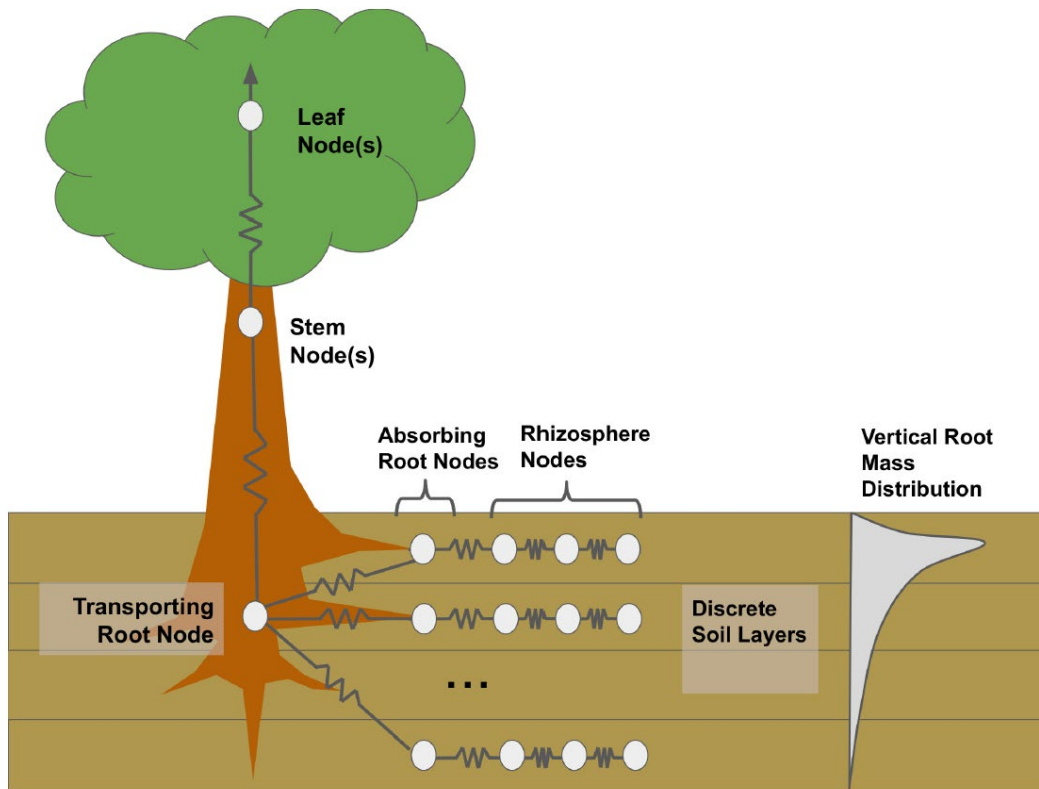


## MODEL DESCRIPTION: updates made to TFS-HYDRO for FATES-HYDRO

### 1. Overview



**Figure S1: Diagram of FATES-HYDRO with simulation of rhizosphere shell, absorbing roots, transporting roots, stem and leaves.** The model is solved for different soil layers with different root distributions.

The FATES-HDRO simulates the water transportation from different nodes including rhizosphere, absorbing root, transporting root, stem and leaf (Fig. S1). Without plant hydrodynamics, FATES default transpiration is estimated at the patch scale (defined by a common time since last disturbance) using a Ball-Berry scheme that is downscaled by a dimensionless ‘beta’ term. Beta is the product of the vertical root distribution and soil water deficit below a predefined threshold, a scheme common to many land surface models. FATES-Hydro calculates this beta term based on leaf water potential, which is dynamically simulated with the plant hydrodynamic module based on the TFS-Hydro v.1 model of Christoffersen et al. (2016).

FATES-Hydro remains, as it was for TFS-Hydro, an individual-based model. It operates on individual trees, which for the FATES vegetation demographic model, are grouped into cohorts

of predefined size class. It solves for water fluxes and potentials for individual trees based on a time-variable flux (transpiration) upper boundary condition and a zero-flux condition at the outer edge of a characteristic rhizosphere, which is abstracted as a series of concentric rings around an absorbing root. As such, while individual trees across cohorts and functional types maintain distinct water potentials, the rhizosphere shells are shared by all individuals within a grid cell (explained below). Below we summarize the main updates and changes to TFS-Hydro that create FATES-Hydro.

## *2. Boundary conditions and sequence of operations between Hydro, FATES and Host Land Model*

While TFS-Hydro was a stand-alone model, FATES-Hydro operates within the FATES vegetation demographic model, which itself plugs into a biophysical Host Land Model (HLM). This nested model structure requires a set of boundary conditions (BCs) that are shared between FATES and the HLM, or between FATES and Hydro. These are passed at every time step: the net change in soil moisture in each soil layer (HLM to Hydro via FATES) and patch transpiration (FATES to Hydro), and root water uptake (from FATES to the HLM). The three BCs are used sequentially as follows.

- 1) The net change in soil moisture in each soil layer, due to the combined effects of infiltration and drainage from the previous time step, is passed to FATES from the HLM and downscaled by Hydro to rhizosphere shells, updating water contents and potentials before solving the combined plant-soil system.
- 2) Then, patch transpiration from FATES is downscaled by Hydro to the individual level, which comprises the upper boundary flux condition (as in TFS-Hydro) and the combined plant-soil system is solved for new water contents and potentials.
- 3) Finally, the resulting net change in soil moisture in each layer (positive in the case of root water uptake, negative when roots release water to soil) is passed by FATES back to the HLM.

## *3. Downscaling*

### *3.1 Layer-specific soil moisture change to rhizosphere shells*

The layer-specific soil moisture change arising from the combined effects of infiltration, inter-layer fluxes, and drainage is downscaled to rhizosphere shells as in TFS-Hydro (see Section 6.3 Supplement S1 of Christoffersen et al. 2016), which we summarize here. The guiding principle is that infiltration, inter-layer fluxes, and drainage all should act so as to dissipate any existing soil to root water potential gradient within a soil layer. Therefore, for layers gaining soil moisture to these processes, water is added to the driest rhizosphere shells first, and for layers losing soil moisture, water is drawn from the wettest rhizosphere layers first. In both cases, the algorithm uses water content to preserve mass balance, orders rhizosphere shells in terms of increasing or decreasing water content, and sequentially adds or subtracts water from these shells until the next driest or wettest shells is matched, respectively.

### *3.2 Patch transpiration to individuals*

Because existing HLMs solve surface temperatures and fluxes at the canopy scale, FATES does not estimate transpiration at the cohort level and only estimates the combined leaf-area weighted stomatal and boundary layer conductance. We estimated each cohort's fraction of total patch transpiration as its fraction of the total patch-level canopy conductance (sum of cohort leaf area-

weighted stomatal and boundary layer conductance). Then, by definition, individuals within cohorts are identical, so cohort-level transpiration is partitioned equally among individuals.

#### 4. Numerical solution as applied to multiple soil layers

The TFS v.1-Hydro model of Christoffersen et al. (2016) used a simple 1-layer soil water bucket model. In the current FATES-Hydro implementation, we modified the original model to work with an arbitrary number of vertical soil layers, on top of the existing fine-scale representation of soil – root water potential gradients (i.e., the rhizosphere). We applied the rhizosphere concentric shell structure within each soil layer, and the maximum soil-root hydraulic conductance within each layer is proportional to layer-specific fine root length density, as in the 1-layer model of Christoffersen et al. (2016).

Because of the addition of the vertical dimension, the system is no longer strictly one-dimensional and requires an amended numerical solution. We kept the original implicit solution, using a first-order Taylor series expansion to estimate fluxes at the next time step and applied it to each soil layer on a sequential basis, described below.

We partitioned the total transpiration flux exiting the canopy for each cohort  $i$  ( $Q_{top,i}\Delta t$ ; kg plant<sup>-1</sup>) over each timestep  $\Delta t$  (s) into  $n_{layer}$  components, where  $n_{layer}$  is the number of soil layers. The resulting transpiration flux for soil layer  $j$  ( $Q_{top,ij}\Delta t$ ) is proportional to the soil-root conductance that layer ( $\sum_{k=1}^{n_{shell}} K_{jk}$ ; kg Pa<sup>-1</sup> s<sup>-1</sup>) relative to the total belowground soil-root conductance, giving:

$$Q_{top,ij}\Delta t = Q_{top,i}\Delta t \frac{\sum_{k=1}^{n_{shell}} K_{jk}}{\sum_{j=1}^{n_{layer}} \sum_{k=1}^{n_{shell}} K_{jk}},$$

For each soil layer and individual within each cohort, we then used  $Q_{top,ij}\Delta t$  as the top boundary condition and solved the 1-dimensional system (outermost rhizosphere shell to absorbing roots in that layer to leaf), updating all plant water contents and potentials each time. As such, the order across soil layers in which the solution is conducted matters – we solved each plant-soil system in order of decreasing total soil-root conductance (i.e., the wettest soil layers with the most fine roots first). While a simultaneous solution of the plant nodes with all soil layers and rhizosphere shells at the same time will give the most accurate solution to this system, it is computationally intensive and the current approach captures gradient-driven water flow at the soil-root boundary while maintaining mass balance throughout the soil-plant system. The reader is referred to Fang et al. (2022) for the description and implementation of the simultaneous numerical solution, as well as a comparison between these two numerical approaches.

#### 5. Upscaling rhizosphere water contents from individuals to grid cell-average

We update mean (site-level) rhizosphere shell moisture contents based on the net change across all individuals and cohorts. This immediately cancels out any developing heterogeneities in rhizosphere water contents around individuals or cohorts of differing transpiration rates. While this is not fully realistic, it is an inherent limitation of a ‘mean field’ representation of soil hydrology associated with a 1-dimensional (vertical) soil hydrology model and is in line with the assumption that belowground soil moisture reserves are mean field in the horizontal dimension.

However, we stress that the current model is a step forward because it allows for a pseudo representation of a horizontal dimension to soil moisture (the radial concentric rhizosphere dimension around individual fine roots) and by extension, limitations of rhizosphere conductance under drought (Sperry et al., 1998), albeit an ‘average’ soil-to-root gradient across all individuals and cohorts.

## 6. Special provisions for plant water content at near residual and saturation

We apply a linear pressure volume relationship to water storage in plant tissues at the very extreme ends of the pressure-volume relationship. Specifically, we identify two matric pressure thresholds, named  $\psi_{\max}$  and  $\psi_{\min}$ .  $\psi_{\max}$  is the pressure at 99.8% of the saturation pressure, and  $\psi_{\min}$  is the pressure within 1% of the residual. When the numerical solver predicts that pressure drops below  $\psi_{\min}$ , we simply extrapolate the derivative of the PV relationship at  $\psi_{\min}$  to lower values. When the solver predicts pressures above  $\psi_{\max}$ , we extrapolate the derivative of the PV relationship at  $\psi_{\max}$  to higher values. In principle, these extrapolations are used to accommodate numerical truncation error in the solver, thereby preventing extreme behavior at the ends of the PV curve, and are very rarely used.

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