in}) = 1 - \exp(-k_r S_{in}), \tag{S.60}$$

$$f(T_a) = 1 - k_t(T_a - T_{opt})^2, \tag{S.61}$$

$$f(D) = \frac{1}{(1 + Dk_d)}, \tag{S.62}$$

$$f(\Phi_x) = \left[1 + \left(\frac{\Phi_{xleaf}}{\Phi_{x50}}\right)^{n_l}\right]^{-1}, \tag{S.63}$$

where k_r, k_t, k_d and n_l are empirical constants, T_{opt} is the air temperature at which $f(T_a)$ is 1, and Φ_{x50} is the leaf water potential at 50% loss of conductivity. $f(\Phi_x)$ represents the inverse polynomial expression commonly used to express the effect of water potential on xylem conductance (Manzoni et al., 2013).

Night time transpiration is modeled as

$$E_n = E_{max} \cdot f(T_a) \cdot f(D) \cdot f(\Phi_x), \tag{S.64}$$

where E_{max} (m s^{-1}) is the maximum night time transpiration, which was estimated in Verma et al. (2014).

S.4 Soil water retention relationships

The relationships between K_s, Φ_s and θ_s are modeled according to van Genuchten (1980) as

$$K_s = \frac{k_{s,sat}}{\rho g}\Theta^{1/2}\left[1-(1-\Theta^{1/n})^m\right]^2, \tag{S.65}$$

$$C_s = \frac{d\theta_s}{d\Phi_s} = \frac{d\theta_s}{\rho g dh_s} = \frac{-\alpha m(\theta_{sat}-\theta_{res})}{\rho g(1-m)}\Theta^{1/m}(1-\Theta^{1/m})^m, \tag{S.66}$$

where,

$$\Theta(z,t) = \frac{\theta-\theta_{res}}{\theta_{sat}-\theta_{res}}, \tag{S.67}$$

$$\theta = \theta_{res} + \frac{(\theta_{sat}-\theta_{res})}{[1+(\alpha|h|)^n]^m}, \tag{S.68}$$

$$m = 1-\frac{1}{n}, \tag{S.69}$$

$$0 < m < 1, \tag{S.70}$$

where K_s (m^2 s^{-1} Pa^{-1}) is the effective soil hydraulic conductivity, $k_{s,sat}$ (m s^{-1}) is the soil hydraulic conductivity under saturated soil conditions, θ_{sat} and θ_{res} indicate the saturated and residual values of the soil volumetric water content, and C_s (Pa^{-1}) is the soil capacitance.

S.5 Hydraulic conductances

S.5.1 Root radial conductance

The exchange of water between soil and roots depends of the amount of roots contained in different soil layers. The fraction of roots at different soil depths is modeled following Vrugt et al. (2001), with the function

$$r(z) = \left(1 - \frac{z}{z_{r_j} - z_{r_i}}\right) \exp\left(\frac{-q_z}{z_{r_j} - z_{r_i}}\, z\right) \quad z_{r_i} \leqslant z \leqslant z_{r_j}, \tag{S.71}$$

where z is the vertical coordinate (positive upwards), z_{r_j} is the elevation of the top of the roots, and z_{r_i} is the elevation of the bottom of the roots, with $z_{r_j} - z_{r_i}$ the root depth. Using Eq.(S.71), the root water uptake is written as

$$S(z,t) = k_{s,rad}\ f(\theta) \cdot A_{ind}(z) \cdot \frac{r(z)}{\int_{z_{r_i}}^{z_{r_j}} r(z)dz} \cdot (\Phi_s - \Phi_r), \tag{S.72}$$

where $f(\theta)$ [-] is a water stress reduction function, Φ_s, and Φ_r, are water potentials (Pa) for the soil and roots, respectively, $k_{s,rad}$ ($\mathrm{m^3 s^{-1} m_{root}^{-2} Pa^{-1}}$) is the soil-to-root radial conductance per unit of root surface area, and A_{ind} is the lateral root surface area index. The $f(\theta)$ function is written as,

$$f(\theta) = \begin{cases} 0 & \theta \leq \theta_1, \qquad \text{(S.73)} \\ \dfrac{(\theta - \theta_1)}{(\theta_2 - \theta_1)} & \theta_1 < \theta \leq \theta_2, \qquad \text{(S.74)} \\ 1 & \theta > \theta_2, \qquad \text{(S.75)} \end{cases}$$

where θ_1 and θ_2 are the soil water content below which root water uptake is ceased and the soil water content below which root water uptake start decreasing, respectively (Feddes et al., 1976).

S.5.2 Axial conductances

The effective axial conductance of the roots, K_r ($\mathrm{m^2 s^{-1} Pa^{-1}}$), can be defined as

$$K_r = \frac{k_r}{\rho g} \frac{A_r}{A_s}, \tag{S.76}$$

with,

$$k_r(z,t) = k_{sax} \cdot \left(1 - \frac{1}{1 + \exp(a_p(\Phi_r - b_p))}\right), \tag{S.77}$$

where k_{sax} (m s^{-1}) is the specific axial conductivity for the root system, and a_p (Pa^{-1}) and b_p (Pa) are parameters for the root xylem cavitation curve, which describes the vulnerability of xylem to cavitation.

The effective hydraulic conductance of the axial stem xylem, K_x (m^2 s^{-1} Pa^{-1}), is defined similarly as Eq. (S.76), as

$$K_x = \frac{k_x}{\rho g} \frac{A_x}{A_s}, \tag{S.78}$$

with

$$k_x(\Phi_x(z,t)) = k_{max} \cdot \left(1 - \frac{1}{1 + \exp(a_p(\Phi_x - b_p))}\right), \tag{S.79}$$

where k_{max} (m s^{-1}) is the maximum conductivity of saturated stem xylem, and a_p (Pa^{-1}) and b_p (Pa) are the shape parameters of the cavitation curve.

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