

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

Dear Prof. Romano, dear Nunzio,

Please find enclosed our replies to the comments of the reviewers on the revised version of our manuscript. The main changes we made to the manuscript are in the introduction section to clarify the objectives of the paper. We follow the suggestion of the second reviewer to shift the focus from the 'development of a new root water uptake model' towards the upscaling of 3D flow in the root architecture to an effective 1D approach. In contrast to other root hydraulic models that are used in 1D model, the model that we derived uses a quasi-exact (quasi since we still use a discretized version of the flow equation but that was addressed in the previous round of revisions) solution of the 3D root water flow model. In order to interpret this solution in bio-physical terms, we casted it in a form that uses root system hydraulic properties. In this way, we can identify and diagnose how the exact model differs from one of the simpler models that are commonly used in 1D models. It also allows to demonstrate that using these exact root system properties in the simplified model improves the prediction skills of this model compared to the case where these properties are derived from the root segment properties in a top-down approach without considering the root architecture. We are strongly convinced that: 1) exact upscaling the 3D model, 2) casting it in a form that uses root system hydraulic properties, and 3) comparing it with models that make simplifying assumptions about the root system topology are three important novel aspects in this paper. We hope that we resolved the confusion about a 'new model' and made clear that we derived a *new solution* of a 3D root water uptake model that uses root system hydraulic properties. This solution can easily be interpreted physically and can be used to derive some general properties of root water uptake from soil profiles with vertical variations in soil hydraulic heads. It also shows that unlike what reviewer 2 is suggesting, an upscaled version of a general 3D model is not exactly equivalent to reparameterized root water uptake models that use simplified root system topologies. However, when the reparameterization is done in a bottom-up approach, the approximation by one of these models, i.e. the parallel root model, can be quite accurate (but not exact).

You find below the comments of the reviewers with our replies given in blue text and what we changed to the paper in blue italic text.

Kind regards

Jan Vanderborght in behalf of all the co-authors.

## Reviewer 1:

### General comments

I found this revision of the article is now fluent and much easier to read and understand. Most of my preceding comments have been adequately accounted for and replied and I'm just left with a few minor comments below that don't need any revision. I'm convinced that the paper will be of great interest for all people involved in water balance modeling, and it opens the way for a real account, on a formal basis, of how to consider a root system ( especially in hydrology modelling) at different scales.

Thank you very much.

### Specific comments

L158 from solving the Laplacian on the weighted directed graph of soil and root nodes: Rather the Laplacian matrix ? To me, Laplacian is confusing with operator in equation 1, but it is not that equation which is solved on the graph but the flux equations.

*This was changed to: ...are obtained from solving the Laplacian matrix of the weighted directed graph of soil and root nodes*

L177  $SUF (N_{root} \times 1)$  [but also L185 for Heff..] : As  $SUF$  is a node related property, its dimension should be  $N_{root} + 1$ , if  $N_{root}$  is the number of root segments (as stated before) ? May be state that root collar node is not considered in equations (or rather separately) and such that root nodes are  $N_{root}$  length.

To avoid confusion, we explained clearer how we defined the root system network, collar node, root node and soil nodes:

*The entire network is connected to one outlet node that represents the root collar where the hydraulic head,  $H_{collar}$ , or the flux boundary condition is defined. Since branches of a root architecture do not re-join distally (further away from the collar), there is only one segment that connects a certain node with the proximal (closer to the collar) part of the root system or each node is the distal node of only one element (except for the collar node). Therefore, the network of  $N_{root}$  root segments connects  $N_{root}$  root nodes with each other and the root collar. The root nodes (but not the collar node), are connected by  $N_{root}$  soil-root segments to  $N_{root}$  soil nodes.*

Then we relate  $SUF$  to root nodes (instead of root 'system') so that it should be clear that the dimension of  $SUF$  should be  $N_{root} \times 1$ . ...the root system conductance,  $K_{rs} (L^2 T^{-1})$ , and the standard uptake fraction vector  $SUF (N_{root} \times 1)$  of the root nodes....

L324, 329: For this results about  $K_{comp}$ ,  $SUF$  refer to table 2 and 3

We added references to the tables.

L459-460, 462 Explain how  $K_{comp}$  profile and  $C7$  matrix is used here as diagnosis of approximation of a parallel model, and if logical...

In this part, we are comparing the  $SUF$ s of the top-down parameterized big root and parallel root models with the  $SUF$  of the exact model. For the top-down parameterized models, also  $K_{rs}$  and  $SUF$

may deviate from the exact model. For the bottom up parameterized parallel root model, the parallel root model only differs from the exact model in terms of  $K_{comp}$  and  $C_7$ . We discussed later that according the figure 11 and based on  $K_{comp}$  and  $C_7$ , the largest discrepancies between the exact and bottom up parameterized parallel root model were expected for the sunflower root system. But these discrepancies were small when compared with the discrepancies between the exact model and the top down parameterized root models. Therefore we concluded that: *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 top down parallel root model with infinite axial conductance).*

L436 the SUF was be calculated directly => SUF was directly calculated ...

Thank you. We corrected this.

## Reviewer 2:

I carefully read the authors' response and the new manuscript.

Let me divide my comments in two parts.

First part - general impression:

What surfaces from the revision documents is a lack of care in drafting the documents. There are a few leftovers from comments apparently addressed to the co-authors that should not appear in the revised documentation.

For example, besides a large number of MS-WORD reference errors "Error! Reference source not found", the answer to the question of Rev #1 labeled as L50-65 is evidently a sentence addressed to the co-authors not meant to be in the final revision.

These mishaps are definitely not that important from the scientific point of view, but provide a general impression of carelessness, as is the large number of misprints such as expect vs except, connection vs. connecting, etc., and make the reading rather difficult in many sections.

Thank you for finding these. We have read the paper many times but some errors will always slip through.

The manuscript is in better shape in terms of readability.

Thank you. The readability of the manuscript should have improved again after this round.

Second part: Scientific.

I have to be franc here, and I apologize if I am overly "didactic" in my comments. Now that I can read the manuscript with somewhat more clarity than before, I do not find so much novelty in what is done in the paper. From the introduction (from lines 127 on) the authors state that "The objective of the paper is to derive with a bottom up approach a model that describes root water uptake considering the hydraulics of the 3D root architecture". The second objective is as follows. "This model will be scaled up to a 1D model that could be readily implemented in land surface models." After that there are numerical experiments.

Two comments are in order:

1. First objective, I have the following major reservations:

Big-root, parallel root, explicit 3D root geometry, axial flow, parallel flow, flow in series, are all processes contained in a single model framework, i.e. a stationary diffusion equation (or in mathematical terms the weighted graph Laplacian) defined on a given graph (the 3D root network). The solution of this model depends upon the topology of the graph, i.e., the (assumed or measured or modeled) 3D distribution of root sections and bifurcation nodes. Since the latter is assumed given in this manuscript, I do not understand the novelty of the contribution, besides providing a "physical-biological" interpretation of the inversion of the graph Laplacian.

I still have some difficulties in understanding the differences the authors make between the different parallel/big/general root models. To me the difference is only on the root network geometry and not at all on the processes. The weighted graph Laplacian can be interpreted as the combination of Ohm's and Kirchoff laws, i.e., force balance (Ohm's or Darcy's or Henry's law) and mass/energy balance (Kirchoff). The distinction between parallel/big/general root models is only given by the root architecture. Within the theory of diffusion equations, it is well known that we can find a re-parametrization, or more precisely in our case a redistribution of the edges of the graph (i.e., of the root architecture) and of the weights of the graph Laplacian (i.e., conductivities and edge lengths) that will connect each node of the graph directly with the sink node where the base of the plant trunk is located (the collar in the authors' jargon). This would be what the authors call a "parallel root" model that is completely equivalent in terms of sap dynamics to a "big root" model. So in the relevant terms of model results, indistinguishable.

In essence, this interpretation is given in the manuscript in an imprecise way and this casts doubts on the reader on the scientific novelty/relevance of the authors' work.

This impression is reinforced by the authors' answer to comment 3 of Rev 2.

Hence, as far as the first explicit objective, there seems to be no scientific novelty, but rather a contribution to additional confusion in the "linear diffusive" root modeling frameworks.

The reviewer is correct that the physical model or concept is the same for all 'models'. The difference between the different 'models' that we consider is in the topology of the root network. To make this clear, we added in the previous revision:

*Although the topology of the root system may also be considered as a parameterization of a model that describes water flow in the soil root system, we consider the root topology here as specific 'model' that is fixed a-priori in a kind of top-down approach and that is subsequently parameterized based on measurements of soil water potential, leaf water potential, transpiration fluxes and information about the root system such as the root density distribution and hydraulic properties of root segments. Two a-priori proposed root system topologies can be distinguished: big root and parallel root models.*

We agree that the definition of the first objective being the 'derivation of a model that describes root water uptake considering the hydraulics of the 3D root architecture' does not capture what we actually did and is not novel since 3D root architecture models have been developed and solved before. We reformulated therefore the objective towards the development of '*an exact upscaled 1D model that describes root water uptake considering the hydraulics of the 3D root architecture and that could be readily implemented in land surface models.*' In order to interpret the 3D root architecture model and its upscaled version, we cast the 3D model in a form that uses two root system hydraulic characteristics that have a simple physical interpretation (what the reviewer is referring to as 'providing a "physical-biological" interpretation of the inversion of the graph Laplacian'.) This has been done already for a parallel root system by Couvreur et al. 2012 but an exact formulation of root water uptake for a general root system model in terms of these characteristics is still missing. By casting the solution of a general root system in a form that uses these two hydraulic root system characteristics, a few general features of root water uptake processes can be inferred. Doing so, we can show that these characteristics are sufficient to describe the total root water uptake from the water potentials in the collar and the distribution of water potentials in the soil. We

can also show that the deviation of the uptake from a profile with a heterogeneous soil hydraulic head distribution from the uptake under a uniform hydraulic head distribution, which is also referred to as water uptake redistribution, only depends on the root hydraulic architecture and the soil hydraulic head distribution but not on the transpiration or the collar water potential. Since these root system characteristics fully define the parallel root model, additional terms or factors in the equation for the exact root system can be used as diagnostics of the deviation between the parallel root system model and the exact 3D model or its upscaled version that are due to differences in root system topology. A second consequence of the parallel root model being fully defined by the two root hydraulic characteristics is that it can be parameterized straightforwardly in a bottom-up approach. We wanted to test to what extent using exact root system hydraulic characteristics obtained in a bottom-up approach in combination with an approximation of the root topology by the parallel root system improves the description of the root water uptake compared to the case when the root hydraulic characteristics are derived in a top-down approach using either a big root or a parallel root topology.

We reformulated the objectives of the paper to:

*The objective of this paper is to derive with a bottom-up approach an exact upscaled 1D model that describes root water uptake considering the hydraulics of the 3D root architecture and that could be readily implemented in land surface models. The model will be compared with parallel root and big root models that are currently used in 1D models. In order to interpret the models and their differences, we will cast in a first part the solutions of the models in a form that uses two hydraulic root system characteristics: the root system conductance and the root water uptake distribution for a uniform soil water potential or hydraulic head distribution. This was already done for a parallel root system by Couvreur et al. 2012 but an exact formulation of root water uptake in terms of these characteristics for a general root system model, including a 3D root model and its upscaled version and a big root model, is still missing. We will show that these characteristics are for all models sufficient to describe the total root water uptake as a function of soil and collar water potentials or hydraulic heads. We will further show that these root system characteristics fully define the parallel root model. Additional terms or factors in the equation for the exact root system can be used as diagnostics of the deviation between the parallel root system model and the exact 3D model or its upscaled version that are due to differences in root system topology. A second consequence of the parallel root model being fully defined by the two root hydraulic characteristics is that it can be parameterized straightforwardly in a bottom-up approach. In a second part, we will compare the upscaled exact model with the parallel and big root models that can be parameterized in two different ways: a top-down parameterization in which parameters are derived from the root segment distribution and root segment hydraulic parameters assuming a-priori big root or parallel root topologies, versus a bottom-up parameterization of the parallel root model that uses exact hydraulic root system characteristics obtained from solving the flow equations in the 3D hydraulic root architecture (Figure 1). For the parallel root system model, we can evaluate to what extent the simulated uptake is impacted by the simplified root system topology while using exact hydraulic root system characteristics. First, the models will be compared for a very simple hypothetical root system that represents a hybrid form of the two 'asymptotic' root architectures (parallel root versus big root model). Second, the models will be compared for single roots with realistic distributions of root segment properties and for realistic root architectures of plants with a tap root or a fibrous root system.*

Before the upscaling, the purpose was to give a 'biological and physical interpretation of the inverse Laplacian'. As written above, the main outcome of this interpretation is that two root system hydraulic properties can be defined that are sufficient to describe the total uptake by the root system

for any distribution of the soil water potentials in the root zone: the root system conductance and the uptake distribution for a uniform soil hydraulic head distribution. It was found that this uptake distribution must be used to weigh the local hydraulic heads and derive an effective hydraulic head. We suppose that this is what the reviewer refers to with 'Within the theory of diffusion equations, it is well known that we can find a re-parametrization, or more precisely in or case a redistribution of the edges of the graph (i.e., of the root architecture) and of the weights of the graph Laplacian (i.e., conductivities and edge lengths) that will connect each node of the graph directly with the sink node where the base of the plant trunk is located (the collar in the authors jargon). This would be what the authors call a "parallel root" model that is completely equivalent in terms of sap dynamics to a "big root" model.'

But, we respectfully disagree that this leads to fully equivalent models. The total uptake that is simulated by the different models is indeed the same for all possible distributions of the water potentials but the distribution of the uptake in the soil profile is not. We added:

*This implies that any root system can be represented by a parallel root system with the same  $SUF$  and  $K_{rs}$  that simulates the same total root water uptake for any distribution of soil water hydraulic heads. However, comparing Eq. [22] with Eq. [17] shows that the compensatory uptake between the root system and its parallel root analogue differs and that  $diag(\mathbf{K}_{comp})$  and  $\mathbf{C}_7$  can be used as diagnostics for the difference in compensatory uptake.*

It was also found that the compensatory uptake when hydraulic heads are not uniformly distributed is independent of the total uptake or the transpiration. This is an important outcome since it differs from approaches that have been implemented to describe root water uptake compensation, hydraulic lift, root water redistribution in simulation models. To make this clearer, we added references to other studies in the discussion section:

*Unlike how it is defined in other approaches (Simunek and Hopmans, 2009; Jarvis, 2011), this compensation term does not depend 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.*

## 2. Second objective: upscaling

Here the paper becomes interesting. The authors' attempt is worthwhile, but it is not explained clearly and concisely:

The objective here is well explained by the authors in their response to question 4 of rev 2 and in lines 128-129 of the introduction "This model will be scaled up to a 1D model that could be readily implemented in land surface models." However, it does not surface clearly neither from the introduction nor from the model derivations sections, which are too mixed up with the comparison between parallel/big root/3d general modeling frameworks. As a result it does not seem the main objective of the paper and thus the impression on the lack of novelty is pervasive.

We reformulated the objectives so that it is hopefully clear now that the main emphasis of the paper is on the macroscale model, which is also central in Figure 1. However, this macroscale model can be

set-up in different ways: exact from upscaling of the 3D root architecture model, using a big root model or using a parallel root model with two ways of parameterizing the parallel root model. The confusing part here is that the big root and parallel root models that are used at the macroscopic scale use indeed the same concept as the 3D model that represents the real root hydraulic architecture but the topology of the root system in the big root and parallel root models is drastically simplified. We make it clearer now that big root and parallel root models are used in 1D models and are compared with upscaled exact models.

*Root hydraulics has been implemented in 1D land surface models using big root or parallel root models to represent emerging processes like hydraulic redistribution and root water uptake compensation,...*

*The model will be compared with parallel root and big root models that are currently used in 1D models.*

But, the 3D model was recast into a form that uses the root system characteristics  $SUF$  and  $K_{rs}$  before the model was scaled up. Therefore, in order to draw analogies with the parallel root model, we in fact also considered a '3D parallel root model' that has as many parallel roots that are connected to the root collar as there are root nodes in the 3D exact model. Later we scaled up the model. We added in the in the upscaling part:

*When the 3D root architecture is a parallel root architecture, then the upscaled model has the same form as Eq. **Error! Reference source not found.** in which the upscaled  $SUF$  is used. This upscaled model represents an upscaled parallel root system with each root connecting one soil layer with the to the root collar. It should be noted that we did not derive an 'upscaled' root system topology for the exact model. In the following, we will always refer to the upscaled parallel root model. The upscaling was performed here assuming 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. The upscaled parallel root model then represents a root system with parallel roots that each connect one region with the root collar.*

Going beyond this point, it is the parametrization here that comes into play. It is impossible to come up with the complete identification of the conductivities for i) flow from the soil into the root, ii) axial flow in the root at all points (xylems are highly heterogeneous), iii) upward flow by capillarity (or whatever process or combination of processes form the upward driving force). These parametrizations act at drastically different scales, from thin (capillary) to main roots. This type of discussion is left at a "subliminal" level, but should be instead at the center of the idea that we can come up with an "upscaled" model and try to determine the "upscaled" parameters (to be used in 1D models) directly from measurements.

We referred already to approaches that have been used successfully to derive parameters of the root system and of root segments. We added in the conclusion that the bottom-up approach allows to ingest information about the large variation in root properties in models. When information about the variability of root segment properties is available, this could be achieved with stochastic simulation. Using tissue and cell scale models in combination with anatomical data, a high throughput characterization of root segment hydraulic properties and their variability could be achieved. In a paper by Sixtine Passot, we have already outlined the framework of a multiscale model

for root water uptake. The current paper would contribute to the connection between root segment properties, root architecture and root system properties at the macroscopic scale. We extended the following part in the discussion section:

*Overviews of hydraulic properties of different crops, herbaceous species, and trees are given in Bouda et al. (2018) and Draye et al. (2010). But, variations of root hydraulic properties between different root orders or with root age can be very large (Rewald et al., 2011). Root segment hydraulic properties could be derived either from: direct measurements on root segments (Schneider et al., 2017;Zhu and Steudle, 1991;Meunier et al., 2018b); 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 modeling (Rothfuss and Javaux, 2017;Cai et al., 2018;Meunier et al., 2018a;Couvreur et al., 2020), or using anatomical information about root tissues in combination with flow modeling (Couvreur et al., 2018;Heymans et al., 2020). The latter approach implies a further downscaling to tissue and cellular levels, which could be used to characterize the variability of root segment properties efficiently. A framework for such a multi-scale approach is presented in Passot et al. (2018). With stochastic simulations of hydraulic RSAs, the impact of the variability of root segment properties on root system scale properties and upscaled root water uptake could be derived using the approach presented in this paper.*

In conclusion I still would require major revisions to this paper.