



From hydraulic root architecture models to macroscopic representations of root hydraulics in soil water flow and land surface models.

Jan Vanderborght¹, Valentin Couvreur², Felicien Meunier^{3,4}, Andrea Schnepf¹, Harry Vereecken¹, Martin Bouda^{2,5}, and Mathieu Javaux^{1,2}.

5 ¹ Forschungszentrum Jülich GmbH, IBG-3 (Agrosphäre), Wilhelm-Johnen-Str., 52428 Jülich, Germany.

² University of Louvain, Earth and Life Institute, 1348 Louvain-la-Neuve, Belgium

³ CAVElab - Computational and Applied Vegetation Ecology, Department of Environment, Ghent University, Ghent, Belgium

⁴ Department of Earth and Environment, Boston University, Boston, USA

⁵ Institute of Botany of the Czech Academy of Sciences, Pruhonice, Czechia

10 *Correspondence to:* Jan Vanderborght (j.vanderborght@fz-juelich.de)

Abstract: Root water uptake is an important process in the terrestrial water cycle. How this process depends on soil water content, root distributions, and root properties is a soil-root hydraulic problem. We compare different approaches to implement root hydraulics in macroscopic soil water flow and land surface models. By upscaling a three dimensional hydraulic root architecture model, we derived an exact macroscopic root hydraulic model. The macroscopic model uses three characteristics: the root system conductance, K_{rs} , the standard uptake fraction, **SUF**, that represents the uptake from a soil profile with a uniform hydraulic head, and a compensatory matrix that describes the redistribution of water uptake in a non-uniform hydraulic head profile. Two characteristics, K_{rs} and **SUF**, are sufficient to describe the total uptake as a function of the collar and soil water potential; and water uptake redistribution does not depend on the total uptake or collar water potential. We compared the exact model with two hydraulic root models that make a-priori simplifications of the hydraulic root architecture: the parallel and big root model. The parallel root model uses only two characteristics, K_{rs} and **SUF**, that can be calculated directly following a bottom up approach from the 3D hydraulic root architecture. The big root model uses more parameters than the parallel root model but these parameters cannot be obtained straightforwardly with a bottom up approach. The big root model was parameterized using a top down approach, i.e. directly from root segment hydraulic properties assuming a-priori a single big root architecture. This simplification of the hydraulic root architecture led to less accurate descriptions of root water uptake than by the parallel root model. To compute root water uptake in macroscopic soil water flow and land surface models, we recommend the use of the parallel root model with K_{rs} and **SUF** computed in a bottom up approach from a known 3D root hydraulic architecture.

1 Introduction

Plant transpiration, which corresponds with about 40% of the precipitation on land (Oki and Kanae, 2006; Trenberth et al., 2007; Good et al., 2015) is an important component of the terrestrial water cycle. It drives water flow from the soil into the plant and plays an important physiological role for distributing minerals from the soil to the above ground part of the plant and for regulating the temperature of the leaves. Understanding where and when plants take up water from the soil is important to unravel the interaction between climate, soil and plant growth, manage soil water, and select or breed plants that are optimally performing in a certain soil-climate environment. Therefore, root water uptake is a sensitive process in land surface and crop



35 models (Gayler et al., 2013; Wöhling et al., 2013; Vereecken et al., 2015; Ferguson et al., 2016; Vereecken et al., 2016; Whitley et al., 2017).

There are several ways to distinguish and classify root water uptake models: macroscopic versus microscopic, mechanistic versus empirical, and bottom-up versus top-down (Feddes et al., 2001; Hopmans and Bristow, 2002). Here, we will focus on models that describe water flow in the soil-root system mechanistically based on soil and plant hydraulics, i.e. based on water potential gradients in each system, on root and soil conductances, and on exchange or radial soil-root conductances. When water flow is described mechanistically in the soil-plant system, processes with an important impact on root water uptake emerge from the model simulations and do not have to be parameterized (Javaux et al., 2013). These include hydraulic redistribution when water uptake from the wetter part of the root zone is released in the drier part and root water uptake compensation when root water uptake shifts to wetter zones (Katul and Siqueira, 2010). The differences between different modeling approaches that we consider are related to the spatial representation of the root system and its architecture or topology.

A first approach to model this system is to start with a simplified concept of the root system or its topology and then parameterize this model based on measurements of soil water potential, leaf water potentials, transpiration fluxes and information about the root system such as the root density distribution and hydraulic properties of root segments. In this kind of top-down approach, two a-priori proposed root system topologies can be distinguished: big root and parallel root models. Big root models are 1D models in which the root system is represented by one vertical ‘big root’. In this model, all root segments in a layer at a certain depth are grouped in one ‘tube’ and these tubes are connected in series with each other. Nimah and Hanks (1973) used this approach for simulating root water uptake but simplified the head losses due to axial flow. The axial root hydraulic conductivity, which determines head losses due to flow in the root system, and the radial conductivity, which determines the exchange between the soil and the root in the big root model, were linked to properties of the root system such as: the root radial conductance per root surface area; the axial conductivity per root cross sectional area; the distributions of root cross sectional and surface area in the soil profile; and the unsaturated soil hydraulic conductivity (Amenu and Kumar, 2008; Quijano and Kumar, 2015).

The second simplified root topology model is what we define as the ‘parallel root model’. In the ‘parallel root model’, the root system is conceptualized to consist of branches of different lengths that take up water near their tips and that are all connected in parallel to a root collar node (Gou and Miller, 2014). The parallel root system considers a connection in series between the radial and axial conductances of a single root branch. Thus, this model can also account for axial root conductances or for head losses due to flow along the root branch (Hillel et al., 1976). Although it is not identical to the parallel root model, a model that shows similarities with the parallel root model is the model by Ryel et al. (2002) which has been implemented in several land surface models.

A further simplification is to neglect the axial resistance so that the water potential in the root xylem is everywhere the same (Gardner and Ehlig, 1962; Wilderott, 2003; de Jong van Lier et al., 2008; Siqueira et al., 2008; de Jong van Lier et al., 2013; Manoli et al., 2014; Daly et al., 2018). This simplification wipes out the difference between the ‘big root’ and ‘parallel root’ models.

The second approach starts from an explicit 3D representation of the root architecture and the distribution of root segment conductances and describes the flow in the branched root network that is coupled to flow in the soil (Doussan et al., 1998; Doussan et al., 2006; Javaux et al., 2008). Hydraulic characteristics of the root system such as the root system conductance and the root water uptake distribution for a uniform soil water potential distribution can be derived using analytical solutions of the flow equations in the root system. These characteristics were derived for single roots with constant (Landsberg and Fowkes, 1978) or with varying root hydraulic properties (Meunier et al., 2017b), and for branched root systems (Roose and Fowler, 2004; Meunier et al., 2017c). The solutions provide a direct or a bottom-up link between the root architecture and the



hydraulic properties of root segments on the one hand and the hydraulic root system characteristics on the other hand (Meunier et al., 2017a). By making assumptions about the axial conductance of the root system, Couvreur et al. (2012) derived an approximate model that simulates the uptake for arbitrary soil water potential distributions within the root zone and that uses these hydraulic root system characteristics. The form of the obtained model is similar to that of the parallel root model but it uses root system characteristics that were derived from an exact or numerical solution of the flow in the 3D hydraulic root architecture. In other words, even though the model formulation is similar to the parallel root model, the systems' properties were not derived in a top down approach by a-priori assuming a parallel root model. The model was formulated originally to simulate the 3D distribution of the water uptake in the soil by a 3D root architecture. When it is assumed that the soil water potentials do not vary in the horizontal direction, the model can be scaled up to a 1D formulation of the same form to calculate vertical water uptake profiles (Javaux et al., 2013; Couvreur et al., 2014a). Another approach was followed by Bouda and Saiers (2017) who derived an upscaled 1D root water uptake model using a so-called root system architecture stencil that is calibrated on solutions of water flow in a 3D root architecture. Bouda (2019) showed recently that the root system architecture stencil they derived based on solutions of water flow in 3D root system architectures is similar to an analytically exact solution of the big root model.

Both big root and parallel root models are approximations of the real 3D root architecture and the connectivity of the individual root segments and topology of the root system may have an important impact on the root system functioning (Bouda et al., 2018). Analytical solutions of water uptake by single roots, which are represented as 'leaky tubes' with uniform radial and axial conductances, demonstrated that the axial conductance may limit the water absorption at the distal ends of roots and that water uptake takes place along the entire root length (Landsberg and Fowkes, 1978). The solutions obtained with these models question assumptions made in parallel root models about negligible axial root resistances or about negligible uptake along the root and suggest that a big root model may be a better option. On the other hand, root tissue maturation generally leads to a decrease of radial root conductivity towards the older proximal end of roots so that root water absorbance can be larger near the root tips. A fibrous root system architecture with several lateral roots that are connected at the root collar and that take up water near the root tips might be represented better by a parallel root model than by a big root model, even when axial resistances cannot be neglected. In case of several parallel root branches, the xylem water potentials may differ between the different branches at a given depth and a big root model is not able to account for these variations in xylem water potentials. Upscaling of water flow in 3D root architectures to models that describe 1D root water uptake profiles in soils is crucial to implement root hydraulics in land surface models that describe exchanges of water and energy between the land surface and the atmosphere at catchment, continental and global scales. Also for crop models, which predict crop growth and yield at the field scale, an upscaling to 1-D uptake profiles is necessary. Root hydraulics has been implemented in land surface models to represent emerging processes like hydraulic redistribution and root water uptake compensation, which have an important impact on transpiration, assimilation and biogeochemical cycles during dry spells and seasons (Quijano et al., 2013; Liu et al., 2020). Yan and Dickinson (2014) and Fu et al. (2016) implemented the parallel root like model of Ryel whereas Tang et al. (2015) implemented a big root model. Kennedy et al. (2019) implemented a parallel root model in CLM and Sulis et al. (2019) implemented an approach proposed by Couvreur et al. (2012), which is for a certain parameterization equivalent to a parallel root model. Nguyen et al. (2020) demonstrated that differences in drought stress and crop growth in different soils with different soil hydraulic properties could be predicted by a crop model that considers root hydraulics whereas commonly used empirical relations failed. Root hydraulics are also important to describe the interaction of different species that share the same soil volume. Quijano et al. (2012) developed a multispecies model that simulates root water uptake by different species from a shared soil water reservoir based on their big root model. Each species was represented by its own big root model and the different big root models took up water from the shared soil water profile. The model demonstrated the impact of hydraulic redistribution on the uptake by the different species and their mutualistic dependencies. Water taken up deep in the soil profile



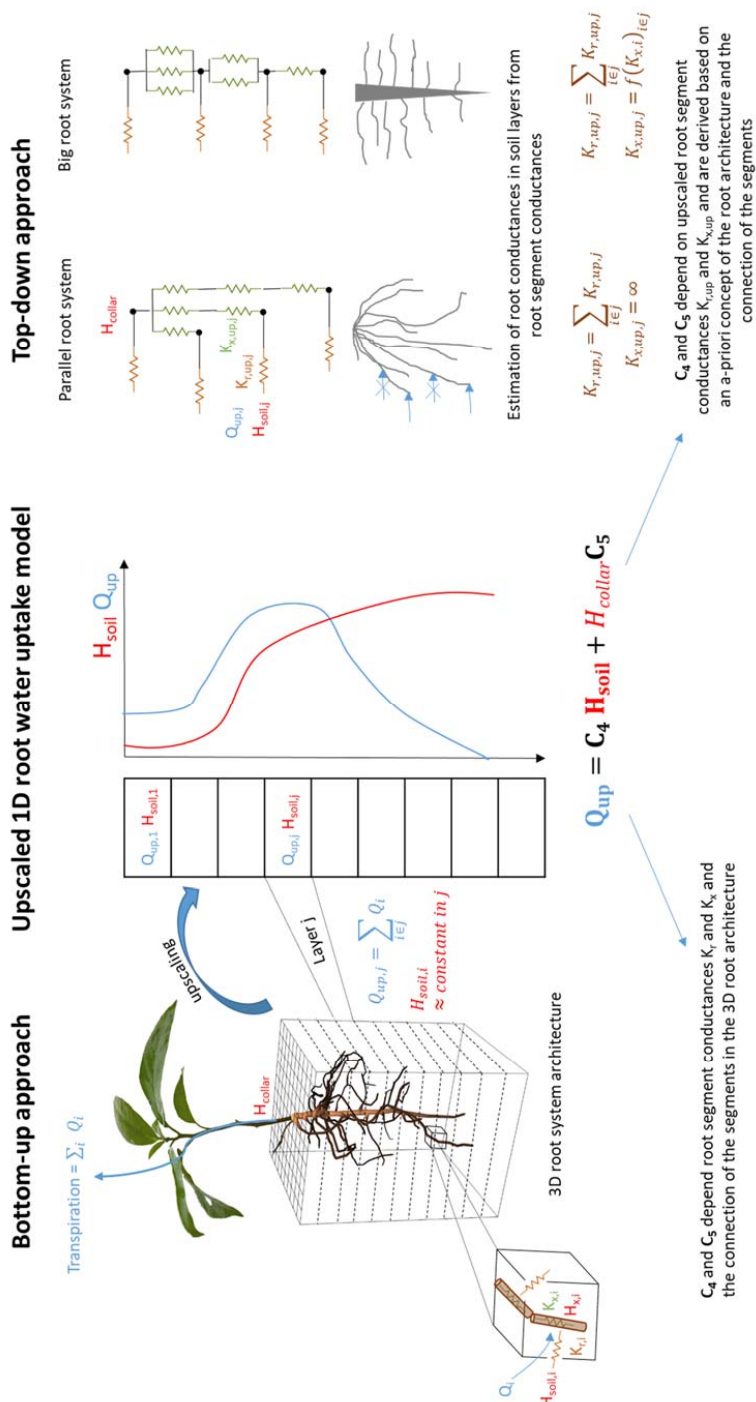
by deep rooting trees was released in the shallower soil layers where it could be accessed by shrubs or understory vegetation.

120 Similar conclusions were drawn by Manoli et al. (2014) and Manoli et al. (2017) using a parallel root system model. Although all models reproduced the impact of root hydraulics on ecosystems fluxes, a model comparison by Zhu et al. (2017), who compared Ryel's model with a big root model and an empirical root water uptake compensation model, highlighted that different models led to fairly different results. However, the nature of these differences is not well understood.

The objective of this paper is to derive with a bottom up approach a model that describes root water uptake considering the

125 hydraulics of the 3D root architecture. This model will be scaled up to a 1D model that could be readily implemented in land surface models. The model will be compared to currently used parallel root and big root models that are parameterized using a top-down approach (Figure 1). In a first part, the model will be demonstrated for a very simple hypothetical root system that represents a hybrid form of the two 'asymptotic' root architectures (parallel root versus big root model). In a second part, the model will be demonstrated for single roots with realistic distributions of root segment properties and realistic root

130 architectures of plants with a tap root or a fibrous root system.



31
 32
 33

Figure 1: Bottom-up approach versus top-down approaches for a parallel and a big root system model to derive and parameterize an upscaled one dimensional root water uptake model.



2 Set up of equations

135 In our model, the root system is discretised in a set of root segments or elements which are connected with each other in nodes. The N_{root} nodes of the root network are connected to N_{root} soil nodes and the entire system is connected to an extra outlet node that represents the root collar where the hydraulic head, H_{collar} , or the flux boundary condition is defined. Water flows in this network due to water potential differences between two connected nodes, i.e. between two root nodes or between a soil node and a root node. The root segments have a certain length and a certain conductance for water flow in the xylem in the axial direction, K_x ($L^2 T^{-1}$) and for radial flow from the soil to the xylem, K_r ($L^2 T^{-1}$). The axial flow in the xylem, $\mathbf{J}_x[i]$ ($L^3 T^{-1}$), of the root segment i that connects a distal node i with a proximal node j , and that has an axial conductance $\mathbf{K}_x[i]$ ($L^2 T^{-1}$), is related to the pressure head differences between the two nodes:

$$\mathbf{J}_x[i] = \mathbf{K}_x[i](\mathbf{H}_x[i] - \mathbf{H}_x[j]) \quad [1]$$

We use bold symbols for vectors and matrices that represent the set of fluxes, conductances, and hydraulic heads in the nodes of the soil-root network. Since branches of a root architecture do not re-join distally, there is only one segment that connects a certain node with the proximal part of the root system and its conductance is uniquely defined by the distal node number of the segment. $\mathbf{H}_x[i]$ (L) is the hydraulic head of the water in the xylem that includes both the pressure potential and the elevation potential. It is expressed as the height of a virtual water column that is connected to and in equilibrium with the water at node i . The flow from the soil to the root node i , $\mathbf{Q}[i]$ ($L^3 T^{-1}$), is related to the pressure head difference between the water in the soil and in the xylem of node i :

$$\mathbf{Q}[i] = \mathbf{K}_r[i](\mathbf{H}_{\text{soil}}[i] - \mathbf{H}_x[i]) \quad [2]$$

155 where $\mathbf{K}_r[i]$ ($L^2 T^{-1}$) is the radial conductance of the root and $\mathbf{H}_{\text{soil}}[i]$ is the hydraulic head of the soil water that is in contact with node i . The root segment hydraulic properties as defined above are extensive properties that depend on the size of the root segment. Intensive properties k_x ($L^3 T^{-1}$) and k_r (T^{-1}) (called hereafter intrinsic conductance) can be defined as:

$$\mathbf{k}_x[i] = \mathbf{K}_x[i]\mathbf{l}[i] \quad [3]$$

$$\mathbf{k}_r[i] = \frac{\mathbf{K}_r[i]}{2\pi r[i]\mathbf{l}[i]} \quad [4]$$

where $\mathbf{l}[i]$ and $r[i]$ are the length and radius of the root segments, respectively.

For each root node, two equations can be set up: one equation that closes the water balance in this node and one equation that calculates the flow \mathbf{Q} from the soil to this node. When the hydraulic heads in the soil nodes \mathbf{H}_{soil} ($N_{\text{root}} \times 1$) and the hydraulic head in the root collar, H_{collar} , are prescribed, the xylem water potentials in the root system, \mathbf{H}_x ($N_{\text{root}} \times 1$) and the flow from the soil nodes to the root nodes \mathbf{Q} are obtained by solving the following equation:

$$\left[\mathbf{IM} \cdot \text{diag}(\mathbf{K}) \cdot \mathbf{IM}_{\text{collar}}^T \right] \begin{bmatrix} H_{\text{collar}} \\ \mathbf{H}_x \\ \mathbf{H}_{\text{soil}} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{Q} \end{bmatrix} \quad [5]$$

160 where the connections of the nodes in the system with other root nodes and with the soil nodes are described by the connectivity matrix \mathbf{IM} ($2N_{\text{root}} \times 2N_{\text{root}}$) and an extended connectivity matrix that includes the connections of the xylem nodes to the collar, $\mathbf{IM}_{\text{collar}}^T$ ($2N_{\text{root}} \times 2N_{\text{root}}+1$) $\text{diag}(\mathbf{K})$ ($2N_{\text{root}} \times 2N_{\text{root}}$) is the diagonal conductance matrix with the first N_{root} elements representing the axial conductances of the root segments, K_x , and the last N_{root} elements the radial root segment conductances (or soil-root conductances). The setup of the equation and the connectivity matrices are described in more detail in the Appendix. The first



N_{root} equations in Eq. [5] close the water balances in root nodes and from solving these, the xylem water potentials in the root nodes are obtained. Plugging the obtained xylem water potentials in the last N_{root} equations, the fluxes towards each root node can be obtained from Eq. [5] (see Appendix) as:

$$\mathbf{C}_4 \mathbf{H}_{\text{soil}} + \mathbf{C}_5 H_{\text{collar}} = \mathbf{Q} \quad [6]$$

where \mathbf{C}_4 ($L^2 T^{-1}$) is an $N_{\text{root}} \times N_{\text{root}}$ symmetric matrix and \mathbf{C}_5 ($L^2 T^{-1}$) an $N_{\text{root}} \times 1$ column. The relations between \mathbf{C}_4 , \mathbf{C}_5 and the root segment conductivities (stored in $\text{diag}(\mathbf{K})$) and the segment connectivities (defined in \mathbf{IM}) is given in Table 1. This equation can be written in another form that uses macroscopic characteristics of the root system, K_{rs} and \mathbf{SUF} , and an effective root zone hydraulic head H_{eff} that were introduced by (Couvreur et al., 2012):

$$\mathbf{Q} = K_{rs} \mathbf{SUF} (H_{\text{eff}} - H_{\text{collar}}) + \mathbf{C}_4 (\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}}) \quad [7]$$

where K_{rs} is the root system conductance ($L^2 T^{-1}$), \mathbf{SUF} is the ($N_{\text{root}} \times 1$) standardized uptake fraction vector (-), H_{eff} (L) is the effective soil water hydraulic head around the system, \mathbf{H}_{eff} is a ($N_{\text{root}} \times 1$) vector filled with H_{eff} . The derivation of Eq. [7] is given in the appendix. Here we summarize the main properties of the equation. The first term on the right-hand side of Eq. [7] represents the uptake from the soil profile when the soil water hydraulic head is uniform in the soil and equal to H_{eff} , and $\mathbf{SUF}(i)$ represents the fraction of the total uptake by a certain root node for a uniform soil water hydraulic head. For a non-uniform distribution of soil water hydraulic heads, H_{eff} is a weighted average of the soil water hydraulic heads, \mathbf{H}_{soil} . When \mathbf{H}_{soil} are weighted by the uptake fractions under uniform hydraulic head conditions, \mathbf{SUF} , to calculate H_{eff} , the sum of the fluxes of the second term of the right hand side of Eq. [7] is zero. The second term on the right-hand side represents the amount of water that is taken up more (less) by a certain root node than in case the soil water hydraulic head is equal to H_{eff} when the soil water hydraulic head around the node is larger (smaller) than H_{eff} . This second term represents the compensatory uptake and we name the \mathbf{C}_4 matrix the compensatory matrix. Of note is that the second term only depends on the hydraulic root architecture (defining \mathbf{C}_4 and \mathbf{SUF}) and on the soil water hydraulic head distribution. It neither depends on the water potential at the root collar nor on the transpiration rate. As a consequence, root water uptake compensation changes over time only due to changes in the soil water hydraulic heads but not due to e.g. diurnal changes in transpiration rate. Another interesting consequence of the fact that the sum of the fluxes calculated by the second term is zero is that the total uptake by the root system or transpiration rate T ($L^3 T^{-1}$) can be calculated based on the root system conductance and effective soil water hydraulic head only:

$$T = \sum_i \mathbf{Q} = K_{rs} (H_{\text{eff}} - H_{\text{collar}}) \quad [8]$$

In Table 1, relations between K_{rs} , \mathbf{SUF} , \mathbf{C}_4 , H_{eff} and the root hydraulic architecture are given.



Table 1: Equations to calculate the root system hydraulic conductance, K_{rs} , the standard uptake fraction, SUF , the compensatory uptake matrix, C_4 , and the effective soil water hydraulic head, H_{eff} , from the hydraulic root architecture.

$C = \mathbf{IM} \cdot \mathit{diag}(\mathbf{K}) \cdot \mathbf{IM}_{\text{collar}}^T (2N_{\text{root}} \times 2N_{\text{root}} + 1)$	[9]
$C_1 = C[1 : N_{\text{root}}, 1]$	[10]
$C_2 = C[1 : N_{\text{root}}, 2 : N_{\text{root}} + 1]$	[11]
$C_3 = C[1 : N_{\text{root}}, N_{\text{root}} + 2 : 2N_{\text{root}} + 1]$	[12]
$C_4 = \mathit{diag}(\mathbf{K}_r) [\mathbf{I} + C_2^{-1} C_3] (N_{\text{root}} \times N_{\text{root}})$	[13]
$C_5[i] = -\sum_j C_4[i, j]$	
$K_{rs} = \sum_i \sum_j C_4[i, j]$	[14]
$SUF[i] = \frac{\sum_j C_4[i, j]}{\sum_i \sum_j C_4[i, j]}$	[15]
$H_{eff} = \mathbf{SUF}^T \mathbf{H}_{\text{soil}}$	[16]

195 K_{rs} and SUF can be calculated directly from the compensatory matrix C_4 . In the following, we will present a reformulated form of Eq. [7] that resembles the equation that is obtained for a parallel root system. For the derivation, we refer to the appendix and we focus here on the results.

As is derived in the appendix, the matrix C_4 in Eq. [7] can be ‘factorized’ in a product of two diagonal matrices: one with a diagonal that is equal to the SUF vector and one with a diagonal that represents a ‘compensatory conductivity vector’ \mathbf{K}_{comp} ; and one matrix C_7 which is close to the identity matrix \mathbf{I} :

$$200 \quad \mathbf{Q} = K_{rs} (\mathbf{H}_{eff} - \mathbf{H}_{collar}) \mathbf{SUF} + \mathit{diag}(\mathbf{SUF}) \mathit{diag}(\mathbf{K}_{\text{comp}}) C_7 (\mathbf{H}_{\text{soil}} - \mathbf{H}_{eff}) \quad [17]$$

The diagonal elements of C_7 are 1 and for each row of C_7 , the sum of the off-diagonal elements is equal to zero. When $H_{eff} = H_{collar}$, i.e. there is no net uptake but only redistribution of water through the root system, and when the soil water hydraulic head of node i is ΔH higher than the soil water hydraulic head in all other nodes ($\mathbf{H}_{\text{soil}}[i] - \Delta H = \mathbf{H}_{\text{soil}}[j \neq i]$), then the flow from node i to all other nodes in the root system, $\Delta Q[i]$, is:

$$205 \quad \Delta Q[i] = \mathbf{k}_{\text{comp}}[i] \Delta H \quad [18]$$

where $\mathbf{k}_{\text{comp}}[i]$ ($L^3 T^{-1}$) represents the conductivity of the root system to transfer water from all other root elements to the root node i . From the definition of H_{eff} , it follows that:

$$\mathbf{H}_{\text{soil}}[i] - H_{eff} = (1 - \mathbf{SUF}[i]) \Delta H \quad [19]$$

Plugging this into Eq. [17] and considering that the sum of the off-diagonal elements of a row in C_7 is zero and that the soil hydraulic heads $\mathbf{H}_{\text{soil}}[j \neq i]$ are all the same, it follows that:

$$\Delta Q[i] = \mathbf{SUF}[i] \mathbf{K}_{\text{comp}}[i] (1 - \mathbf{SUF}[i]) \Delta H \quad [20]$$

By comparing Eqs. [18] and [20], we find that $\mathbf{SUF}[i](1 - \mathbf{SUF}[i]) \mathbf{K}_{\text{comp}}[i] = \mathbf{k}_{\text{comp}}[i]$.



210 For a root system in which all root nodes are connected in parallel to the root collar, $\mathbf{k}_{\text{comp}}[i]$ is equal to the equivalent
 conductance of a connection in series of a conductance from root node i to the collar, which is $\text{SUF}[i] K_{rs}$, and a conductance
 from the collar to all other nodes, $(1 - \text{SUF}[i]) K_{rs}$:

$$\mathbf{k}_{\text{comp}}[i] = \left((\text{SUF}[i] K_{rs})^{-1} + ((1 - \text{SUF}[i]) K_{rs})^{-1} \right)^{-1} = \text{SUF}[i] (1 - \text{SUF}[i]) K_{rs} \quad [21]$$

This implies that for a parallel root system, $\mathbf{K}_{\text{comp}} = \mathbf{K}_{rs}$. It can further be shown that \mathbf{C}_7 is the identity matrix for a parallel root
 system (see appendix) so that Eq. [7] can be written as:

$$\mathbf{Q} = K_{rs} (\mathbf{H}_{\text{eff}} - \mathbf{H}_{\text{collar}}) \text{SUF} + K_{rs} \text{diag}(\text{SUF}) (\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}}) \quad [22]$$

215

The parallel root system is fully defined by the SUF and K_{rs} and the compensatory uptake is defined when the uptake
 distribution from a soil profile with a uniform soil water hydraulic head is known. Since in a non-parallel root system the
 connection of a single root node to all other root nodes is at least as good as the series connection of this node to the collar and
 the connection of the collar with all other root system nodes, it follows that $\mathbf{K}_{\text{comp}}[i] \geq K_{rs}$. Negative off-diagonal elements
 220 in a row of \mathbf{C}_7 represent nodes which are better connected with each other than with other nodes while positive numbers
 indicate a worse connection.

3 Upscaling:

From the matrix equations, it follows that the upscaling of the relations between the uptake rates \mathbf{Q} and soil water hydraulic
 heads \mathbf{H}_{soil} is trivial for cases when the soil water hydraulic heads are uniform in certain regions of the soil. When we assume
 225 that the soil water hydraulic heads do not change in the horizontal direction, then we can simply group and sum up all SUF
 values for the soil root nodes that are in the same soil horizontal soil layer and derive an upscaled SUF vector that describes
 the relative uptake from each soil layer when the soil water hydraulic heads are uniformly distributed (Couvreur et al., 2014a)
 (Figure 2). The upscaled matrix \mathbf{C}_4 that is multiplied by a vector of soil water hydraulic heads in the different soil layers is
 simply obtained by:

230

$$\mathbf{C}_{4,\text{upscaled}}[i, j] = \sum_{k \in \text{layer}_i} \sum_{l \in \text{layer}_j} \mathbf{C}_4[k, l] \quad [23]$$

The dimensions of the upscaled matrices are reduced so that the number of equations that need to be solved is reduced to the
 number of layers in which the soil water hydraulic heads are uniform. This implies a massive reduction in the computational
 cost compared with the cost of solving equations for a large number of root segments that make up a 3D root architecture.
 235 Under the assumption that the soil water hydraulic heads are constant within a layer, the obtained equations are exact,
 independent of the soil water hydraulic heads, and need to be derived from the large set of equations for a given 3D root
 architecture only once. They can be used afterwards to calculate uptake from the layers for other collar and soil hydraulic
 heads. Based on the upscaled \mathbf{C}_4 and SUF , the upscaled \mathbf{C}_7 and \mathbf{K}_{comp} can be derived. It must be noted that \mathbf{C}_7 and \mathbf{K}_{comp} cannot
 be scaled up directly by summing up elements in the \mathbf{C}_7 matrix and \mathbf{K}_{comp} vector. The upscaling was performed here assuming
 240 uniform soil water hydraulic heads in the horizontal direction. It can be applied for any region where soil water hydraulic heads
 are assumed to be uniform.



$$\mathbf{Q} = K_{rs} (H_{eff} - H_{collar}) \mathbf{SUF} + \mathbf{C}_4 (\mathbf{H}_{soil} - \mathbf{H}_{eff})$$

245 **Figure 2: Upscaling of the SUF and C_4 matrix by simply taking the sum of elements that correspond with nodes where the soil water hydraulic heads are the same. Nodes with the same water hydraulic heads are grouped in layers and are marked with the same color. The elements of the marked blocks of the Q and SUF vectors and in the C_4 matrix are summed up.**

4 Demonstrations:

In order to demonstrate the model, its upscaling, and comparison with big root and parallel root approximations, we considered in a first step an abstract ‘hybrid’ parallel-big root system, which is a mixture of the parallel and big root systems. It consists of three parallel branches of different length that each take up water along their length and not only at the root tip as supposed in the parallel root system. Since the water fluxes in each of the three branches are different because of their different length, the water hydraulic heads in the xylem at a given depth differ between the three roots even when the soil water hydraulic heads do not vary at a given depth. Therefore, this ‘hybrid’ root system represents an intermediate model that matches with neither the parallel root nor the big root model perfectly. This model should demonstrate the upscaling and the difference between the two approximate models. We used a dummy parameterization of the root hydraulic properties and of the vertical distribution of the soil water hydraulic heads (i.e. the parameters were chosen to represent certain differences but the actual values of the parameters and their units were not of interest). We considered a case in which all the root segments had the same radial conductance and a case in which the radial conductance at the root tips were a factor 10 larger.

In a second step, we considered a single root with either constant or changing root hydraulic parameters along the root axis. In a third step, we considered root systems that correspond in terms of complexity and parameterization to more realistic root systems and represent three different crops: grass, maize and sunflower.



4.1 Simple hybrid root system:

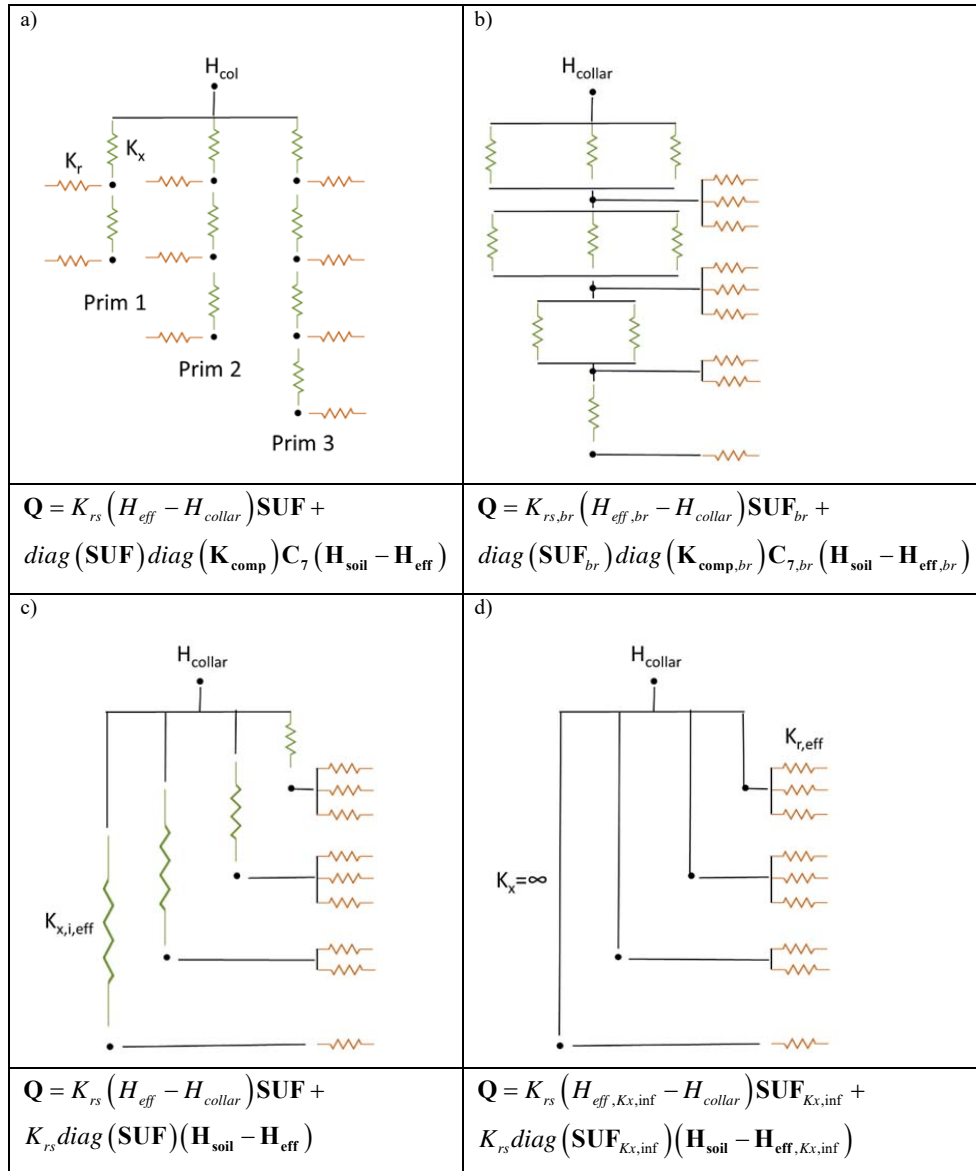


Figure 3: Hybrid parallel-big root system consisting of three primary root branches of different length a); and approximations by: the big root model b); the parallel root model with the same SUF and K_{rs} as the hybrid model c); and the parallel root model with an infinite axial conductance and the same K_{rs} as the hybrid model. The approximate models describe upscaled root water uptake within a horizontal soil layer. The SUF, K_{rs} , \mathbf{K}_{comp} and C_7 of the big root model are calculated from the segment axial and radial conductances that are arranged following the big root topology. The SUF and K_{rs} of the parallel root model c) are matched to those of the upscaled hybrid model by adapting $K_{x,eff}$ of the segment that connects the xylem node at a certain depth to the collar node. The K_r of the segments of the parallel root model with infinite K_x are scaled to $K_{r,eff}$ so that the K_{rs} matches the K_{rs} of the hybrid root system. The equations below the resistance nets represent the equations that calculate the upscaled water uptake Q in a horizontal layer.

265

270

Figure 3 a) shows the hybrid parallel-big root system that consists of three primary root branches of different length. This root system was scaled up to a model that describes uptake from a horizontal soil layer where the soil water hydraulic head is uniform (the exact model) and was approximated by upscaled parallel and big root systems. The big root approximation



assumes that the root segments are organized and connected following the a-priori defined big root architecture so that the axial and radial conductance in a certain layer is the sum of the axial and radial conductances of the individual root segments in that layer (Figure 3 b). This parameterization of the big root model comes down to a top down parameterization based on root segment conductances in a soil layer. For the parallel root approximation, we considered a root system with the same **SUF** and K_{rs} as the upscaled hybrid model (Figure 3 c). For a given distribution of radial conductances, K_{rs} and **SUF** can be defined by adapting effective $K_{x,eff}$ of virtual root branches that connect a certain depth with the root collar. This parameterization, which is based on calculations for the 3D hydraulic root architecture, corresponds with a bottom up parameterization. For the upscaled parallel root model, the number of parameters that needs to be defined is equal to $ndepths+1$ where $ndepths$ is the number of soil layers. In contrast, the big root model requires $2ndepth$ parameters. Unlike for the parallel root system, there is no simple relation between K_{rs} and **SUF** on the one hand and the compensatory uptake term on the other for the big root model. Therefore, the structure of the big root model does not lend itself to calculating its parameters directly from characteristics of the 3D hydraulic root architecture in a bottom up approach. The third model that we considered is a parallel root model in which the **SUF** is derived in a top down approach directly from the distribution of the radial conductances assuming an infinitely large axial conductance (parallel root approximation with infinite K_x). The K_{rs} of this root system was adjusted to the K_{rs} of the hybrid root system, which comes down to a scaling of the radial conductance of all root nodes with the same factor.

We considered two parameterizations of the root hydraulic conductances. In the first case, the conductances of all root segments are uniform: $K_x=10$ and $K_r=1$. In the second case, the radial root hydraulic conductance is larger at the root tips ($K_r=1$) than in the other parts along the primary roots ($K_r=0.1$). To evaluate the effect of a non-uniform hydraulic head in the soil, the soil water hydraulic heads varied from top to bottom as: -0.5, 0, 0.5, 1 and were assumed to be the same for root nodes at the same depth. The hydraulic head at the root collar was set to -1. The K_{rs} , **SUF** and K_{comp} and their upscaled values for the hybrid root system and the three approximations are given in Table 2 and Table 3 for the root system with homogeneous root segment conductances and for the root system with higher radial conductances at the root tips, respectively. The root water uptake profiles that are simulated by the different models for the two parameterizations of the root segment conductivities are given in Figure 4 and Figure 5.

The upscaled **SUF** profiles that were estimated for a parallel root system considering only the distribution of radial conductances (infinite K_x parallel root model) overestimate the **SUF** deeper in the soil profile and underestimate it at shallower depths. The resistance to axial flow reduces the uptake from more distal root segments compared to the uptake at more proximal root segments. The big root model can better account for the impact of the axial resistance on the **SUF** distribution. However, the assumption of equal xylem hydraulic head in all root segments at a certain depth leads to an underestimation of the uptake in a soil profile with homogeneous hydraulic head in the proximal root segments. This underestimation was not important when the radial conductance was larger near the root tips. The upscaled **SUF**, which represents the uptake by all root segments at a certain depth, was equal to the sum of the **SUFs** of the individual root segments at that depth.

For a non-uniform distribution of the soil water hydraulic head, which increased with depth, the uptake at greater depths increased and that at shallower depths decreased as compared to the uptake under uniform soil water hydraulic head. All models reproduced this compensation of root water uptake. The parallel root approximation, which used the exact root system **SUF** and K_{rs} , underestimates the root water uptake compensation whereas the big root model overestimates it. The parallel root model uses K_{rs} to calculate the compensatory uptake and K_{rs} was smaller than K_{comp} . The big root model overestimates the compensation since it assumes that all root segments in a certain layer are directly connected to all the root segments in the overlying or underlying layers and that the xylem hydraulic heads are the same in all root segments at a certain depth. This implies that redistribution flow between the soil layers via the root system can occur directly without flow having to pass the collar first before it returns to another layer. The K_{comp} that is derived for the big root model is only slightly higher, except for

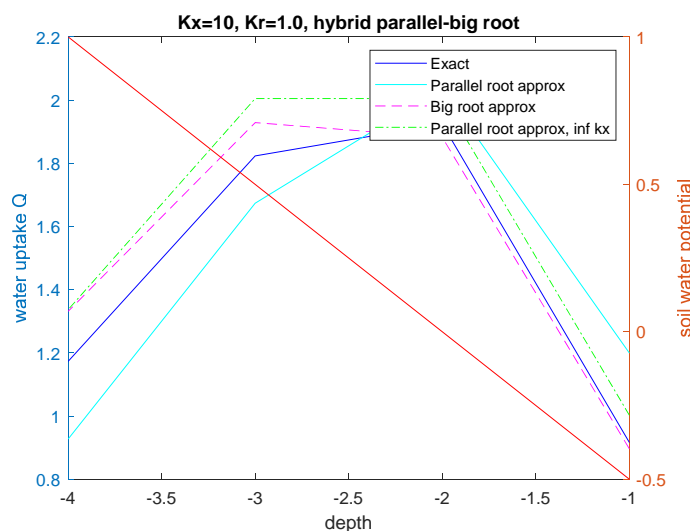


the deepest root node, than the K_{comp} of the exact model. The larger uptake simulated by the big root model from the deeper layer is therefore linked to the larger SUF in the deeper soil layers. This is also the case for the infinite K_x parallel root model for which the higher SUF and higher soil water hydraulic head at greater depths lead to a larger simulated water uptake, especially deeper in the profile.

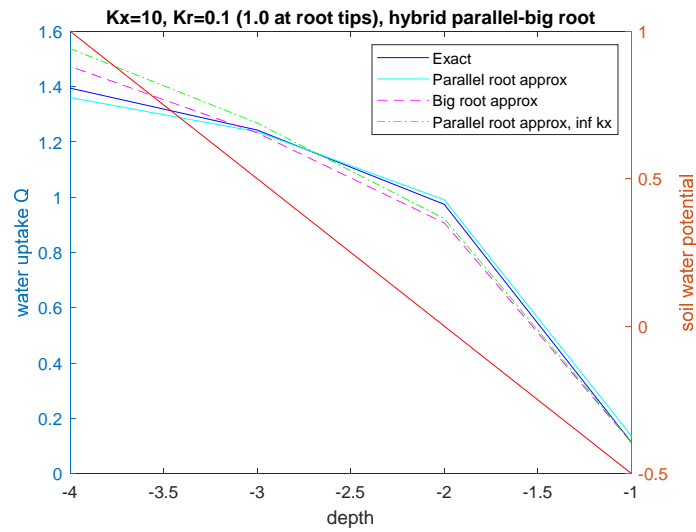
320 Also of interest is that the upscaled K_{comp} values are not equal to the average of the K_{comp} values of the root nodes in a soil layer. For the top layer, the upscaled K_{comp} is even larger than the largest K_{comp} value of the three primary root branches. Larger radial resistance away from the root tips led to a root system that behaves more like a parallel root system (Figure 5). This is reflected in the K_{comp} values that are closer to K_{rs} and the C_7 matrix that is closer to the identity matrix than the C_7 matrix of the hybrid parallel-big root system with uniform root segment hydraulic properties (Table 3). The higher radial

325 root segment conductances near the root tips make that water transfer between two soil layers via root tips in these layers soil, which passes through the root collar, is more efficient than water transfer via a root tip segment and a root segment that is directly connected to it. In the big root model, the root tip segment with higher radial conductance in one layer is assumed to be directly linked to the root tip segment in another layer so that the water flow between these layers occurs more efficiently than via the root collar. This is reflected in the higher K_{comp} and the larger deviation of the C_7 matrix from the

330 identity matrix for the big root model than for the hybrid parallel-big root model which lead to an overestimation of the root water uptake compensation by the big root model.



335 **Figure 4:** Upscaled water uptake profile (left axis) and soil water potential distribution (right axis, red line) for the hybrid parallel-big root system, the approximate parallel root model, big root model, and the parallel root model assuming an infinite axial conductance, K_x .



340 **Figure 5:** Upscaled water uptake profiles (left axis) and soil water potential distribution (right axis, red line) for the hybrid parallel-big root system, the approximate parallel root model, big root model, and the parallel root model assuming an infinite axial conductance, K_x . The radial conductance along the primary root branches vary along the branches (radial conductance is 1 at root tips and 0.1 at other nodes).



Table 2: K_{rs} , SUF, K_{comp} and upscaled values and C_7 matrices for the hybrid parallel-big root system, the big root system and the parallel root system with infinite K_x .

	Hybrid Parallel-Big root				Big root	Parallel
	$K_r=1, K_x=10, K_{rs}= 6.0147$				$K_{rs}= 6.1122$	Inf $K_x,$ $K_{rs}= 6.0147$
	Prim. root 1	Prim. root 2	Prim. Root 3	Upscaled		
Depth	SUF	SUF	SUF	$SUF_{upscaled}$	$SUF_{upscaled}$	$SUF_{upscaled}$
1	0.1396	0.1391	0.1273	0.3988	0.3908	0.33
2	0.1269	0.1108	0.1010	0.3387	0.3299	0.33
3		0.1007	0.0848	0.1855	0.1920	0.22
4			0.0771	0.0771	0.0873	0.11
	K_{comp}	K_{comp}	K_{comp}	$K_{comp_upscaled}$		
1	6.65	7.13	7.44	7.52	7.68	
2	6.70	7.98	8.94	8.41	8.65	
3		8.09	10.09	9.35	9.39	
4			10.26	10.26	10.00	

345 C_7 matrix of the upscaled hybrid parallel-big root system

1	0	0	0
0.042	1	-0.030	-0.012
0.078	-0.014	1	-0.064
0.106	0.017	-0.123	1

C_7 matrix big root system

1	0	0	0
0.044	1	-0.030	-0.014
0.071	-0.022	1	-0.050
0.091	0	-0.091	1



350 **Table 3: K_{rs} , SUF, K_{comp} and upscaled values and C_7 matrices for the hybrid parallel-big root system with variable root radial root segment conductances along the roots, for the big root system, and for the parallel root system with infinite K_x .**

	Hybrid Parallel-Big root				Big root	Parallel
	$K_r=1, K_x=0.1, K_{rs}= 2.7673$				$K_{rs}= 2.7673$	Inf K_x , $K_{rs}= 2.7673$
	Prim. root 1	Prim. root 2	Prim. root 3	Upscaled		
Depth	SUF	SUF	SUF	$SUF_{upscaled}$	$SUF_{upscaled}$	
-1	0.0328	0.0328	0.0328	0.0984	0.0984	0.0833
-2	0.2984	0.0298	0.0298	0.3580	0.3576	0.3333
-3		0.2709	0.0270	0.2979	0.2979	0.3056
-4			0.2457	0.2457	0.2462	0.2778
	K_{comp}	K_{comp}	K_{comp}	$K_{comp_upscaled}$		
-1	3.0274	3.0295	3.0313	3.0485	3.0485	
-2	2.8067	3.3170	3.3213	2.9419	3.3373	
-3		2.8815	3.6389	2.9847	3.5590	
-4			2.9892	2.9892	3.5898	

C_7 matrix of the upscaled hybrid parallel big-root system

1	0	0	0
-0.004	1	0.002	0.002
-0.002	0.007	1	-0.005
-0.002	0.008	-0.006	1

C_7 matrix of the big root system

1	0	0	0
0.009	1	-0.005	-0.004
0.014	0.017	1	-0.031
0.015	0.02	-0.035	1

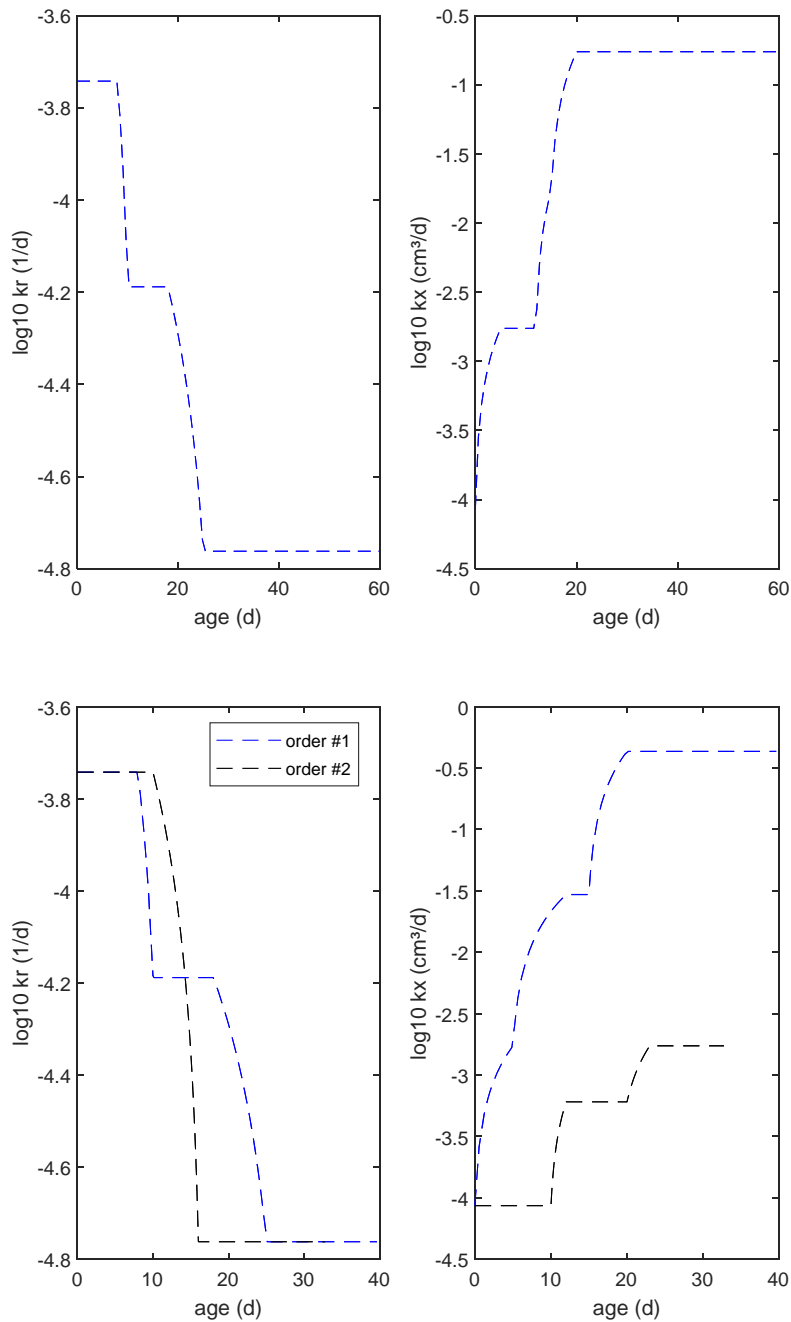
4.2 Single root branches

We considered two single root branches, one with homogeneous (intrinsic) root segment conductances ($k_x= 0.171 \text{ cm}^3 \text{ d}^{-1}$, $k_r= 1.81 \cdot 10^{-4} \text{ d}^{-1}$) and one with conductances that changed along the root axis due to maturation of the root tissue (Figure 6). This generally leads to an increase in axial conductance and a decrease in radial conductance with age or distance from the root tip (Doussan et al., 1998; Doussan et al., 2006; Zarebanadkouki et al., 2016; Couvreur et al., 2018; Meunier et al., 2018b). The root was assumed to be 50 cm long with 1cm long segments with uniform conductances. The soil collar potential was assumed to be -4000 cm and the soil water hydraulic head varied linearly between -3000 cm at the soil surface and 0 cm at the lowest depth of the root system. The upscaled model considered 2 cm long segments.

As to be expected, the big root system matches nearly perfectly with the exact model (Figure 7). The deviations are due to the upscaling and the variations of soil water and xylem hydraulic heads along a root segment that is represented by a single node (Bouda, 2019). The infinite K_x parallel root model that derives the SUF based on the radial root segment conductances overestimates the SUF in the distal part of the root since the impact of the axial resistance to flow is not considered. For a

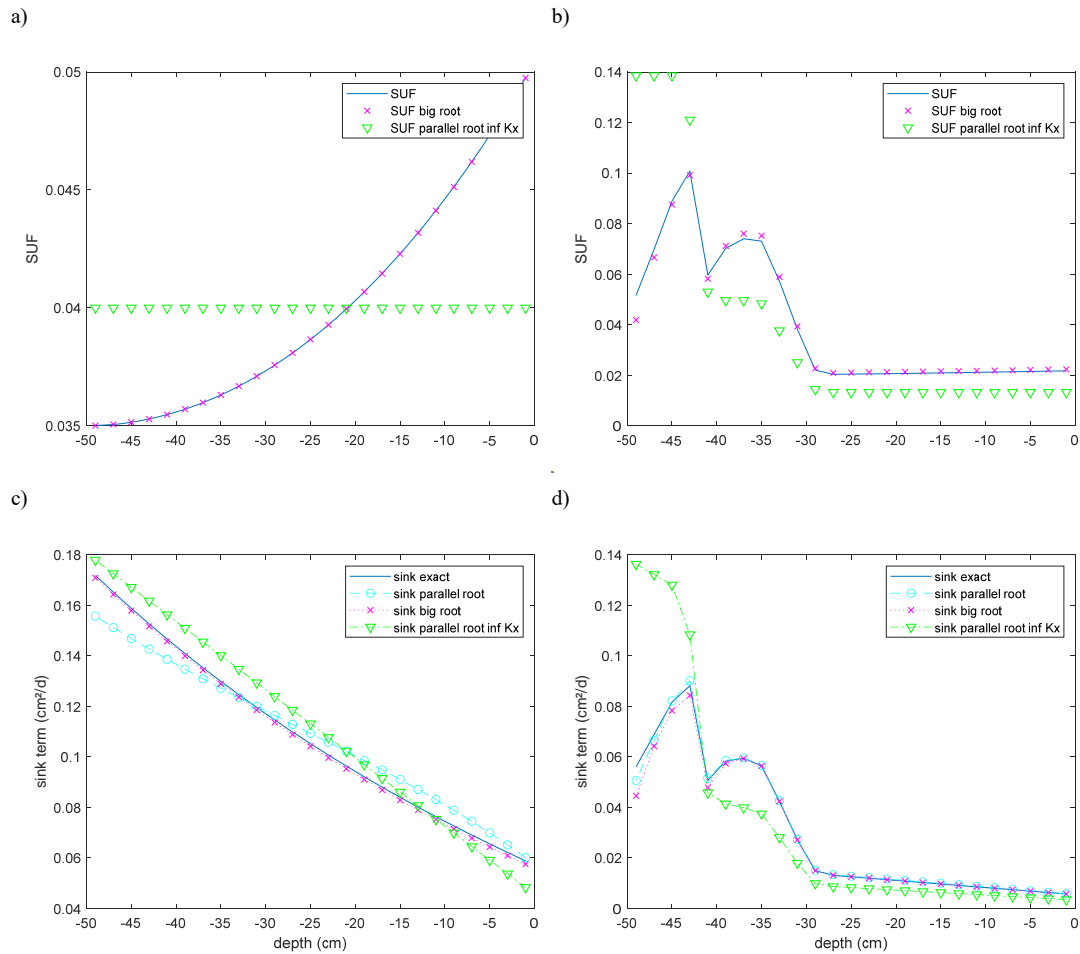


365 larger soil water hydraulic head near the distal end of the root, the overestimation of the SUF in this region results in an
overestimation of the root water uptake from the deeper soil and an overestimation of the apparent root water uptake
compensation. The opposite is the case for the parallel root system that uses the exact SUF and underestimates the uptake near
the distal end of the root due to an underestimation of the root water uptake compensation. However, for a root with non-
uniform root segment conductances, uptake simulated with this parallel root system represents nearly perfectly the exact uptake
370 and even slightly better than the big root system. Even for a single root, which can be considered to be a 'perfect' big root
system, the parallel root model may perform quite well when this model uses the exact SUF. This is even better when root
segment conductivities vary along the root. The K_{comp} profiles and C_7 matrices, which are shown for the two root systems in
Figure 8, may be used as diagnostics of the approximation of the root water uptake by the parallel root model. Rather than the
absolute values of the ratios of K_{comp}/K_{rs} and of the entries in the C_7 matrix, the distributions of these values along the root
375 profile seem to indicate whether a parallel root model can describe the uptake profile. For the root with uniform root segment
conductances, larger values of K_{comp}/K_{rs} and off-diagonal entries in C_7 that deviated from zero were distributed more over the
entire root length whereas for the root with non-uniform root segment conductivities, these larger values and deviations were
concentrated near the root tips.

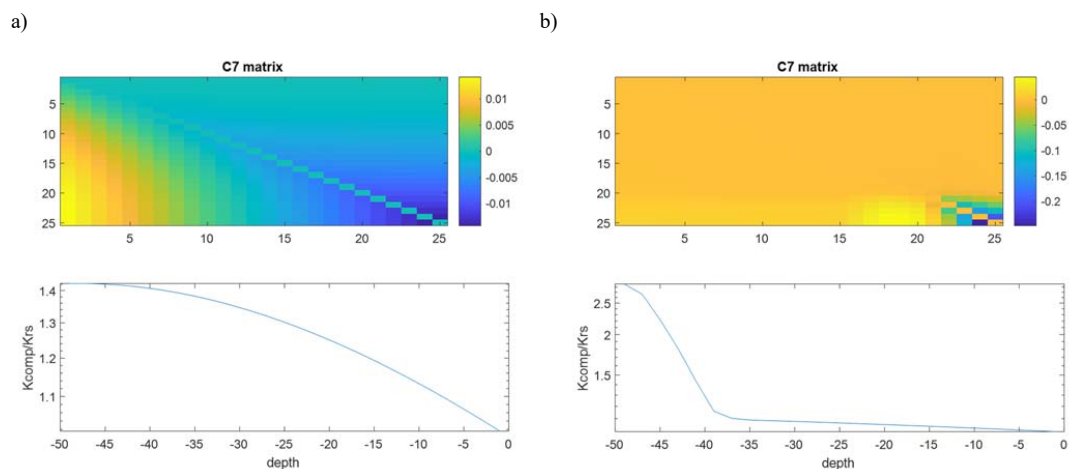


380

Figure 6: Radial (left), k_r , and axial (right), k_x , intrinsic root conductivities as a function of the root segment age for the single root (top) and root system architectures (bottom).



385 **Figure 7: Standard uptake for homogeneous soil water potential (SUF) (a,b) and sink term for a linear increase of water potential with depth (c,d) of a single root branch with uniform (a,c) and age dependent (b,d) root segment conductances. Approximations are calculated for the parallel root, the big root, and parallel root using infinite axial conductance models. Sink terms are divided by the thickness of the soil layer, 2cm, over which the root segment sink terms are summed.**



390 **Figure 8:** C_7 matrices and profiles of the ratio of K_{comp}/K_{rs} of the single root with uniform (a) and non uniform (b) root segment hydraulic conductances along the root. The labels on the axes of the C_7 matrices represent the root segment numbers, which increase from the proximal to the distal end of the root, i.e. from top to bottom. For visualization, the diagonal elements of the C_7 matrix were set to 0.



395 **4.3 Realistic root systems:**

We generated root systems of three different plants: maize, sunflower and grass using the CRootBox shiny app (<https://plantmodelling.shinyapps.io/shinyRootBox/>) (Schnepf et al., 2018) . The intrinsic radial and axial root segment conductances depended on the root order and varied with age (Figure 6). We assumed that this relation between root age and segment conductance did not vary between the crops. It should be noted that the root architectures and intrinsic root segment

400 conductances were chosen to illustrate the difference between the different root water uptake modelling approaches for more realistic root systems. However, the derived root system characteristics should not be interpreted as the characteristics of a certain crop. As for single root branch simulations, the collar water potential was -4000 cm, the soil water potential at the soil surface -3000 cm and 0 cm at the maximal rooting depth of the root system. The SUF and root water uptake distributions were scaled up to and derived for 2cm thick horizontal soil layers yielding 1D vertical profiles.

405 For the parameterization of the big root model, we calculated the axial conductance of the big root for each soil layer i , $K_{x,\text{bigroot},i}$ from the length, orientation, and intrinsic axial conductances of all the root segments in that layer as follows. First we calculate an ‘effective’ intrinsic axial conductance for flow in the vertical direction in a soil layer, $k_{x,\text{eff},i}$:

$$k_{x,\text{eff},i} = \frac{\sum_j l_j |\cos(\alpha_j)| k_{x,j}}{\sum_j l_j} \quad [24]$$

where l_j is the length of the j th root segment, $k_{x,j}$ its intrinsic root conductance and α_j the angle of the segment with the vertical. To obtain $K_{x,\text{bigroot},i}$, we multiplied the effective intrinsic axial conductance by the number of roots that cross the layer and

410 divided it by the layer thickness. The number of roots that cross the layer is calculated from the sum of the vertical increments of the root segments divided by the layer thickness so that we obtained:

$$K_{x,\text{bigroot},i} = \frac{k_{x,\text{eff},i} \sum_j l_j |\cos(\alpha_j)|}{\Delta z_i^2} \quad [25]$$

The radial conductance of the big root system in layer i , $K_{r,\text{bigroot},i}$ was calculated by simply adding up the radial conductances of the root segments.

415 For the parallel root system, we considered as above two parameterizations. The first used the SUF and K_{rs} values of the exact upscaled model. The second parameterization, the parallel root model with infinite K_x , assumes that the axial conductance is very high compared to the radial conductance so that the SUF can be calculated directly from the distribution of the radial root segment conductances:

$$SUF [i] = \frac{K_{r,\text{bigroot},i}}{\sum_i K_{r,\text{bigroot},i}} \quad [26]$$

To account for the effect of resistance to axial flow, the exact K_{rs} is used in the parallel root model with infinite K_x . It should

420 be noted that Eqs. [24], [25], and [26] use information about root segments such as their orientation, age and root type dependent conductance, and surface which is mostly not used or available to parameterize hydraulic root water uptake models. Mostly, the root segment conductances and root radii are assumed to be constant so that root length density is used to estimate the hydraulic properties. Since we focus in this paper on the differences between different model structures, we used the more detailed information to avoid differences due to differences in information that was used for parameterization.



425 The root system conductances that are estimated from the root segment conductances considering the 3D hydraulic root architectures, K_{rs} , or using a big root representation, $K_{rs, \text{bigroot}}$, are given in Table 4. The root system conductances for sunflower are considerably smaller than those of maize and grass. This is attributed to sunflower having only one single tap (primary) root with a high intrinsic axial conductance (Figure 6) versus maize and grass having many primary roots. $K_{rs, \text{bigroot}}$ is larger than the exact K_{rs} . The upscaling approach for the big root model (Eqs. [24] [25]) in combination with the assumption that

430 the root architecture can be represented by a single big root leads to an overestimation of the root system conductance. This was also observed for the simple hybrid big-parallel root model (Table 2) but is more outspoken for more complex and realistic root systems.

Looking at the **SUF**, the parallel root system model that assumed no axial resistance to flow overestimated the **SUF** deeper in the soil profile. Not considering axial resistance to flow leads to an overestimation of the uptake capacity of the distal ends of

435 roots. For the **SUF** of the big root model, the opposite was observed. Here, axial resistance to flow from the distal ends of the deep primary roots to the collar is apparently overestimated. In the big root model, the xylem water potentials in the secondary and primary roots in a certain layer are assumed to be equal. However, because of the lower axial conductance of secondary roots (see Figure 6), the xylem water heads can be considerably higher in the secondary than in the primary roots in a certain layer. Assuming similar xylem water heads in secondary and primary roots in a certain soil layer reduces the xylem heads in

440 the secondary roots and generates too much uptake by the secondary roots in that layer. An overestimation of uptake in a more ‘downstream’ soil layer will lead to an underestimation in the more ‘upstream layers’. These effects may explain the underestimation of the **SUF** below approximately 50 cm depth in the maize and sunflower root systems that is compensated by an overestimation in shallower depths. For the grass root system, which consists of several short primary roots with high axial conductance, **SUF** is almost not sensitive to the assumed root architecture.

445 The non-uniform soil water hydraulic heads resulted in an increased uptake deeper in the soil profile (compare the shape of the **SUF** and sink term profiles in Figure 10). For the grass root system, the sink distributions for the different models are very similar. The higher uptake predicted by the big root model is due to the higher $K_{rs, \text{bigroot}}$ than the true K_{rs} . For the other root system models, the differences between the sink term distributions of the exact model, the big root model, and the parallel root model with infinite axial conductance are caused by differences in K_{rs} , **SUF**, and compensatory uptake resulting from approximations of K_{comp} and the C_7 matrix (Figure 11). The parallel root model that uses the exact K_{rs} and **SUF** profile but approximates K_{comp} by K_{rs} and C_7 by the identity matrix, predicts almost the same sink term distribution profile as the exact model. The parallel root model slightly underestimates the compensatory root water uptake, i.e. too much uptake near the soil surface and too little deeper in the soil profile. The K_{comp}/K_{rs} trace and C_7 matrix of the root systems (Figure 11) suggest the largest deviations between the sink term distributions of the exact and parallel root system for the sunflower root system. This

450 corresponds with the results shown in Figure 10. The impact of approximations of K_{comp} and the C_7 matrix on the sink term distribution is apparently of second order importance compared to the impact of the estimated K_{rs} (big root model) and **SUF** (big root model and parallel root model with infinite axial conductance).

460 **Table 4: Root system conductances, K_{rs} and root system conductances of the big root model, $K_{rs, \text{bigroot}}$ estimated from root segment conductances,**

	K_{rs} (cm ² /d)	$K_{rs, \text{bigroot}}$ (cm ² /d)
Maize	0.0576	0.0781
Sun flower	0.00555	0.0068
Grass	0.045	0.0489

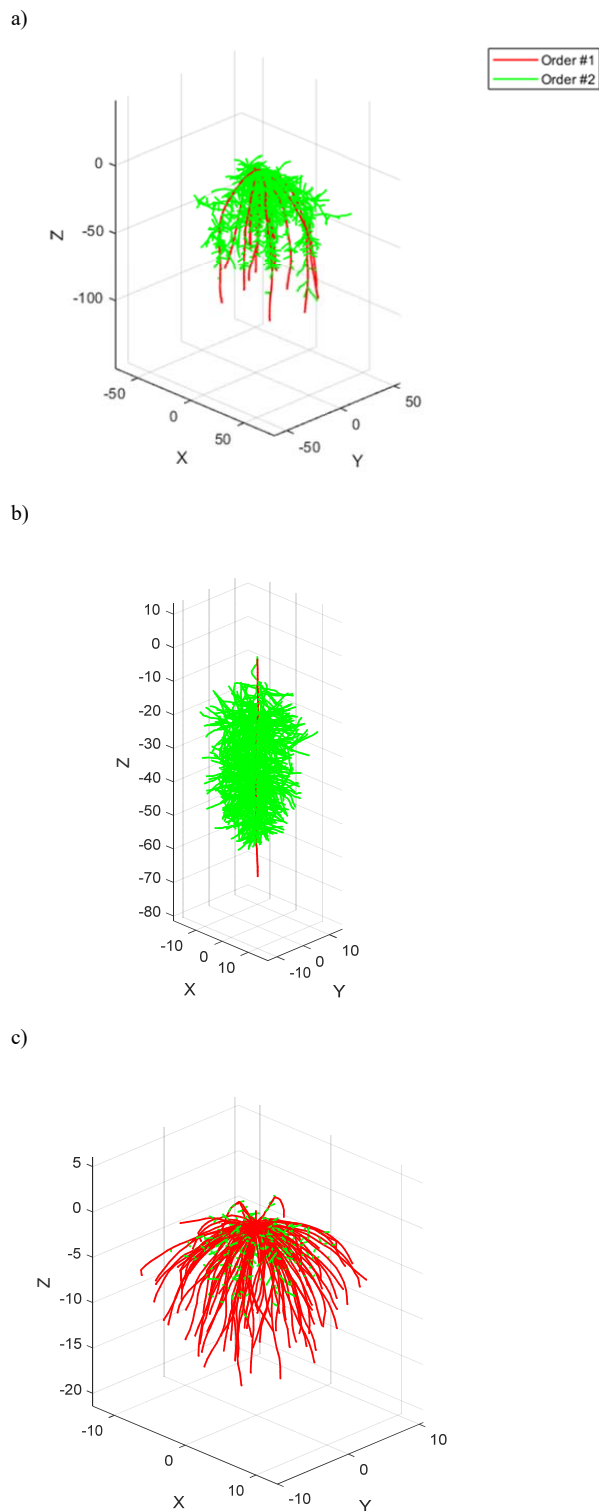
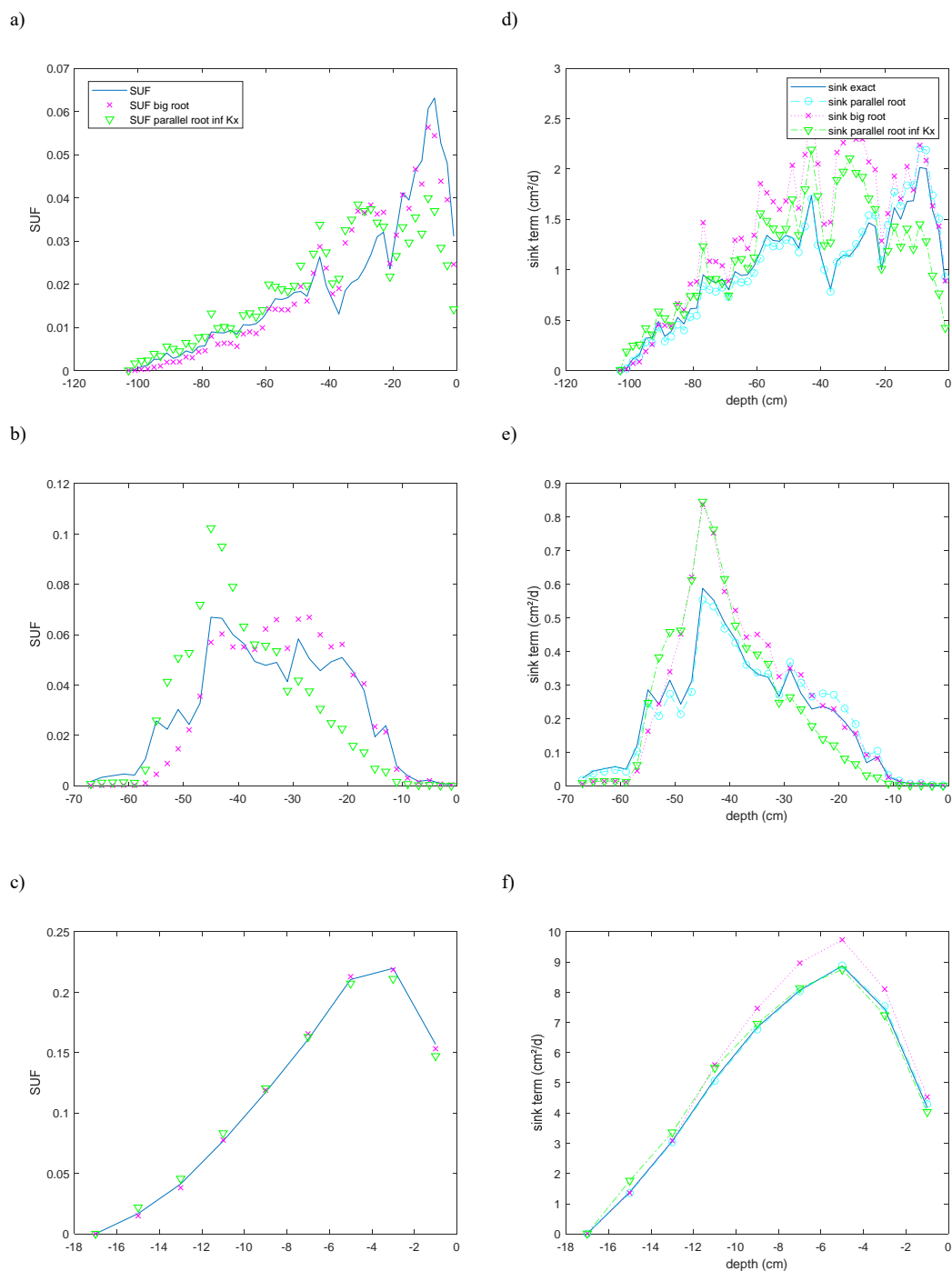


Figure 9: Root systems generated with the CRootbox shiny app: a) maize, b) sunflower, c) grass. Colors refer to the root order.



465 **Figure 10:** Depth profiles of scaled up Standardized Uptake Fractions (SUF) (a-c) and sink term distribution normalized by the
 considered soil layer thickness (2 cm) for a non-uniform soil water potential distribution (-3000 cm at the soil surface and 0 cm at
 the maximal root depth) (d-f) for maize (a,d), sunflower (b,e) and grass (c,f) root systems shown in Figure 9.

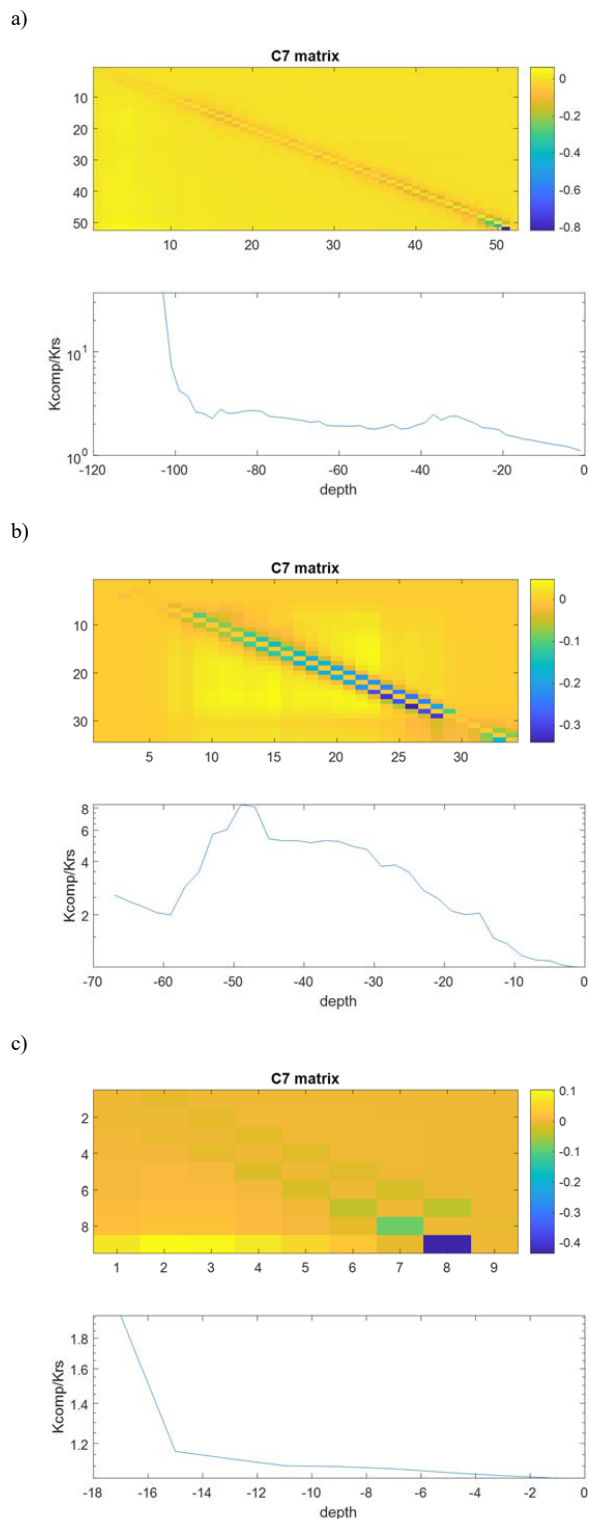


Figure 11: C₇ matrices and ratios of K_{comp}/K_{rs} for the maize a), sunflower b), and grass c) root systems



5 Discussion and Conclusion

We analysed the equation that describes water flow in a network of root segments, which constitutes a root system architecture and reformulated it into a form that lends itself to upscaling and to deriving simpler or parsimonious root water uptake models. In line with Couvreur et al. (2012), we deduced that the total uptake by a root system is a simple function of a weighted soil water hydraulic head and the weights are equal to the water uptake by the RSA in a uniform soil water hydraulic head field. The root system conductance, K_{rs} , and the uptake distribution for uniform soil water hydraulic head, i.e. the standardized uptake fraction **SUF**, are the two properties of the root system that define the relation between the transpiration, the collar hydraulic head, and the distribution of the soil water potentials. This implies that for any distribution of soil water hydraulic heads that leads to the same weighted hydraulic head, transpiration rate and collar hydraulic head are uniquely related.

We found that the uptake distribution is the sum of the uptake for the case of a uniform soil water hydraulic head, i.e. the weighted hydraulic head, and a correction or compensation term that depends on the difference between the local and weighted soil water hydraulic head. This compensation term does not depend directly on the collar hydraulic head or transpiration rate, which is a consequence of the compensation being a passive redistribution process that is not influenced by the transpiration rate as long as the soil water hydraulic heads do not change by the plant water uptake.

When soil water hydraulic heads are assumed to be uniform in certain regions, e.g. in horizontal soil layers, the upscaling of the root water uptake model is trivial and leads to the same form as the detailed model. Whether soil water hydraulic heads remain uniform during root water uptake depends on spatial distribution of the root segments and on the water redistribution in the soil that cancels out spatial variations in root water uptake (Couvreur et al., 2014a). Further work is needed to evaluate this assumption and to develop upscaling methods when soil water hydraulic heads cannot be assumed to be uniform in the horizontal direction.

The simplified root architectures that are used in land surface models, big root and parallel root models, are special cases of RSAs and the root water uptake models for these architectures can be cast in the same form as the model for a general RSA. For the parallel root model, we could show that the root water uptake model is fully defined by the K_{rs} and **SUF** of the root system. K_{rs} and **SUF** of the parallel root system model that is used in a 1D LSM assuming horizontally uniform soil water hydraulic heads can be derived directly and exactly from upscaled K_{rs} and **SUF** of a general root system. The impact of the root segment connections and their root hydraulic properties are directly represented in the K_{rs} and **SUF**, which can be calculated and scaled up without making any simplifying assumptions about the RSA. The bottom-up approach to parameterize a parallel root model from 3D RSA models is therefore straightforward. For the big root model, we could not find such a simple relationship and upscaling was carried out by first deriving the effective conductances of the big root based on the intrinsic conductances of the root segments in a certain layer. From the obtained effective conductances of the big root model, the K_{rs} and **SUF** were derived. Since the derivation of effective conductances cannot account exactly for the 3D RSA and its hydraulic properties, the obtained K_{rs} and **SUF** for the big root model are approximations. Another approach that could be pursued is to derive upscaled K_{rs} and **SUF** directly from the 3D RSA (as was done for the parallel root model) and fit the effective conductances. However, for each layer, only one **SUF** value is available whereas two effective conductances (radial and axial) need to be estimated. This implies that more information about water uptake by the 3D RSA is required, such as compensatory uptake, in order to parameterize the effective conductances of the big root model. The big root model lends itself less for a bottom-up parameterization approach than the parallel root model. K_{rs} and **SUF** of the parallel root model could also be estimated from intrinsic root segment conductances without solving the 3D RSA model. But then it needs to be assumed that the axial root segment conductances are large so that they do not limit the uptake. This assumption led, for the considered root segment hydraulic properties, to an overestimation of the uptake by the distal parts of the roots.



When the exact K_{rs} and SUF are used in the parallel root system model, the approximations in the parallel root system model lead to an underestimation of redistribution of the water uptake for non-uniform distributions of the soil water hydraulic head.

510 However, the typical distribution of radial conductances along a root with lower radial conductances in older more proximal root segments than in younger distal segments that result from aging of root tissues make that the underestimation of the root water uptake redistribution by the parallel root system model is not so important. Even the redistribution of the uptake along a single long root with age dependent root segment conductances can be represented well with a parallel root system model that uses the exact K_{rs} and SUF . The big root model overestimates the root water uptake redistribution. But, the estimated root

515 water uptake profiles by this model seem to be affected more by the approximate estimation of K_{rs} and SUF from the root segment hydraulic properties. We therefore conclude that bottom-up approaches that start from 3D root architecture models and that use age dependent and/or root order dependent hydraulic properties of root segments are promising approaches to parameterize root water uptake modules of LSMs or crop models. This approach is more reliable than the top-down approach that starts from an upscaled root water uptake model (big root or parallel root model) and derives the effective parameters of

520 these models from root segment hydraulic properties. Since we used information about root segment hydraulic properties and their orientation, the top-down estimated parameters will deviate even more from the correct parameters when proxies of the hydraulic RSA, which are mostly limited to root length density distributions, are used. An often used argument against RSA models and the proposed bottom-up approach, is that they require a lot of input parameters which are hardly available. Indeed, root density distributions are mostly the only information that is available about the RSA. However, root distributions could

525 be used to constrain parameters (Garré et al., 2012; Vansteenkiste et al., 2014) or parameters groups (Pages et al., 2012; Morandage et al., 2019) of RSA models. Next to the RSA architecture, also information about the root segment hydraulic properties is required. This information could be derived either from direct measurements on root segments (Schneider et al., 2017) or using information on water fluxes in the soil-plant system (e.g. water contents, collar water hydraulic heads, stable water isotopes in the soil and plant xylem) in combination with inverse modelling (Rothfuss and Javaux, 2017; Cai et al.,

530 2018; Meunier et al., 2018a; Couvreur et al., 2020).

The uptake profiles and their approximations by the simplified models were calculated for a given non-uniform soil water hydraulic head distribution. Even though the approximations of the uptake profiles are very good, it still requires testing how this evolves over time and affects the dynamics of root water uptake.

In the current study, we considered a linear flow model in the root system (i.e. root segment hydraulic conductances are not a

535 function of the water pressure heads). Cavitation in the root xylem or changes in radial conductances due to for instance aquaporin activation are not considered. Since we focussed on the root system hydraulic architecture, we did not consider water potential gradients in the rhizosphere between the bulk soil and the soil-root interface. These gradients can be important and generate an additional non-linear resistance to radial flow. It is still debated whether root xylem cavitation or rhizosphere resistance triggers the non-linear system behavior but there seems to be more and more evidence that the rhizosphere non-linearities are crucial (Carminati et al., 2020). Most root water uptake modules that consider root hydraulics in LSMs already

540 include the non-linear rhizosphere resistances. How the root water uptake model and its upscaled and simplified versions that are based on a bottom-up analysis of the hydraulic root architecture can be coupled with approaches that consider non-linear resistances to radial flow in the soil (e.g. (Gardner and Ehlig, 1962; Hillel et al., 1976; de Jong van Lier et al., 2008; de Jong van Lier et al., 2013)) requires further research. Different proposals were made and implemented by (Couvreur et al.,

545 2014b; Meunier et al., 2018a) but a crucial aspect is how these approaches can be scaled up to 1D models.



6 Appendix

For a given node i in the discretized root network, the mass balance is:

$$\mathbf{K}_x[i](\mathbf{H}_x[i] - \mathbf{H}_x[\text{prox}(i)]) - \sum_{j \in \text{distal}(i)} \mathbf{K}_x[j](\mathbf{H}_x[j] - \mathbf{H}_x[i]) - \mathbf{K}_r[i](\mathbf{H}_{\text{soil}}[i] - \mathbf{H}_x[i]) = 0 \quad [\text{A } 1]$$

550 where $\text{prox}(i)$ represents the proximal node of the segment connected to node i and $\text{distal}(i)$ the distal node of a segment that is connected to i . Note that $\mathbf{H}_x[\text{prox}(i)]$ may also be H_{collar} when node i is connected to the root collar. The flow from a soil node i to xylem node i is:

$$\mathbf{K}_r[i](\mathbf{H}_{\text{soil}}[i] - \mathbf{H}_x[i]) = \mathbf{Q}[i] \quad [\text{A } 2]$$

When we define $\mathbf{dH}[i]$ as the difference between the pressure head of node i , which can also be a soil node, and its proximal node, then it follows that:

$$\mathbf{IM} \cdot \text{diag}(\mathbf{K}) \cdot \mathbf{dH} = \begin{bmatrix} \mathbf{0} \\ \mathbf{Q} \end{bmatrix} \quad [\text{A } 3]$$

555 where \mathbf{IM} is the $(2N_{\text{root}} \times 2N_{\text{root}})$ connectivity matrix with $\mathbf{IM}[i,i]=1$, $\mathbf{IM}[i,j]=-1$ when j is a distal node of i and $\mathbf{IM}[i, N_{\text{root}}+i] = -1$, which represents the connection of the root node i with the soil node i . Since the soil nodes are connected to only one root node and are always distal nodes in the network, the lower left $(N_{\text{root}} \times N_{\text{root}})$ submatrix is a zero matrix, and the lower right $(N_{\text{root}} \times N_{\text{root}})$ submatrix of \mathbf{IM} is the identity matrix. $\text{diag}(\mathbf{K})$ is a diagonal conductivity matrix with the first N_{root} diagonal elements representing the xylem conductivities and the last N_{root} elements the radial conductances. The differences in pressure heads \mathbf{dH} can be expressed as:

$$\mathbf{dH} = \mathbf{IM}_{\text{collar}}^T \begin{bmatrix} H_{\text{collar}} \\ \mathbf{H}_x \\ \mathbf{H}_{\text{soil}} \end{bmatrix} \quad [\text{A } 4]$$

The first column of $\mathbf{IM}_{\text{collar}}^T$ represents the connections to the collar and $\mathbf{IM}_{\text{collar}}^T[i,1] = -1$ when root node i is connected to the collar while $\mathbf{IM}_{\text{collar}}^T[:, 2 : N_{\text{root}} + 1] = \mathbf{IM}^T$. Plugging Eq. [A 4] in Eq. [A 3] leads to Eq. [5].

From the first N_{root} equations in Eq. [5], the unknown hydraulic heads in the xylem, \mathbf{H}_x , can be derived when the soil water hydraulic heads, \mathbf{H}_{soil} , and the collar hydraulic head, H_{collar} , are known. The xylem hydraulic heads are obtained from:

$$H_{\text{collar}} \mathbf{C}_1 + \mathbf{C}_2 \mathbf{H}_x + \mathbf{C}_3 \mathbf{H}_{\text{soil}} = \mathbf{0} \quad [\text{A } 5]$$

$$\mathbf{H}_x = -\mathbf{C}_2^{-1} [\mathbf{C}_3 \mathbf{H}_{\text{soil}} + H_{\text{collar}} \mathbf{C}_1]$$

565 where

$$\mathbf{C} = \mathbf{IM} \cdot \text{diag}(\mathbf{K}) \cdot \mathbf{IM}_{\text{collar}}^T \quad [\text{A } 6]$$

$$\mathbf{C}_1 = \mathbf{C}[1 : N_{\text{root}}, 1] \quad \mathbf{C}_1[i] = -\mathbf{K}_x[i] \quad \text{if } \text{prox}(i) = \text{collar} \quad [\text{A } 7]$$

$$\mathbf{C}_2 = \mathbf{C}[1 : N_{\text{root}}, 2 : N_{\text{root}} + 1] \quad \mathbf{C}_2[i, j] = \mathbf{K}_x[i] + \sum_{j \in \text{distal}(i)} \mathbf{K}_x[j] + \mathbf{K}_r[i] \quad [\text{A } 8]$$

$$\mathbf{C}_2[i, j] = -\mathbf{K}_x[i] \quad \text{if } \text{prox}(i) = j$$

$$\mathbf{C}_2[i, j] = -\mathbf{K}_x[j] \quad \text{if } j \in \text{distal}(i)$$



$$\mathbf{C}_3 = \mathbf{C}[1:N_{root}, N_{root} + 2:2N_{root} + 1] \quad \mathbf{C}_3[i, i + N_{root}] = -\mathbf{K}_r[i] \quad [\text{A } 9]$$

Note that \mathbf{C}_2 and \mathbf{C}_3 are symmetric matrices.

For the fluxes, we can write using the lower part of the \mathbf{C} matrix that:

$$\mathbf{Q} = \mathbf{C}[N_{root} + 1:2N_{root}, :] \begin{bmatrix} \mathbf{H}_{collar} \\ \mathbf{H}_x \\ \mathbf{H}_{soil} \end{bmatrix} \quad [\text{A } 10]$$

This can be written out as:

$$\mathbf{Q} = \mathbf{C}_{L1}\mathbf{H}_{collar} + \mathbf{C}_{L2}\mathbf{H}_x + \mathbf{C}_{L3}\mathbf{H}_{soil} \quad [\text{A } 11]$$

570 where

$$\mathbf{C}_{L1} = \mathbf{C}[N_{root} + 1:2N_{root}, 1] \quad [\text{A } 12]$$

$$\mathbf{C}_{L2} = \mathbf{C}[N_{root} + 1:2N_{root}, 2:N_{root} + 1] \quad [\text{A } 13]$$

$$\mathbf{C}_{L3} = \mathbf{C}[N_{root} + 1:2N_{root}, N_{root} + 1, 2N_{root} + 1] \quad [\text{A } 14]$$

working out Eq. [A 6], it is found that all entries in \mathbf{C}_{L1} are 0, $\mathbf{C}_{L2} = -\text{diag}(\mathbf{K}_r)$ and $\mathbf{C}_{L3} = \text{diag}(\mathbf{K}_r)$, so that Eq. [A 11] corresponds with:

$$\mathbf{Q} = \text{diag}(\mathbf{K}_r)[\mathbf{H}_{soil} - \mathbf{H}_x] \quad [\text{A } 15]$$

which is the matrix form of Eq. [A 2]. Plugging Eq. [A 5] into the general form of Eq. [A 11] gives:

$$\mathbf{C}_4\mathbf{H}_{soil} + \mathbf{C}_5\mathbf{H}_{collar} = \mathbf{Q} \quad (N_{root} \times 1) \quad [\text{A } 16]$$

where

$$\mathbf{C}_4 = -\mathbf{C}_{L2}\mathbf{C}_2^{-1}\mathbf{C}_3 + \mathbf{C}_{L3} \quad [\text{A } 17]$$

$$\mathbf{C}_5 = \mathbf{C}_{L1} - \mathbf{C}_{L2}\mathbf{C}_2^{-1}\mathbf{C}_1 \quad [\text{A } 18]$$

575 which simplify due to the simple forms of \mathbf{C}_{L1} , \mathbf{C}_{L2} , and \mathbf{C}_{L3} to yield:

$$\mathbf{C}_4 = \text{diag}(\mathbf{K}_r)[\mathbf{I} + \mathbf{C}_2^{-1}\mathbf{C}_3] \quad (N_{root} \times N_{root}) \quad [\text{A } 19]$$

$$\mathbf{C}_5 = \text{diag}(\mathbf{K}_r)\mathbf{C}_2^{-1}\mathbf{C}_1 \quad (N_{root} \times 1) \quad [\text{A } 20]$$

Note that since \mathbf{C}_2 and \mathbf{C}_3 are symmetric matrices, also \mathbf{C}_4 is a symmetric matrix.

When we consider the case of a uniform soil hydraulic head, H_{eff} , then we can write

$$\mathbf{Q}[i] = H_{eff} \sum_j \mathbf{C}_4[i, j] + H_{collar} \mathbf{C}_5[i] \quad [\text{A } 21]$$

580 When $H_{eff} = H_{collar}$, there is neither flow from the soil to the collar nor flow through the root system from one soil node to the other. From this follows that:

$$\sum_i \mathbf{C}_4[i, j] = -\mathbf{C}_5[i] \quad [\text{A } 22]$$

If we consider now the total root water uptake, then



$$Q_{tot} = \sum_i \mathbf{Q}[i] = -\sum_i \mathbf{C}_5[i] (H_{eff} - H_{collar}) \quad [A 23]$$

From this follows that we can derive the root system conductance K_{rs} directly from:

$$K_{rs} = \frac{Q_{tot}}{(H_{eff} - H_{collar})} \quad [A 24]$$

$$K_{rs} = -\sum_i \mathbf{C}_5[i] = \sum_i \sum_j \mathbf{C}_4[i, j]$$

585 The standardized uptake fraction $\mathbf{SUF}[i]$, which is defined as the fraction of the uptake by a root node to the total root water uptake under uniform soil water hydraulic head, is related to the matrix \mathbf{C}_4 and vector \mathbf{C}_5 as:

$$\mathbf{SUF}[i] = \frac{\mathbf{Q}[i]}{Q_{tot}} = \frac{\sum_j \mathbf{C}_4[i, j]}{\sum_i \sum_j \mathbf{C}_4[i, j]} = \frac{\mathbf{C}_5[i]}{\sum_i \mathbf{C}_5[i]} \quad [A 25]$$

So we can write for uniform soil water hydraulic heads:

$$\mathbf{Q}[i] = K_{rs} \mathbf{SUF}[i] (H_{eff} - H_{collar}) \quad [A 26]$$

590 For the general case that the soil water hydraulic heads are not uniform, we can define the effective soil water hydraulic head, H_{eff} , as:

$$H_{eff} = \mathbf{SUF}^T \mathbf{H}_{soil} \quad [A 27]$$

After adding and subtracting $\mathbf{C}_5 H_{eff} = K_{rs} \mathbf{SUF} H_{eff} = K_{rs} \mathbf{SUF} \cdot \mathbf{SUF}^T \mathbf{H}_{soil}$ in Eq. [A 16], we obtain the following equation for the root water uptake \mathbf{Q} :

595

$$\mathbf{C}_6 \mathbf{H}_{soil} + K_{rs} (H_{eff} - H_{collar}) \mathbf{SUF} = \mathbf{Q} \quad [A 28]$$

$$\mathbf{C}_6 = \mathbf{C}_4 - K_{rs} \mathbf{SUF} \cdot \mathbf{SUF}^T \quad [A 29]$$

From the definitions of \mathbf{C}_6 , \mathbf{C}_4 , \mathbf{SUF} and K_{rs} follows that the sum of the elements in the rows of \mathbf{C}_6 is zero for all rows. This implies that when \mathbf{C}_6 is multiplied with an n root \times 1 vector with constant elements, a zero vector is obtained. Therefore, we can reformulate the equation for the root water uptake as:

600

$$\mathbf{C}_6 (\mathbf{H}_{soil} - \mathbf{H}_{eff}) + K_{rs} (H_{eff} - H_{collar}) \mathbf{SUF} = \mathbf{Q} \quad [A 30]$$

Since $\mathbf{SUF}^T \mathbf{H}_{soil} = H_{eff}$ and since the sum of all elements in \mathbf{SUF} is one so that $\mathbf{SUF}^T \mathbf{H}_{eff} = H_{eff}$, it follows also that:

$$\mathbf{C}_4 (\mathbf{H}_{soil} - \mathbf{H}_{eff}) + K_{rs} (H_{eff} - H_{collar}) \mathbf{SUF} = \mathbf{Q} \quad [A 31]$$

The definition of H_{eff} (Eq. [A 27]) makes that sums of all the fluxes in the first term of Eq. [A 30] and in the first term of Eq. [A 31] are both zero. Considering Eq. [A 31], we can write:



$$\begin{aligned} \sum_i C_4 (\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}}) &= \sum_i \sum_j C_4 [i, j] \mathbf{H}_{\text{soil}} [j] - \sum_i \left(\sum_j C_4 [i, j] \right) \left(\sum_i \text{SUF} [i] \mathbf{H}_{\text{soil}} [i] \right) \quad [\text{A } 32] \\ &= \sum_i \sum_j C_4 [i, j] \mathbf{H}_{\text{soil}} [j] - \sum_i \sum_j C_4 [i, j] \left(\frac{\sum_i \sum_j C_4 [i, j] \mathbf{H}_{\text{soil}} [i]}{\sum_i \sum_j C_4 [i, j]} \right) \\ &= \sum_i \sum_j C_4 [i, j] \mathbf{H}_{\text{soil}} [j] - \sum_i \sum_j C_4 [i, j] \mathbf{H}_{\text{soil}} [i] \\ &= 0 \end{aligned}$$

605 since $C_4[i,j]=C_4[j,i]$

Eqs. [A 30] and [A 31] have a similar form as the equation that was proposed by Couvreur et al. (2012) to describe water uptake by a root network. In order to draw the analogy and identify differences between the two approaches, we will discuss the nature of the C_6 matrix and how it can be transformed or approximated. From the definition of C_6 , it also follows that the sum of all the elements in the vector $C_6 (\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}})$ is zero. Therefore, this vector represents the perturbations of the uptake ΔQ at a certain depth due to the perturbation of the soil water hydraulic head at this depth compared to the uptake when the soil water hydraulic head is uniform in the root zone. When there is no net uptake, i.e. when $H_{\text{eff}} = H_{\text{collar}}$, then $C_6 (\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}})$ represents the redistribution water fluxes through the root system due to spatial variations in \mathbf{H}_{soil} . When we consider now that the soil water hydraulic head around node i is ΔH higher than the hydraulic head in all other nodes, then we can define $\Delta Q[i] = k_{\text{comp}}[i] \Delta H$. $k_{\text{comp}}[i]$ represents the compensatory root system conductance to transfer water from node i towards all other nodes when there is a hydraulic head difference between the soil water at node i and the soil water next to all other nodes in the root system. $\Delta Q(i)$ and $k_{\text{comp}}[i]$ are related to the C_6 matrix and SUF vector as:

$$\Delta Q[i] = \left((1 - \text{SUF}[i]) C_6 [i, i] - \text{SUF}[i] \sum_{j \neq i} C_6 [i, j] \right) \Delta H \quad [\text{A } 33]$$

$$k_{\text{comp}} [i] = \frac{\Delta Q[i]}{\Delta H} = \left((1 - \text{SUF}[i]) C_6 [i, i] - \text{SUF}[i] \sum_{j \neq i} C_6 [i, j] \right) = C_6 [i, i] \quad [\text{A } 34]$$

620

since

$$C_6 [i, i] + \sum_{j \neq i} C_6 [i, j] = 0 \quad [\text{A } 35]$$

We assume now a root system in which all soil nodes are connected via one radial and one axial resistance to the collar node so that the overall resistance to flow from one soil-root node to the collar is equal to the sum of the axial plus radial resistances. We call this root system the ‘parallel root system’. The radial and axial resistances for each soil node can however be different. Also a root system in which there is no resistance to axial flow can be considered as a system in which all soil nodes are connected directly to the root collar. But, it is important to keep in mind that systems with a significant axial root resistance can also be considered, as long as there is a direct connection between the soil node and the root collar without additional

625



intermediate nodes that connect to the soil. For instance, fibrous root systems with only primary roots, in which uptake takes only place near the root tip but not at the more basal ends, can also be represented by this root system model. For such a root system, it follows that:

$$\mathbf{k}_{\text{comp}}[i] = \text{SUF}[i](1 - \text{SUF}[i])K_{rs} \quad [\text{A } 36]$$

In the same vein, it can be deduced that for such a parallel root system:

$$\frac{C_6[i, j]}{C_6[i, i]} = -\frac{\text{SUF}[j]}{(1 - \text{SUF}[i])} \quad \text{for } i \neq j \quad [\text{A } 37]$$

The j^{th} column of the C_6 matrix represents to what extent water from the j^{th} node can flow to the other nodes in the system. For a parallel root system, in which the flow must pass through the collar node, the flow from node j to node i is proportional to the conductance for the flow from node j to the collar node and hence to $\text{SUF}[j]$. Based on this, we can write the C_6 matrix for this root system as:

$$C_6 = \text{diag}\left(\frac{C_6[i, i]}{1 - \text{SUF}[i]}\right)(\mathbf{I} - \mathbf{ones} \cdot \text{SUF}^T) = K_{rs} \text{diag}(\text{SUF}[i])(\mathbf{I} - \mathbf{ones} \cdot \text{SUF}^T) \quad [\text{A } 38]$$

Since $\text{SUF}^T \mathbf{H}_{\text{soil}} = \mathbf{H}_{\text{eff}}$, it follows that for a parallel root system:

$$C_6(\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}}) = K_{rs} \text{diag}(\text{SUF}[i])(\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}}) \quad [\text{A } 39]$$

640

This implies that we can obtain the following equation to simulate root water uptake for the parallel root system:

$$K_{rs} \text{diag}(\text{SUF}[i])(\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}}) + K_{rs}(H_{\text{eff}} - H_{\text{collar}})\text{SUF} = \mathbf{Q} \quad [\text{A } 40]$$

which is identical to the equation proposed by Couvreur et al. 2012.

For a general root system, we can rewrite the general equation which takes a similar form as the equation that we obtained for the parallel root system.

645

$$\text{diag}(\mathbf{K}_{\text{comp}}[i])\text{diag}(\text{SUF}[i])C_7(\mathbf{H}_{\text{soil}} - \mathbf{H}_{\text{eff}}) + K_{rs}(H_{\text{eff}} - H_{\text{collar}})\text{SUF} = \mathbf{Q} \quad [\text{A } 41]$$

$$\mathbf{K}_{\text{comp}}[i] = \frac{C_6[i, i]}{\text{SUF}[i](1 - \text{SUF}[i])} = \frac{\mathbf{k}_{\text{comp}}[i]}{\text{SUF}[i](1 - \text{SUF}[i])} \quad [\text{A } 42]$$

$$C_7 = \text{diag}\left(\frac{(1 - \text{SUF}[i])}{C_6[i, i]}\right)C_6 + \mathbf{ones} \cdot \text{SUF}^T \quad [\text{A } 43]$$

For the parallel root system, C_7 equals the identity matrix and $\mathbf{K}_{\text{comp}}[i]$ equals K_{rs} .

650 For the general root system, we find that $\mathbf{K}_{\text{comp}}[i]$ is larger than K_{rs} . This means that for a certain ΔH between soil node i and all other nodes, there is more redistribution in the general root system than in the parallel root system. In the general root



system, the flow from one soil-root interface to another soil-root interface does not always have to pass through the collar but can take a shorter way. The diagonal terms of C_7 are equal to 1 and the off-diagonal terms of each row of C_7 sum up to 0. A negative value of the j th column for the i th row in C_7 means that there is more redistribution between node i and j in the general root system than in case the root system would be a parallel root system with the same uptake distribution under uniform soil water potential and the same K_{rs} . This happens when the two nodes are connected more strongly with each other than with the other nodes in the system.

7 Author contributions:

VC initiated the study on the exact macroscopic representation and upscaling of root water uptake. Model development was done by JV, VC, FM, MJ, and MB and programming was done by JV, VC and FM. Codes were checked by AS. All authors contributed to the conceptualization of the paper. JV wrote the paper, which was critically reviewed by all co-authors.

8 Acknowledgements

This work has partially been funded by the German Research Foundation under Germany's Excellence Strategy, EXC-2070 – 390732324 – PhenoRob and in the framework of projects P3 and P24 of the priority programme 2089 'Rhizosphere spatiotemporal organization – a key to rhizosphere functions'. VC was supported by the Belgian National Fund for Scientific Research (FRS-FNRS; grant no. 1208619F), the Interuniversity Attraction Poles Program of the Belgian Science Policy Office (grant no. IAP7/29) and the Communauté française de Belgique-Actions de Recherches Concertées (grant no. ARC16/21-075), the EPPN2020 731013 and EMPHASIS-PREP 739514 projects. MB was supported by long-term research development project No. RVO 67985939 of the Czech Academy of Sciences and the project CZ.02.2.69/0.0/0.0/18_070/0009075 of the Czech Ministry of Education (OP RDE).



675 **8.1 References**

- Amenu, G. G., and Kumar, P.: A model for hydraulic redistribution incorporating coupled soil-root moisture transport, *Hydrology and Earth System Sciences*, 12, 55-74, 10.5194/hess-12-55-2008, 2008.
- Bouda, M., and Saiers, J. E.: Dynamic effects of root system architecture improve root water uptake in 1D process-based soil-root hydrodynamics, *Adv. Water Resour.*, 110, 319-334, 10.1016/j.advwatres.2017.10.018, 2017.
- 680 Bouda, M., Brodersen, C., and Saiers, J.: Whole root system water conductance responds to both axial and radial traits and network topology over natural range of trait variation, *J. Theor. Biol.*, 456, 49-61, 10.1016/j.jtbi.2018.07.033, 2018.
- Bouda, M.: A Big Root Approximation of Site-Scale Vegetation Water Uptake, *Journal of Advances in Modeling Earth Systems*, 11, 4597-4613, 10.1029/2019ms001806, 2019.
- Cai, G. C., Vanderborght, J., Couvreur, V., Mboh, C. M., and Vereecken, H.: Parameterization of Root Water Uptake Models
685 Considering Dynamic Root Distributions and Water Uptake Compensation, *Vadose Zone J.*, 17, 10.2136/vzj2016.12.0125, 2018.
- Carminati, A., Ahmed, M. A., Zarebanadkouki, M., Cai, G., Lovric, G., and Javaux, M.: Stomatal closure prevents the drop in soil water potential around roots, *New Phytol.*, 226, 1541-1543, <https://doi.org/10.1111/nph.16451>, 2020.
- Couvreur, V., Vanderborght, J., and Javaux, M.: A simple three-dimensional macroscopic root water uptake model based on
690 the hydraulic architecture approach, *Hydrol. Earth Syst. Sci.*, 16, 2957-2971, 10.5194/hess-16-2957-2012, 2012.
- Couvreur, V., Vanderborght, J., Beff, L., and Javaux, M.: Horizontal soil water potential heterogeneity: simplifying approaches for crop water dynamics models, *Hydrol. Earth Syst. Sci.*, 18, 1723-1743, 10.5194/hess-18-1723-2014, 2014a.
- Couvreur, V., Vanderborght, J., Draye, X., and Javaux, M.: Dynamic aspects of soil water availability for isohydric plants: Focus on root hydraulic resistances, *Water Resour. Res.*, 50, 8891-8906, 10.1002/2014wr015608, 2014b.
- 695 Couvreur, V., Faget, M., Lobet, G., Javaux, M., Chaumont, F., and Draye, X.: Going with the Flow: Multiscale Insights into the Composite Nature of Water Transport in Roots, *Plant Physiol.*, 178, 1689-1703, 10.1104/pp.18.01006, 2018.
- Couvreur, V., Rothfuss, Y., Meunier, F., Bariac, T., Biron, P., Durand, J. L., Richard, P., and Javaux, M.: Disentangling temporal and population variability in plant root water uptake from stable isotopic analysis: when rooting depth matters in labeling studies, *Hydrology and Earth System Sciences*, 24, 3057-3075, 10.5194/hess-24-3057-2020, 2020.
- 700 Daly, K. R., Tracy, S. R., Crout, N. M. J., Mairhofer, S., Pridmore, T. P., Mooney, S. J., and Roose, T.: Quantification of root water uptake in soil using X-ray computed tomography and image-based modelling, *Plant Cell Environ.*, 41, 121-133, 10.1111/pce.12983, 2018.
- de Jong van Lier, Q., van Dam, J. C., Durigon, A., dos Santos, M. A., and Metselaar, K.: Modeling Water Potentials and Flows in the Soil-Plant System Comparing Hydraulic Resistances and Transpiration Reduction Functions, *Vadose Zone J.*, 12,
705 10.2136/vzj2013.02.0039, 2013.
- de Jong van Lier, Q. D., van Dam, J. C., Metselaar, K., de Jong, R., and Duijnisveld, W. H. M.: Macroscopic root water uptake distribution using a matric flux potential approach, *Vadose Zone J.*, 7, 1065-1078, 10.2136/vzj2007.0083, 2008.
- Doussan, C., Pages, L., and Vercambre, G.: Modelling of the hydraulic architecture of root systems: An integrated approach to water absorption - Model description, *Ann. Bot.*, 81, 213-223, 1998.
- 710 Doussan, C., Pierret, A., Garrigues, E., and Pages, L.: Water uptake by plant roots: II - Modelling of water transfer in the soil root-system with explicit account of flow within the root system - Comparison with experiments, *Plant Soil*, 283, 99-117, 2006.
- Feddes, R. A., Hoff, H., Bruen, M., Dawson, T., de Rosnay, P., Dirmeyer, O., Jackson, R. B., Kabat, P., Kleidon, A., Lilly, A., and Pitman, A. J.: Modeling root water uptake in hydrological and climate models, *Bull. Amer. Meteorol. Soc.*, 82, 2797-2809,
715 2001.



- Ferguson, I. M., Jefferson, J. L., Maxwell, R. M., and Kollet, S. J.: Effects of root water uptake formulation on simulated water and energy budgets at local and basin scales, *Environ. Earth Sci.*, 75, 10.1007/s12665-015-5041-z, 2016.
- Fu, C. S., Wang, G. L., Goulden, M. L., Scott, R. L., Bible, K., and Cardon, Z. G.: Combined measurement and modeling of the hydrological impact of hydraulic redistribution using CLM4.5 at eight AmeriFlux sites, *Hydrology and Earth System Sciences*, 20, 2001-2018, 10.5194/hess-20-2001-2016, 2016.
- 720 Gardner, W. R., and Ehlig, C. F.: SOME OBSERVATIONS ON MOVEMENT OF WATER TO PLANT ROOTS, *Agron. J.*, 54, 453-&, 10.2134/agronj1962.00021962005400050024x, 1962.
- Garré, S., Pagès, L., Laloy, E., Javaux, M., Vanderborght, J., and Vereecken, H.: Parameterizing a Dynamic Architectural Model of the Root System of Spring Barley from Minirhizotron Data, *Vadose Zone J.*, 11, 10.2136/vzj2011.0179, 2012.
- 725 Gayler, S., Ingwersen, J., Priesack, E., Wohling, T., Wulfmeyer, V., and Streck, T.: Assessing the relevance of subsurface processes for the simulation of evapotranspiration and soil moisture dynamics with CLM3.5: comparison with field data and crop model simulations, *Environ. Earth Sci.*, 69, 415-427, 10.1007/s12665-013-2309-z, 2013.
- Good, S. P., Noone, D., and Bowen, G.: Hydrologic connectivity constrains partitioning of global terrestrial water fluxes, *Science*, 349, 175-177, 10.1126/science.aaa5931, 2015.
- 730 Gou, S., and Miller, G.: A groundwater-soil-plant-atmosphere continuum approach for modelling water stress, uptake, and hydraulic redistribution in phreatophytic vegetation, *Ecohydrology*, 7, 1029-1041, 10.1002/eco.1427, 2014.
- Hillel, D., Talpaz, H., and Vankeulen, H.: MACROSCOPIC-SCALE MODEL OF WATER UPTAKE BY A NONUNIFORM ROOT-SYSTEM AND OF WATER AND SALT MOVEMENT IN SOIL PROFILE, *Soil Sci.*, 121, 242-255, 10.1097/00010694-197604000-00009, 1976.
- 735 Hopmans, J. W., and Bristow, K. L.: Current capabilities and future needs of root water and nutrient uptake modeling, in: *Advances in Agronomy*, Vol 77, *Advances in Agronomy*, 103-183, 2002.
- Javaux, M., Schröder, T., Vanderborght, J., and Vereecken, H.: Use of a three-dimensional detailed modeling approach for predicting root water uptake, *Vadose Zone J.*, 7, 1079-1088, 10.2136/vzj2007.0115, 2008.
- Javaux, M., Couvreur, V., Vanderborght, J., and Vereecken, H.: Root Water Uptake: From Three-Dimensional Biophysical Processes to Macroscopic Modeling Approaches, *Vadose Zone J.*, 12, -, 10.2136/vzj2013.02.0042, 2013.
- 740 Katul, G. G., and Siqueira, M. B.: Biotic and abiotic factors act in coordination to amplify hydraulic redistribution and lift, *New Phytol.*, 187, 4-6, 2010.
- Kennedy, D., Swenson, S., Oleson, K. W., Lawrence, D. M., Fisher, R., da Costa, A. C. L., and Gentine, P.: Implementing Plant Hydraulics in the Community Land Model, Version 5, *Journal of Advances in Modeling Earth Systems*, 11, 485-513, 10.1029/2018ms001500, 2019.
- 745 Landsberg, J. J., and Fowkes, N. D.: WATER-MOVEMENT THROUGH PLANT ROOTS, *Ann. Bot.*, 42, 493-508, 10.1093/oxfordjournals.aob.a085488, 1978.
- Liu, Y., Kumar, M., Katul, G. G., Feng, X., and Konings, A. G.: Plant hydraulics accentuates the effect of atmospheric moisture stress on transpiration, *Nature Climate Change*, 10, 691-695, 10.1038/s41558-020-0781-5, 2020.
- 750 Manoli, G., Bonetti, S., Domec, J. C., Putti, M., Katul, G., and Marani, M.: Tree root systems competing for soil moisture in a 3D soil-plant model, *Adv. Water Resour.*, 66, 32-42, 10.1016/j.advwatres.2014.01.006, 2014.
- Manoli, G., Huang, C. W., Bonetti, S., Domec, J. C., Marani, M., and Katul, G.: Competition for light and water in a coupled soil-plant system, *Adv. Water Resour.*, 108, 216-230, 10.1016/j.advwatres.2017.08.004, 2017.
- Meunier, F., Couvreur, V., Draye, X., Vanderborght, J., and Javaux, M.: Towards quantitative root hydraulic phenotyping: novel mathematical functions to calculate plant-scale hydraulic parameters from root system functional and structural traits, *J. Math. Biol.*, 75, 1133-1170, 10.1007/s00285-017-1111-z, 2017a.
- 755



- Meunier, F., Couvreur, V., Draye, X., Zarebanadkouki, M., Vanderborght, J., and Javaux, M.: Water movement through plant roots - exact solutions of the water flow equation in roots with linear or exponential piecewise hydraulic properties, *Hydrology and Earth System Sciences*, 21, 6519-6540, 10.5194/hess-21-6519-2017, 2017b.
- 760 Meunier, F., Draye, X., Vanderborght, J., Javaux, M., and Couvreur, V.: A hybrid analytical-numerical method for solving water flow equations in root hydraulic architectures, *Appl. Math. Model.*, 52, 648-663, 10.1016/j.apm.2017.08.011, 2017c.
- Meunier, F., Rothfuss, Y., Bariac, T., Biron, P., Richard, P., Durand, J. L., Couvreur, V., Vanderborght, J., and Javaux, M.: Measuring and Modeling Hydraulic Lift of *Lolium multiflorum* Using Stable Water Isotopes, *Vadose Zone J.*, 17, 10.2136/vzj2016.12.0134, 2018a.
- 765 Meunier, F., Zarebanadkouki, M., Ahmed, M. A., Carminati, A., Couvreur, V., and Javaux, M.: Hydraulic conductivity of soil-growth lupine and maize unbranched roots and maize root-shoot junctions, *J. Plant Physiol.*, 227, 31-44, 10.1016/j.jplph.2017.12.019, 2018b.
- Morandage, S., Schnepf, A., Leitner, D., Javaux, M., Vereecken, H., and Vanderborght, J.: Parameter sensitivity analysis of a root system architecture model based on virtual field sampling, *Plant Soil*, 10.1007/s11104-019-03993-3, 2019.
- 770 Nguyen, T. H., Langensiepen, M., Vanderborght, J., Hüging, H., Mboh, C. M., and Ewert, F.: Comparison of root water uptake models in simulating CO₂ and H₂O fluxes and growth of wheat, *Hydrol. Earth Syst. Sci.*, 24, 4943-4969, 10.5194/hess-24-4943-2020, 2020.
- Nimah, M. N., and Hanks, R. J.: MODEL FOR ESTIMATING SOIL-WATER, PLANT, AND ATMOSPHERIC INTERRELATIONS .1. DESCRIPTION AND SENSITIVITY, *Soil Sci. Soc. Am. J.*, 37, 522-527, 10.2136/sssaj1973.03615995003700040018x, 1973.
- 775 Oki, T., and Kanae, S.: Global Hydrological Cycles and World Water Resources, *Science*, 313, 1068-1072, 10.1126/science.1128845, 2006.
- Pages, L., Bruchou, C., and Garre, S.: Links Between Root Length Density Profiles and Models of the Root System Architecture, *Vadose Zone J.*, 11, 10.2136/vzj2011.0152, 2012.
- 780 Quijano, J. C., Kumar, P., Drewry, D. T., Goldstein, A., and Misson, L.: Competitive and mutualistic dependencies in multispecies vegetation dynamics enabled by hydraulic redistribution, *Water Resour. Res.*, 48, 10.1029/2011wr011416, 2012.
- Quijano, J. C., Kumar, P., and Drewry, D. T.: Passive regulation of soil biogeochemical cycling by root water transport, *Water Resour. Res.*, 49, 3729-3746, 10.1002/wrcr.20310, 2013.
- Quijano, J. C., and Kumar, P.: Numerical simulations of hydraulic redistribution across climates: The role of the root hydraulic conductivities, *Water Resour. Res.*, 51, 8529-8550, 10.1002/2014wr016509, 2015.
- 785 Roose, T., and Fowler, A. C.: A model for water uptake by plant roots, *J. Theor. Biol.*, 228, 155-171, 10.1016/j.jtbi.2003.12.012, 2004.
- Rothfuss, Y., and Javaux, M.: Reviews and syntheses: Isotopic approaches to quantify root water uptake: a review and comparison of methods, *Biogeosciences*, 14, 2199-2224, 10.5194/bg-14-2199-2017, 2017.
- 790 Ryel, R. J., Caldwell, M. M., Yoder, C. K., Or, D., and Leffler, A. J.: Hydraulic redistribution in a stand of *Artemisia tridentata*: evaluation of benefits to transpiration assessed with a simulation model, *Oecologia*, 130, 173-184, 10.1007/s004420100794, 2002.
- Schneider, H. M., Wojciechowski, T., Postma, J. A., Brown, K. M., Lücke, A., Zeisler, V., Schreiber, L., and Lynch, J. P.: Root cortical senescence decreases root respiration, nutrient content and radial water and nutrient transport in barley, *Plant, Cell & Environment*, 40, 1392-1408, <https://doi.org/10.1111/pce.12933>, 2017.
- 795 Schnepf, A., Leitner, D., Landl, M., Lobet, G., Mai, T. H., Morandage, S., Sheng, C., Zorner, M., Vanderborght, J., and Vereecken, H.: CRootBox: a structural-functional modelling framework for root systems, *Ann. Bot.*, 121, 1033-1053, 10.1093/aob/mcx221, 2018.



- 800 Siqueira, M., Katul, G., and Porporato, A.: Onset of water stress, hysteresis in plant conductance, and hydraulic lift: Scaling soil water dynamics from millimeters to meters, *Water Resour. Res.*, 44, 10.1029/2007wr006094, 2008.
- Sulis, M., Couvreur, V., Keune, J., Cai, G., Trebs, I., Junk, J., Shrestha, P., Simmer, C., Kollet, S. J., Vereecken, H., and Vanderborght, J.: Incorporating a root water uptake model based on the hydraulic architecture approach in terrestrial systems simulations, *Agricultural and Forest Meteorology*, 269-270, 28-45, <https://doi.org/10.1016/j.agrformet.2019.01.034>, 2019.
- 805 Tang, J. Y., Riley, W. J., and Niu, J.: Incorporating root hydraulic redistribution in CLM4.5: Effects on predicted site and global evapotranspiration, soil moisture, and water storage, *Journal of Advances in Modeling Earth Systems*, 7, 1828-1848, 10.1002/2015ms000484, 2015.
- Trenberth, K. E., Smith, L., Qian, T., Dai, A., and Fasullo, J.: Estimates of the Global Water Budget and Its Annual Cycle Using Observational and Model Data, *Journal of Hydrometeorology*, 8, 758-769, 10.1175/jhm600.1, 2007.
- 810 Vansteenkiste, J., Van Loon, J., Garre, S., Pages, L., Schrevens, E., and Diels, J.: Estimating the parameters of a 3-D root distribution function from root observations with the trench profile method: case study with simulated and field-observed root data, *Plant Soil*, 375, 75-88, 10.1007/s11104-013-1942-3, 2014.
- Vereecken, H., Huisman, J. A., Franssen, H. J. H., Brüggemann, N., Bogena, H. R., Kollet, S., Javaux, M., van der Kruk, J., and Vanderborght, J.: Soil hydrology: Recent methodological advances, challenges, and perspectives, *Water Resour. Res.*, 51, 2616-2633, 10.1002/2014wr016852, 2015.
- 815 Vereecken, H., Schnepf, A., Hopmans, J. W., Javaux, M., Or, D., Roose, T., Vanderborght, J., Young, M. H., Amelung, W., Aitkenhead, M., Allison, S. D., Assouline, S., Baveye, P., Berli, M., Brüggemann, N., Finke, P., Flury, M., Gaiser, T., Govers, G., Ghezzehei, T., Hallett, P., Hendricks Franssen, H. J., Heppell, J., Horn, R., Huisman, J. A., Jacques, D., Jonard, F., Kollet, S., Lafolie, F., Lamorski, K., Leitner, D., McBratney, A., Minasny, B., Montzka, C., Nowak, W., Pachepsky, Y., Padarian, J., Romano, N., Roth, K., Rothfuss, Y., Rowe, E. C., Schwen, A., Šimůnek, J., Tiktak, A., Van Dam, J., van der Zee, S. E. A. T.
- 820 M., Vogel, H. J., Vrugt, J. A., Wöhling, T., and Young, I. M.: Modeling Soil Processes: Review, Key Challenges, and New Perspectives, *Vadose Zone J.*, 15, 10.2136/vzj2015.09.0131, 2016.
- Whitley, R., Beringer, J., Hutley, L. B., Abramowitz, G., De Kauwe, M. G., Evans, B., Haverd, V., Li, L. H., Moore, C., Ryu, Y., Scheiter, S., Schymanski, S. J., Smith, B., Wang, Y. P., Williams, M., and Yu, Q.: Challenges and opportunities in land surface modelling of savanna ecosystems, *Biogeosciences*, 14, 4711-4732, 10.5194/bg-14-4711-2017, 2017.
- 825 Wilderott, O.: An adaptive numerical method for the Richards equation with root growth, *Plant Soil*, 251, 255-267, 10.1023/a:1023031924963, 2003.
- Wöhling, T., Gayler, S., Priesack, E., Ingwersen, J., Wizemann, H.-D., Högy, P., Cuntz, M., Attinger, S., Wulfmeyer, V., and Streck, T.: Multiresponse, multiobjective calibration as a diagnostic tool to compare accuracy and structural limitations of five coupled soil-plant models and CLM3.5, *Water Resour. Res.*, 49, 8200-8221, 10.1002/2013WR014536, 2013.
- 830 Yan, B. Y., and Dickinson, R. E.: Modeling hydraulic redistribution and ecosystem response to droughts over the Amazon basin using Community Land Model 4.0 (CLM4), *J. Geophys. Res.-Biogeosci.*, 119, 2130-2143, 10.1002/2014jg002694, 2014.
- Zarebanadkouki, M., Meunier, F., Couvreur, V., Cesar, J., Javaux, M., and Carminati, A.: Estimation of the hydraulic conductivities of lupine roots by inverse modelling of high-resolution measurements of root water uptake, *Ann. Bot.*, 118, 853-864, 10.1093/aob/mcw154, 2016.
- 835 Zhu, S. G., Chen, H. S., Zhang, X. X., Wei, N., Wei, S. G., Yuan, H., Zhang, S. P., Wang, L. L., Zhou, L. H., and Dai, Y. J.: Incorporating root hydraulic redistribution and compensatory water uptake in the Common Land Model: Effects on site level and global land modeling, *J. Geophys. Res.-Atmos.*, 122, 7308-7322, 10.1002/2016jd025744, 2017.